Novel Use of Legendre Transformation in Field Theory and Many Particle Systems

___ On-Shell Expansion and Inversion Method ___

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The Legendre transformation is one of the ways to rewrite the theory by small number of selected variables. It leads naturally to the generalized action functional called the effective action and everything starts from this generating functional. It is applied to various problems of physics ranging from the relativistic field theory to the condensed matter physics. The main techniques used here are the on-shell expansion and the inversion method.

The scheme presented in this article is thus a generating functional formalism of the many particle systems.

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Introduction

The purpose of the present article is to explain some of the novel formal properties and applications of the Legendre transformation using both relativistic field theory and non-relativistic many particle systems. The system can be in either equilibrium (time-independent) or non-equilibrium (time-dependent) states. The most salient feature of the formalism is that everything starts from the generating action functional, just as the classical mechanics can be formulated with the classical action as a starting machinery. In this sense, we are going to explain in the present article the action functional formalism of the many body system.

When we discuss a macroscopic system which contains a huge number of degrees of freedom, it is crucial to rewrite the theory in terms of a small number of coordinates. These variables should include experimentally observable ones and we are interested in a theory written by using these macroscopic coordinates.

There have been known many methods to accomplish the above task; the method of projection operator discusses the dynamical evolution of the system only in the space where all the variables are projected onto the space of the variable we are interested in. In this way we get, for example, the equation of motion for the relevant variable. Or, although quite different technically but essentially equivalent in philosophy to the way of projection operator, we integrate out in path-integral representation all the variables except for those we need. The resulting theory describes the system in terms of the coordinates which are left fixed.

There is another method to meet the purpose; the method of the Legendre transformation. Here we integrate out over all the variables but it is done in the presence of the c-number source term to probe the selected variable. The probe is set to be zero in the end of calculation. The utility of the Legendre transformation is to rewrite the theory in terms of the expectation values of small number of dynamical variables or the order parameters and to get the equation of motion that determines the expectation value of the chosen variables and the solution of them. We are also interested in other physical quantities, such as the excitation spectrum above the solution. Below it is explained how the Legendre transformation does these jobs in a highly systematic way.

In all cases, equilibrium or non-equilibrium, our central concern is the generating functional which is collectively called the effective action $\Gamma$ in what follows. It is defined through the Legendre transformation of another generating functional $W$ of the connected Green's functions. The effective action $\Gamma$ plays the role of action functional in classical analytical mechanics and of the free energy which is written by internal variables in the equilibrium limit. Since there exist already many review type publications on the subjects, here we confine ourselves to novel aspects of the effective action which have recently been developed in our group in order to accomplish the program stated above. Once the Hamiltonian is given, the program can be used regardless of the system we are considering. It is summarized in two key words:
(1) On-shell expansion

(2) Inversion method

The first one is the answer to the question: how to extract physically observable quantities from $I$. Indeed it is the expansion scheme of $I$ where only the physically observable quantities appear in the expansion coefficients. The expansion is performed around a stationary point which determines the ground state of the theory. Then the lowest equation of the on-shell expansion fixes the levels or the modes which are excited above the ground state already found. The higher coefficients represent the scattering amplitudes among the excited modes thus determined. These exhaust the observable information as far as the channel is concerned which we have picked up by selecting the coordinates. For all these investigations we need only elementary formulas of the Legendre transformation, which are summarized in Appendix A.

The second one is rather technical but is invented to answer another question: how to calculate $I$. The inversion method is convenient practically when we rewrite the theory by small number of variables. The method of the Legendre transformation meets this purpose but the rule of the Legendre transformation is known in a diagrammatical language only for the limited class of variables such as non-local product of up to four field operators. We are interested in many other types of operators in actual problems, for instance the density operator which is the local product of two field operators. The inversion method is applicable to any variables. It is actually an extention of the Legendre transformation in the sense that we invert the functional relation between the dynamical variable and the external probe parameter $J$. This $c$-number parameter is not necessarily conjugate to the dynamical variable. When both are conjugate each other, our inversion process corresponds to what is called the "insertion" or the "renormalization of vertices" in graphical theory of statistical mechanics where one replaces the bare vertices by its full order expressions. For actual calculations, we need a small parameter and the inversion process is done in a series of expansion in terms of this small quantity. The parameter can be anything so that the formalism has a wide applicability and the adiabatic expansion of the non-equilibrium phenomenon, for example, can also be discussed by this method.

In the following, above two — On-shell expansion and Inversion method — are combined and applied to various problems and it is our main aim to show that the Legendre transformation is, as a formalism, one of the most convenient and systematic techniques in discussing field theoretical many particle systems.

Following three advantages of our method are emphasized here:

(i) Generalities As has been stressed, the formalism is applicable to any quantum systems; relativistic or non-relativistic, microscopic or macroscopic, zero or non-zero temperature and even to equilibrium or non-equilibrium cases.

(ii) Systematics The method is systematic in two ways. One is the systematic determination of the physical quantities in the form of the on-shell expansion, as stated already: we start from a single function $I'$ and all the approximation schemes are fixed at this level. Usually the approximations are performed separately for each
physical quantity but as will be illustrated below in Chapters XIII and XIV, this sometimes leads to an erroneous answer to the energy levels and we see that an approximation based on \( F \) is essential. The other is a systematic improvement of the lowest equation by taking successively higher-order terms of the inversion formulas. When a small expansion parameter is the coupling constant, the results of the lowest inversion coincide with those of the mean field theory. Therefore, if our process is applied to such a case, it is a way of systematic improvement of the mean field theory. When it is combined with other formalisms, renormalization group for example, it can further be improved in a systematic way.

(iii) Symmetries Another advantage of our approach is that it keeps the symmetry properties of the Hamiltonian even if we truncate the effective action at some finite orders in its perturbation expansion. This is important in the sense that we are led again to erroneous results if we make an approximation which does not respect the symmetry of the Hamiltonian. However, in our scheme this problem is solved in a transparent way; once the approximation is fixed at the level of the starting effective action which automatically respects the symmetry, then the ground state, excited levels and scattering amplitudes are all determined by this effective action in the same approximation without violating the symmetry. We can simply follow the above process of the on-shell expansion. See Chapters VII~XIV, for examples.

In Chapters II~VI and XI we mainly choose relativistic examples but the arguments itself can be applied to non-relativistic cases. The only difference between relativistic and non-relativistic theory lies in the form of dispersion relation. If one replaces the relativistic form \( \omega = \sqrt{p^2 + m^2} \) by an arbitrary one, \( \omega = \omega(p) \), all the formulas hold without further modifications. From Chapters VIII to XIV (except XI) we discuss non-relativistic subjects and one can convince oneself that the formalism works equally well in both theories.

Our primary concern is to explain how to use our method for various problems and we have to say that the arguments on each subject are in a preliminary stage, hoping that the present article stimulates further investigations. Since the subjects treated are rather diverse, changing from chapter to chapter, we have made an effort so that each chapter is readable separately by reproducing now and then some of the important formulas. Rather than collecting many references and results, we present necessary arguments in a self-contained manner as far as space allows us. In this sense the present article looks more like a textbook than a review paper. For the reviews or the textbook of related subjects, see:

Chapter I. Action Functional

Microscopic fundamental law of physics takes the form of variational equation, both in classical and quantum cases. It states that every physical motion, including a static solution as a special case, is realized as an extremum of a functional called the action functional of the system. In quantum theory, the action becomes an operator but we can define $c$-number action functional, called the effective action, whose stationary solution gives the expectation value of an operator. Below we first review the action functional of classical mechanics and then in quantum case the effective action is defined paying particular attention to the correspondence between the classical and quantum theory. The key notion of our investigations is the off-shell and on-shell variations.

§ 1.1. Action functional in classical mechanics

Let us take a classical mechanical system of $N$-degrees of freedom. The coordinates are denoted by $q_i$ ($i=1$ to $N$) and we assume that the action functional $I[q]$ is given through the Lagrangian $L(q_i(t), \dot{q}_i(t))$ as\(^1\)

$$I[q] = \int dt L(q_i(t), \dot{q}_i(t)).$$  \hspace{1cm} (1.1.1)

We use the notation $\dot{q} \equiv (d/dt)q$ throughout this article and the time integration is, for convenience, supposed to be performed in the interval $-\infty \leq t \leq \infty$. By taking infinite time interval, we can freely consider the finite time region $t_i \leq t \leq t_f$. The starting observation is to distinguish two kinds of variations.\(^2\)

Unphysical, or off-shell, variation $\delta q_i(t)$: The stationary requirement of $I[q]$ under the variation,

$$q_i(t) \rightarrow q_i(t) + \delta q_i(t)$$  \hspace{1cm} (1.1.2)

for any $i$ leads to Euler-Lagrange equation of motion,

$$0 = \frac{\delta I[q]}{\delta q_i(t)} = \int dt' \left( \frac{\delta q_i(t')}{\delta q_i(t)} \frac{\partial L}{\partial q_i(t')} + \frac{\delta q_i(t')}{\delta \dot{q}_i(t)} \frac{\partial L}{\partial \dot{q}_i(t')} \right) = \frac{\partial L}{\partial q_i(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i(t)}.  \hspace{1cm} (1.1.3)

Here and hereafter (unless otherwise stated) the summation $\sum_{i=1}^{N}$ is implied over the repeated index and $\delta/\delta q_i(t)$ denotes the functional differentiation which is defined by

$$\frac{\delta q_i(t')}{\delta q_i(t)} = \delta_{t'} \delta(t' - t), \hspace{1cm} \frac{\delta q_i(t')}{\delta \dot{q}_i(t)} = \delta_{t'} \frac{d}{dt} \delta(t' - t).$$

Here $\delta_{t'}$ or $\delta(t' - t)$ is the Kronecker or Dirac $\delta$-function respectively. The variation $\delta q_i(t)$ is an unphysical variation in the sense that if $q_i(t)$ is a physical trajectory satisfying (1.1.3), then $q_i(t) + \delta q_i(t)$ is not. It is obvious that in order to find the stationary trajectory, we have to search for trajectories away from the stationary one.
We call $\delta q_i(t)$ off-shell variation in the following. The reason why the term "off-shell" is used here will become clear when we discuss the field theoretical system.

**Physical, or on-shell, variation $\Delta q_i(t)$:** Now another type of variation is introduced which plays a central role below. Let $q_i^{(0)}(t)$ be one of the solution to (1.1.3) and look for another solution to (1.1.3) in the vicinity of $q_i^{(0)}$. For this purpose, physical or on-shell variation $\Delta q_i(t)$ is defined as follows,

$$q_i^{(0)}(t) \rightarrow q_i^{(0)}(t) + \Delta q_i(t), \quad (1.1.4)$$

where both $q_i^{(0)}(t)$ and $q_i^{(0)}(t) + \Delta q_i(t)$ are physical trajectories. For $\Delta q_i(t)$ to be non-vanishing, two solutions necessarily satisfy different boundary conditions; for instance $\Delta q_i(t_i) \neq 0$ and/or $\Delta q_i(t_f) \neq 0$ for some $t_i, t_f$. Then we get the equation of motion satisfied by $\Delta q_i(t)$ after expanding the following relation in (functional) Taylor series of $\Delta q$,

$$0 = \frac{\delta I[q]}{\delta q_i(t)}_{q_i^{(0)} + \Delta q} = \left( \frac{\delta^2 I[q]}{\delta q_i(t) \delta q_j(t')} \right)_0 \Delta q_j(t') + \cdots. \quad (1.1.5)$$

The symbol $(\cdots)_0$ signifies the value of $(\cdots)$ evaluated at some solution $q_i^{(0)}(t)$ satisfying the stationary condition (1.1.3). The first term of the expansion vanishes because of the definition of $q_i^{(0)}(t)$ and the second term gives us the equation of small oscillation around $q_i^{(0)}(t)$,

$$0 = \int dt' \left( \frac{\delta^2 I[q]}{\delta q_i(t) \delta q_j(t')} \right)_0 \Delta q_j(t') \quad (1.1.6)$$

$$0 = \left( \frac{\partial^2 L}{\partial q_i(t) \partial q_j(t)} \right)_0 \Delta q_j(t) - \frac{d}{dt} \left\{ \left( \frac{\partial^2 L}{\partial q_i(t) \partial q_j(t)} \right)_0 \Delta q_j(t) \right\}$$

$$+ \left( \frac{\partial^2 L}{\partial q_i(t) \partial q_j(t)} \right)_0 \Delta q_j(t) - \frac{d}{dt} \left\{ \left( \frac{\partial^2 L}{\partial q_i(t) \partial q_j(t)} \right)_0 \Delta q_j(t) \right\}. \quad (1.1.7)$$

The boundary value appearing in (1.1.7) is omitted since boundary conditions on

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**Fig. 1.1.** Illustration of unphysical variation $\delta q$.  
**Fig. 1.2.** Illustration of physical variation $\Delta q$.  

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\( \Delta q_i(t) \) are taken into account when we solve (1.1.7). In Figs. 1.1 and 1.2, the above picture of \( \delta q \) or \( \Delta q \) is illustrated which shows clearly the different role played by \( \delta q \) or \( \Delta q \).

Equation (1.1.6) is called the mode determining equation or on-shell equation which determines the time evolution of small deviation \( \Delta q_i(t) \). The terminology “on-shell” comes from the fact that, for field theoretical Lagrangian, Eq. (1.1.6) fixes the dispersion relation of excitation mode of the field. This will be seen later. Our mode determining equation takes the form of zero eigenvalue equation for the matrix

\[
I_0^{(2)}(t, t') = \left( -\frac{\delta^2 I[\bar{q}]}{\delta q_i(t) \delta q_j(t')} \right)_{ij},
\]

(1.1.8)

regarding \( (i, t) \) and \( (j, t') \) as indices specifying rows and columns of the matrix \( I^{(2)} \). By diagonalizing \( I^{(2)} \) in this index space, eigenvector \( \Delta q \) represents the eigenmode of small oscillation around \( q_i^{(0)}(t) \). Equation (1.1.6) holds for any classical mechanical systems.

In Fourier space, Eq. (1.1.6) can be written as

\[
\int d\omega' I_0^{(2)}(\omega, -\omega') \Delta q_j(\omega') = 0,
\]

(1.1.9)

where we have defined \( \Delta q_j(\omega) \equiv \int dt e^{i\omega t} \Delta q_j(t) \). If we take as \( q_i^{(0)}(t) \) a static solution \( q_i^{(0)} \), then \( I_0^{(2)}(t, t') \) is a function of \( t - t' \) and \( I_0^{(2)}(\omega, -\omega') \) has the form \( I_0^{(2)}(\omega) \delta(\omega - \omega') \). Then Eq. (1.1.9) becomes diagonal in \( \omega \)-space,

\[
I_0^{(2)}(\omega) \Delta q_j(\omega) = 0.
\]

(1.1.10)

Recall here that \( I_0^{(2)} \) is an even function of \( \omega \) if the time reversal invariance holds and is real symmetric under \( i \leftrightarrow j \) since it is derived from the second derivative of \( I[q] \). Let \( O_{kn}(\omega) \) be an orthogonal matrix which diagonalizes \( I_0^{(2)}(\omega) \) with diagonal elements \( \lambda^{(k)}(\omega) \) \((k=1 \sim N)\). We assume here the \( \lambda^{(k)} \)'s are non-degenerate. Then the general solution to (1.1.10) is given, using

\[
O_{kn}(\omega) I_0^{(2)}(\omega) O_{nl}(\omega) = \delta_{kl} \delta^{(k)}(\omega),
\]

by

\[
\Delta q_j(\omega) = \sum_k O_{jk}(\omega) C_k \delta^{(k)}(\omega),
\]

(1.1.11)

where \( C_k \) is an arbitrary number. In case the time reversal invariance is maintained in the Lagrangian, the solution to \( \lambda^{(k)}(\omega) = 0 \) occurs in pairs at \( \omega = \omega^{(k)} = \pm \omega^{(k)} \). In this case \( \delta^{(k)}(\omega) \) is replaced by

\[
D^{(k)}_+ \delta(\omega - \omega^{(k)}) + D^{(k)}_- \delta(\omega + \omega^{(k)})
\]

(1.1.12)

with \( D^\pm \) undetermined constants again satisfying \( D^+_* = -D^- \) \((* \text{ represents complex conjugation})\). As a function of time, we get

\[
\Delta q_j(t) = \sum_{k, \sigma} E_{\sigma}^{(k)} e^{-i\omega_{\sigma}^{(k)} t}, \quad (\sigma = \pm)
\]

(1.1.13)

\[
E_{\sigma}^{(k)} = O_{jk}(\omega_{\sigma}^{(k)}) E_{\sigma}^{(k)}, \quad E_{\sigma}^{(k)} \equiv C_k D^{(k)}_\sigma
\]

(1.1.14)
Chapter I. Action Functional

The number of undetermined constants $E_j^{(k)}$ is now $2N$ for each $k$ and they are just fixed by two boundary conditions for each $\Delta q_i(t)$. Our criterion of the stability of $q_i^{(0)}$ is that

all the $\omega^{(k)}$ are real. \hfill (1.1.15)

As a simple example, let us consider the Lagrangian,

$$L = \frac{m}{2} \dot{q}_i^2 - V(q_i),$$ \hfill (1.1.16)

where $m$ is a common mass and $V(q_i)$ represents the potential energy. Equation of motion is given by

$$0 = \frac{\delta I[q]}{\delta q_i(t)} = -m \ddot{q}_i(t) - \left( \frac{\partial V(q(t))}{\partial q_i(t)} \right).$$ \hfill (1.1.17)

Here we take a constant solution $q_i^{(0)}$ which satisfies $\partial V/\partial q_i(t) = 0$ and define $V_{ij} \equiv (\partial^2 V/\partial q_i \partial q_j)_0$. By noting that

$$\left( \frac{\delta I[q]}{\delta q_i(t) \delta q_j(t')} \right)_0 = -m \frac{d^2}{dt^2} \delta(t-t') \delta_{ij} - V_{ij} \delta(t-t'),$$ \hfill (1.1.18)

Eq. (1.1.6) or (1.1.7) becomes in Fourier space as

$$(-m \omega^2 \delta_{ij} + V_{ij}) \Delta q_i(\omega) = 0.$$ \hfill (1.1.19)

The solution to (1.1.19) is given by

$$\Delta q_i(\omega) = \sum_k O_{ik}(\omega^{(k)}) E_{\sigma}^{(k)} \delta(\omega - \omega^{(k)}),$$ \hfill (1.1.20)

where $O_{ik}$ diagonalizes $V_{ij}$ with the eigenvalue $\nu^{(k)}$, $k = 1 \sim N$, and $\omega^{(k)} = \sigma (\nu^{(k)}/m)^{1/2}$ ($\sigma = \pm$). These all agree with the well-known results.

We summarize here the above observations;

$\Delta q \cdots$ unphysical (off-shell) variation leading to the equation of motion,

$\Delta q \cdots$ physical (on-shell) variation corresponding to different boundary conditions.

In what follows, we show that there is a complete parallelism between the classical and quantum system if we take in quantum case the effective action $\Gamma[\phi]$ in place of the classical action $I[q]$. The parallelism is summarized in Table 1.1 in the next section which will become clear by the discussions that follow. In order to study this subject, let us proceed to a quantum system.

§ 1.2. Effective action in quantum field theory

The action functional in quantum system is given by the same action as in the classical case through the replacement of $q_i(t)$ by the operator $\hat{q}_i(t)$. (We use the notation hat $\sim$ to denote the operator.) The equation of motion (1.1.3) holds for
but it is the operator equation in Heisenberg representation; therefore it is another problem to derive the physical information from it.

The question then is whether we can define an action functional which is written in terms of the expectation value of the operator we are interested in, \( \langle \hat{q}_i(t) \rangle \) for example. The effective action is the answer to this problem. We discuss in the following the quantum field theoretical system whose Hamiltonian is given as a space integral of the Hamiltonian density,

\[
\hat{H} = \int d^3x \hat{H}(x) = \int d^3x \hat{H}(\hat{\Pi}(x), \hat{\phi}(x)),
\]

where for simplicity, we have taken as dynamical variables, the Hermite scalar field \( \hat{\phi}(x) \) and its conjugate momentum \( \hat{\Pi}(x) \) which is assumed to have \( N \) components \( \hat{\phi}_i \), \( \hat{\Pi}_i \), \( (i=1 \sim N) \).

Let us first consider the vacuum to vacuum amplitude

\[
\langle 0 | \exp \left( -i \int_{-\infty}^{\infty} dt \hat{H} \right) | 0 \rangle = \int [d\phi] \exp i \int d^4x L(\phi),
\]

where we have set \( \hbar = 1 \) and \( \int [d\phi] \equiv \int \prod \phi(x) \) implies the functional (path) integration by \( \phi(x) \) at every space-time points denoted by \( x \) and \( \int d^4x \) is performed over whole space-time. (Note that in the above functional formula the irrelevant constant factor has been omitted.) The Lagrangian density appearing in the functional integration is defined by the usual rule from the Hamiltonian and it is written by \( \phi(x) \) and \( \partial_{\mu} \phi(x) \),

\[
L(\phi) = L(\phi(x), \partial_{\mu} \phi(x)).
\]

The notations \( x^a = (t, x) \equiv x \) and \( \partial_{\mu} \equiv \partial / \partial x^a \) are used here and hereafter but the arguments below hold of course both for relativistic and non-relativistic system.

The action functional which is a functional of the \( c \)-number field \( \phi_i(x) \) is now defined. For this purpose the \( c \)-number probe \( J \) is introduced in the channel \( \phi_i(x) \) by changing the Hamiltonian density as follows

\[
\hat{H}(x) \rightarrow \hat{H}(t, x) = \hat{H}(x) - J_i(t, x) \phi_i(x).
\]

The probe is assumed to be dependent on both space and time and is set to zero in the end. In this way we are led to consider the generating functional \( W[J] \) defined as follows,

\[
\exp(iW[J]) = \langle 0 | T \exp \left( -i \int dt d^3x \hat{H}_j(t, x) \right) | 0 \rangle
= \int [d\phi] \exp i \int d^4x [L(\phi) + J_i(x) \phi_i(x)],
\]

where the symbol \( T \) implies the time ordering operation. Now expanding in powers of \( J \), we get
\[ W[J] = W_0 + \sum_{n=1}^{\infty} \frac{1}{n!} \int \cdots \int d^4x_1 d^4x_2 \cdots d^4x_n W^{(n)}_{\text{na}}(x_1, x_2, \cdots, x_n) \]
\[
\times J_i(x_1) J_k(x_2) \cdots J_n(x_n), \tag{1.2.2}
\]
\[ W_0 = -\Omega \varepsilon. \tag{1.2.3} \]

Here \( \Omega \) is the whole space time volume, \( \Omega = \int d^4x \), and \( \varepsilon \) the energy density of the ground state. \( W^{(n)}_{\text{na}}(x_1, x_2, \cdots, x_n) \) is the connected time ordered Green’s function defined by
\[
W^{(n)}_{\text{na}}(x_1, x_2, \cdots, x_n) = i^{n-1} \langle 0 | T \hat{\phi}_i(x_1) \hat{\phi}_k(x_2) \cdots \hat{\phi}_n(x_n) | 0 \rangle_c, \tag{1.2.4}
\]
where \( |0\rangle \) denotes the ground state and subscript \( c \) in \( \langle \cdots \rangle_c \) implies the connected part.

In Appendix B, we show why the ground state appears in \( (1.2.4) \). It is related to the range of time integration in \( \int d^4x = \int_0^\infty dt \int d^3x \) in the starting formula \( (1.2.1) \). Strictly speaking we need a convergence factor of time integration. In Appendix B, the time interval is first taken to be finite and the infinite limit is discussed with Feynman prescription \( (B.3) \). It can be shown that the vacuum state is indeed selected out by this process for all orders of perturbation. Leaving the details to Appendix B, let us proceed further.

The coefficient function \( W^{(n)}_{\text{na}}(x_1, \cdots, x_n) \) is the unphysical, i.e., off-shell, quantity from which we have somehow to extract observable information that is contained in the pole of Fourier transform of the Green’s function \( W^{(n)} \); on-shell projection is required. Thus aside from the lowest term \( W_0 \), \( W[J] \) is not made up of physical objects only.

The reason why such an unphysical quantity comes in is simple. For non-vanishing source \( J \neq 0 \), we are not discussing the original theory and only for \( J = 0 \) the correct theory is recovered. The coefficient of Taylor expansion of \( W[J] \) is \( W^{(n)}_{\text{na}}(x_1, \cdots, x_n) \) which is obtained by taking the derivative with respect to \( J \) at \( J = 0 \). This process necessarily involves a quantity with small non-vanishing \( J \) hence the unphysical information creeps into the coefficients. Such an observation suggests the following:

\textit{if the condition \( J = 0 \) is kept throughout the calculation, one can deal with only physical quantities.}

One of the main purposes of this article is to show that the above is indeed possible if one utilizes on-shell expansion of effective action introduced below and that only the physical entities, which exhaust all the observables in the probed channel, appear in the formalism.

Now the effective action \( \Gamma[\phi] \) is a functional of the \( c \)-number field \( \phi(x) \) — the conjugate variable of \( J(x) \). It is defined by the Legendre transformation as follows:
\[
\Gamma[\phi] = W[J] - \int d^4x J_i(x) \phi_i(x), \tag{1.2.5}
\]
\[ \phi_i(x) = \frac{\delta W[J]}{\delta J_i(x)}. \]  \hfill (1.2.6)

In the literature, \( \phi_i(x) \) appearing here is referred to as the ground state (or the vacuum) expectation value of \( \phi_i(x) \) in the presence of \( J_i(x) \). Such a vacuum state is represented by \( |0\rangle \), and \( \phi_i(x) \) is conveniently written as \( \phi_i(x) = \langle 0 | \phi_i(x) | 0 \rangle \). However, we need time-dependent source \( J_i(x) \) so that it is not possible to define the ground state \( |0\rangle \) in a strict sense. This trouble is a superficial one since only the equation coming from \( J_i(x) = 0 \) is used in the following and the role of time-dependent \( J_i(x) \) is to define \( \Gamma[\phi] \) as a starting machinery. The notation \( |0\rangle \) is however convenient and will be used below with the above remark in mind. In this respect the following way of writing \( W[J] \) of (1.2.1) is more transparent:

\[ \exp(iW[J]) = \langle 0 | \text{Exp}\left\{ i \int d^4x J_i(x) \phi_i(x) \right\} | 0 \rangle, \]  \hfill (1.2.7)

where \( \phi_i(x) \) is an operator whose time development is governed by the Hamiltonian without source \( J_i(x) \) and \( |0\rangle \) is also the ground state in the absence of \( J_i(x) \). Equation (1.2.7) is also used below.

Now the essential point of the Legendre transformation is to invert (1.2.6) in favour of \( J \) and express \( J_i(x) \) as a functional of \( \phi_i(x) \); \( J_i(x) = J_i[x, \phi] \), which is inserted in (1.2.5). (Later in Chapter VII, extracting this essential part, the generalization of the Legendre transformation called inversion method is explained.) Several identities of the Legendre transformation are summarized in Appendix A. By (A.5),

\[ \frac{\delta \Gamma[\phi]}{\delta \phi_i(x)} = -J_i[x, \phi]. \]  \hfill (1.2.8)

The original theory is recovered for \( J = 0 \) so that the solution \( \phi_i^{(0)}(x) \) to

\[ \frac{\delta \Gamma[\phi]}{\delta \phi_i(x)} = 0 \]  \hfill (1.2.9)

determines the true ground state expectation value; \( \phi_i^{(0)}(x) = \langle 0 | \phi_i(x) | 0 \rangle \). The solution \( \phi_i^{(0)} \) is independent of \( x \) if the translational invariance is maintained by the ground state. However we keep \( x \)-dependence of \( \phi_i^{(0)}(x) \) for the formula to assure the generalities.

Expanding \( \Gamma[\phi] \) around \( \phi_i^{(0)}(x) \) by writing

\[ \phi_i(x) = \phi_i^{(0)}(x) + \delta \phi_i(x), \]  \hfill (1.2.10)

we get again the off-shell expansion,

\[ \Gamma[\phi] = \Gamma[\phi^{(0)}] + \sum_{n \geq 2} \frac{1}{n!} \int \cdots \int d^4x_1 \cdots d^4x_n \Gamma^{(n)}_{i_1 \cdots i_n}(x_1, \ldots, x_n) \delta \phi_{i_1}(x_1) \cdots \delta \phi_{i_n}(x_n), \]  \hfill (1.2.11)

\[ \Gamma^{(n)}_{i_1 \cdots i_n}(x_1, \ldots, x_n) = \left( \frac{\delta^n \Gamma[\phi]}{\delta \phi_{i_1}(x_1) \cdots \delta \phi_{i_n}(x_n)} \right)_0. \]  \hfill (1.2.12)

Here \((\cdots)_0\) implies \((\cdots)\) evaluated at \( \phi = \phi^{(0)} \). It is well-known (see Appendix A) that
Table 1.1. Classical-quantum correspondences.

<table>
<thead>
<tr>
<th>Classical Mechanical System</th>
<th>Quantum Mechanics or Fields</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I[q]$ classical action</td>
<td>$\Gamma[\phi]$ effective action</td>
</tr>
<tr>
<td>$\delta q$ unphysical variation</td>
<td>$\delta \phi$ off-shell variation</td>
</tr>
<tr>
<td>$\frac{\delta I[q]}{\delta q(t)} = 0$ equation of motion</td>
<td>$\frac{\delta \Gamma[\phi]}{\delta \phi(x)} = 0$ equation of motion</td>
</tr>
<tr>
<td>$q^{(0)}(t)$ trajectory</td>
<td>$\phi^{(0)}(x) = \langle 0</td>
</tr>
<tr>
<td>$\Delta q(t)$ physical variation</td>
<td>$\Delta \phi(x)$ on-shell variation</td>
</tr>
<tr>
<td>$= \text{deviation of the trajectory}$</td>
<td>$= \text{wave function of the excited state}$</td>
</tr>
<tr>
<td>$\int dt \left( \frac{\delta^2 I[q]}{\delta q(t) \delta q(t')} \right) \Delta q(t') = 0$ mode-determining equation</td>
<td>$\int dx' \left( \frac{\delta^2 \Gamma[\phi]}{\delta \phi(x) \delta \phi(x')} \right) \Delta \phi(x') = 0$ mode-determining (on-shell) equation</td>
</tr>
<tr>
<td>$\rightarrow$ higher orders in $\Delta q(t)$ non-linear interaction among the modes</td>
<td>$\rightarrow$ higher orders in $\Delta \phi(t)$</td>
</tr>
<tr>
<td>$\rightarrow$ on-shell quantities are determined</td>
<td>$\rightarrow$ excited states are determined</td>
</tr>
</tbody>
</table>

$I^{(n)}_{\text{tot}}(x_1, \ldots, x_n)$ is the off-shell one-particle irreducible (1PI) $n$-point Green’s function with the external legs amputated. Appearance of off-shell quantities is due to the fact that the variation $\delta \phi_i(x)$ defined in (1.2.10) produces $\phi_i(x)$ which is not a solution to (1.2.9) but to (1.2.8) with non-vanishing $J$.

On-shell expansion of $\Gamma[\phi]$ is obtained by an exact parallelism with the classical case (1.1.4). We look for another “trajectory” satisfying (1.2.9) in the vicinity of $\phi_i^{(0)}(x)$. For this purpose, we write

$$\phi_i(x) = \phi_i^{(0)}(x) + \Delta \phi_i(x),$$

and requires that $\phi_i(x)$ stays always on the surface in the functional space defined by $J_i[x, \phi] = 0$. By this process, we see clearly the relationship between the condition $J = 0$ and the on-shell condition, i.e. the pole of the Green’s function. The next chapter is devoted to these investigations.

References

1) For classical analytical dynamics see, for example, the textbook: H. Goldstein, *Classical Mechanics* (Addison Wesley, New York, 1950).
5) The followings are introductory reviews of the effective action:
Chapter II. On-Shell Expansion of Effective Action

On the basis of the notion of on-shell variation introduced in the previous chapter, the present chapter is devoted to the discussion of one of the main points of our paper. It is the problem of how to extract physically observable quantities from the effective action. We will see that on-shell expansion solves this problem by fixing the following three objects step by step,

(I) the ground state,
(II) excited states above the ground state determined in (I),
(III) scattering matrix elements among excited states determined in (II).

All these quantities are determined in a systematic way and they exhaust all the observable information as far as the channel is concerned which we are probing by introducing the source term. Fock space can be reconstructed from the c-number generating functional $\Gamma[\phi]$. This is an alternative and more explicit approach to the reconstruction theorem of Wightman.\(^1\) The content presented in Table 1.1 will thus be clarified.

§ 2.1 Basic formulation

In this section we assume that the field $\phi_i(x)$ is multicomponent Hermite field. It can be a relativistic Klein-Gordon field or the photon field or the non-relativistic phonon field.

Now in order to examine another solution of (1·2·9) in the form of (1·2·13), we first write $\Delta \phi_i(x)$ as\(^3\)–\(^5\)

$$
\Delta \phi_i(x) = \Delta \phi_i^{(1)}(x) + \Delta \phi_i^{(2)}(x) + \Delta \phi_i^{(3)}(x) + \cdots,
$$

(2·1·1)

assuming that $\Delta \phi_i^{(n)}(x)$ ($n=1, 2, \cdots$) is of order $[\Delta \phi_i^{(1)}(x)]^n$. Each $\Delta \phi_i^{(n)}(x)$ is then determined successively by requiring that

$$
\left[ \frac{\delta \Gamma[\phi]}{\delta \phi_i(x)} \right]_{\phi \rightarrow \phi^{(0)} + \Delta \phi} = 0
$$

(2·1·2)

$$
= \sum_{n=1}^\infty \frac{1}{n!} \int \cdots \int d^4 x_1 \cdots d^4 x_n \Gamma^{(n+1)}_{i_1, i_2, \cdots, i_n}(x_1, x_2, \cdots, x_n) \Delta \phi_{i_1}(x_1) \Delta \phi_{i_2}(x_2) \cdots \Delta \phi_{i_n}(x_n)
$$

(2·1·3)

holds for every term of $O[\Delta \phi^{(1)}]^n$. Then we find the following set of equations,

$$
\Gamma^{(2)}_{i j}(x, y) \Delta \phi_j^{(1)}(y) = 0,
$$

(2·1·4a)

$$
\Gamma^{(2)}_{i j}(x, y) \Delta \phi_j^{(2)}(y) + \frac{1}{2!} \Gamma^{(3)}_{i j k}(x, y, z) \Delta \phi_j^{(1)}(y) \Delta \phi_k^{(1)}(z) = 0,
$$

(2·1·4b)
Chapter II. On-Shell Expansion of Effective Action

\( I^{(3)}_{g}(x, y)\Delta \phi^{(3)}(y) + 2 \times \frac{1}{2!} I^{(3)}_{g,s}(x, y, z) \Delta \phi^{(1)}_{i}(y) \Delta \phi^{(2)}_{s}(z) \)

\[ + \frac{1}{3!} I^{(9)}_{g,s,t}(x, y, z, w) \Delta \phi^{(1)}_{i}(y) \Delta \phi^{(1)}_{s}(z) \Delta \phi^{(1)}_{t}(w) = 0, \quad (2.1.4c) \]

eq etc. Here and hereafter the summation \( \Sigma \), or the integration \( \int d^4 y \) over the repeated indices or valubales are implied and we recall that all the coefficients are evaluated at \( \phi_i(x) = \phi_i^{(0)}(x) \), as defined in (1.2.12).

**The lowest order:** The requirement (2.1.4a) turns out to be the zero eigenvalue equation for \( \Delta \phi^{(1)}_{i}(y) \):

\[ I^{(2)}_{g,xy} \Delta \phi^{(1)}_{i}(y) = 0. \quad (2.1.5) \]

We will use in the following this type of notation for \( I^{(2)} \) in order to emphasize the matrix character. Thus

\[ \text{Det}(I^{(2)}_{g,xy}) = 0, \quad (2.1.6) \]

where the determinant is taken regarding \( ix \) and \( jy \) as the indices of the matrix \( I^{(2)} \). We call (2.1.5) or (2.1.6) generalized on-shell condition. In order to see the reason, let us take the space-time translation-invariant case \( \phi^{(0)}(x) = \phi^{(0)} \) where \( I^{(2)}_{g,xy} \) is a function of \( x - y \). Then the Fourier representation of (2.1.4a) takes the form,

\[ I^{(2)}_{g}(p^0, p) \Delta \phi^{(1)}_{i}(p^0, p) = 0. \quad (2.1.7) \]

Here we have denoted four momentum as \( p = (p^0, p) \) and the one dimensional Fourier transformation is defined as \( \int dx f(x) \exp i p x = \hat{f}(p) \). This is nothing but the on-shell criterion in the sense that it determines the dispersion relation \( p^0 = \omega(p^2) \) of the spectrum. It defines (three-dimensional) surface, i.e., shell, in the four-dimensional space spanned by the whole values of \( \omega \) and \( p \).

For the case of time-independent but space inhomogeneous solution \( \phi^{(0)}(x) \), on-shell condition (2.1.7) is slightly modified as

\[ \int d^3 q I^{(2)}_{g}(p^0, p, q) \Delta \phi^{(1)}_{i}(p^0, q) = 0, \quad (2.1.8) \]

which also fixes the energy levels in the situation considered. If the time-inhomogeneous background field is further considered, Eq. (2.1.4a) becomes

\[ \int d^3 q d^3 q I^{(2)}_{g}(p^0, p, q, q) \Delta \phi^{(1)}_{i}(q^0, q) = 0. \quad (2.1.9) \]

This determines the mode which is excited upon the time-dependent solution \( \phi^{(0)}(x) \) and its wave function has in general the distribution in frequency \( q_0 \). Notice that such a situation cannot be included in the conventional on-shell criterion based on the pole structure of the Green's function. For composite channels, where \( \tilde{\phi}(x) \) is replaced by \( \tilde{\phi}(x) \tilde{\phi}(y) \) for example, the above observations hold with minor modifications. This will be discussed in § 2.4.

In order to make the arguments transparent, we now fix the dispersion relation by taking a relativistic field theory. However, as has been stressed in the Introduction,
the formulas that follow apply for any case if we replace the relativistic dispersion relation \( \omega(p^2) = \sqrt{p^2 + m^2} \) by an arbitrary form \( \omega(p^2) \) and also replace the Klein-Gordon operator \( \Box + m^2 \) by \( \partial^\mu \partial_\mu + \omega(\Box) \) \((\Box = \partial^\mu \partial_\mu = \partial^2 \partial t^2 - \Box^2)\).

Thus we assume \( \phi_i(x) \) to be multi-component Hermite Klein-Gordon field. Then in Fourier space, (2·1·5) takes the form

\[
\Gamma^{(2)}_{ij}(\vec{p}^2) \Delta \phi_j^{(1)}(\vec{p}) = 0. \tag{2·1·10}
\]

Here we have defined

\[
\Gamma^{(2)}_{ij}(\vec{p}^2) = \int d^4(x-y) e^{i(p-x)y} \Gamma^{(2)ij}_{k_1k_2}
\]

with \( p^2 = p_\mu p^\mu = (p^0)^2 - \vec{p}^2, \quad px = p^0 x^0 - \vec{p} \cdot \vec{x} \). Note here the identity of the Legendre transformation (A·8) which is given in Fourier space as

\[
\Gamma^{(2)}_{ij}(\vec{p}^2) = - W^{(2)-1}_{ij}(\vec{p}^2). \tag{2·1·11}
\]

Equations (2·1·10) and (2·1·11) mean that \( \Delta \phi_i^{(1)}(\vec{p}) \) has a support only at the pole of \( W_{ij}(\vec{p}^2) \), and \( \Delta \phi_j^{(1)}(\vec{p}) \) is the eigenvector corresponding to the pole of \( W^{(2)}_{ij}(\vec{p}^2) \). We note here that \( \Gamma^{(2)}_{ij} \) or \( W^{(2)}_{ij} \) is a symmetric matrices since it is the second derivative of \( \Gamma \) or \( W \) and that it is real if we assume the Wick rotation. We thus work in the Euclidean metric and in the end the analytic continuation is done to the physical region. This makes the arguments simple.

Let \( O_{ij}(\vec{p}^2) \) be an orthogonal matrix which diagonalizes \( \Gamma^{(2)}_{ij}(\vec{p}^2) \) and \( W^{(2)}_{ij}(\vec{p}^2) \) as

\[
[O^{-1}(\vec{p}^2) \Gamma^{(2)}_{ij}(\vec{p}^2) O(\vec{p}^2)]_{ij} \equiv \Gamma^{(2)}_{ij}(\vec{p}^2) = \delta_{ij} \gamma_i(\vec{p}^2),
\]

and let the solution of \( \gamma_i(\vec{p}^2) = 0 \) be \( p^2 = m_i^2 \). We first solve \( \Gamma^{(2)}_{ij}(\vec{p}^2) \Delta \bar{\phi}_j(\vec{p}) = 0 \) with a solution \( \Delta \bar{\phi}_j(\vec{p}) = C_j(p) \delta(p^2 - m_j^2) \), where \( C_j(p) \) is an arbitrary function. Then the pole part of \( W^{(2)}_{ij}(\vec{p}^2) \) is given by

\[
W^{(2)}_{ij}(\vec{p}^2) = O_{ij}(\vec{p}^2) \frac{1}{\gamma(m_k^2)(m_k^2 - p^2)} O_{ij}^*(\vec{p}^2) \tag{2·1·12}
\]

with \( \gamma(p^2) = dp \gamma(p^2)/dp^2 \). The general solution of (2·1·10) is thus

\[
\Delta \phi_j^{(1)}(\vec{p}) = O_{ij}(\vec{p}^2) C_j(p) \delta(p^2 - m_k^2) \tag{2·1·13}
\]

\[
\equiv C_k(p) \Delta \phi_j^{(1)}(\vec{p}). \tag{2·1·14}
\]

In this way Eq. (2·1·5) determines the shell \( p^2 = m_k^2 \) where \( \Delta \phi_i^{(1)}(\vec{p}) \) has a non-vanishing value. We assume \( m_k^2 > 0 \). (The Goldstone particle with \( m_k^2 = 0 \) is expected if the theory has a continuous symmetry and if \( \phi_i^{(0)} \) breaks it, see § 3.5.) We also assume \( \gamma(m_k^2) > 0 \) because otherwise the particle of mass \( m_k \) becomes a negative-norm state by (2·1·12). Since there are two solutions \( p^0 = \pm \sqrt{(p^2 + m_k^2)^{1/2}} \equiv \pm \omega(p^2) \) for on-shell condition \( p^2 = m_k^2 \), we can always write

\[
C_k(p) = C_k^+(p) \theta(p^0) + C_k^-(p) \theta(-p^0)
\]

\[
\equiv \sum_{\delta = \pm} C_k^\delta(\delta p^0) \theta(\delta p^0). \tag{2·1·15}
\]
These coefficients $C_k^{\pm}(\pm p)$ are to be determined by the boundary conditions on $\Delta \phi_i^{(3)}(x)$. We have to specify, for example, $\Delta \phi^{(1)}(t_0, x)$ and $d\Delta \phi^{(1)}(t_0, x)/dt_0$ at some time $t_0$. For each $k$, $\Delta \phi_j(k, \psi)$ in (2.1.14) is an eigenvector corresponding to the particle with mass $m_k$. Since $W_{k,x,y}$ is the causal two point Green's function, Eq. (2.1.5) coincides with the usual definition of the particle spectrum. In $x$-space, $\Delta \phi_j^{(1)}(x)$ is written as a sum of modes thus determined

$$\Delta \phi_j^{(1)}(x) = \int d^2pO_{jk}(m_k^2)[\tilde{C}_k^+(p)e^{-ip\cdot x} + \tilde{C}_k^-(p)e^{ip\cdot x}],$$

$$\tilde{C}_k^{\pm}(p) = \frac{1}{(2\pi)^4} \frac{1}{2i\not{p}_0} C_k^{\pm}(p),$$

$$\not{p}_0 = \sqrt{\not{p}^2 + m_k^2}, \quad \not{p}_k \cdot x = \not{p}_k \cdot x_0 - \not{p} \cdot x. \quad (2.1.16)$$

For single component case, the formula is simplified into

$$\Delta \phi^{(1)}(x) = \int d^2p[\tilde{C}^+(p)e^{-ip\cdot x} + \tilde{C}^-(p)e^{ip\cdot x}],$$

$$\not{p}_0 = \sqrt{\not{p}^2 + m^2}. \quad (2.1.17)$$

**Higher order terms:** We proceed to higher orders. By (2.1.4b), $\Delta \phi_i^{(3)}(x)$ is given by

$$\Delta \phi_i^{(3)}(x) = \frac{1}{2!} W_{x,y}^{(2)} \Gamma_{y,z}^{(3),iw} \Delta \phi_k^{(1)}(z) \Delta \phi_i^{(1)}(w)$$

$$= \frac{1}{2!} W_{x,y}^{(3)} \bar{W}_{y,z}^{(2)-1} \bar{W}_{z,x}^{(2)-1} \Delta \phi_j^{(2)}(y') \Delta \phi_k^{(1)}(z'), \quad (2.1.18)$$

where we have used (A.22):

$$\Gamma_{x,y,z}^{(3)} = W_{x,y}^{(3)} \bar{W}_{y,z}^{(2)-1} \bar{W}_{z,x}^{(2)-1} \bar{W}_{x,y}^{(2)-1}. \quad (2.1.19)$$

The arrow above $W^{(2)-1}$ indicates that $W^{(2)-1}$ operates to the left in the sense that in Fourier space the pole of $W^{(3)}$ is canceled first by $W^{(2)-1}$ and then $\Delta \phi^{(1)}$ is operated from the right. In the solution (2.1.18), we do not have to add the solution of the homogeneous equation $\Gamma^{(2)}(p')\Delta \phi_j^{(2)}(p) = 0$ since in the sum (2.1.1) it can be absorbed by redefining $\Delta \phi_i^{(1)}(x)$.

For $\Delta \phi_i^{(3)}(x)$, a new feature arises; we recover the one-particle-reducible graphs and get $W^{(4)}$. We differentiate (2.1.19) with respect to $\phi_i(w)$ and obtain the relation between $\Gamma^{(4)}$ and $W^{(4)}$, $W^{(3)}$, $W^{(2)}$, as in (A.23). Using this formula, $\Delta \phi_i^{(3)}$ in (2.1.4c) can be solved as

$$\Delta \phi_i^{(3)}(x) = \frac{1}{3!} W_{x,y,z}^{(4),iw} \bar{W}_{y,z}^{(2)-1} \bar{W}_{z,x}^{(2)-1} \bar{W}_{x,y}^{(2)-1} \Delta \phi_j^{(2)}(y') \Delta \phi_k^{(1)}(z') \Delta \phi_l^{(1)}(w'). \quad (2.1.20)$$

By a straightforward mathematical induction we can easily show that the recovery of the one-particle reducible graphs persists for general $\Delta \phi_i^{(n)}(x)$ and it is given by
\[
\Delta \phi_i^{(n)}(x) = \frac{1}{n!} W_{i, x, x_1, \ldots, x_n}^{(n+1)} \overline{W}_{i, x, x_1, \ldots, x_n}^{(2)} \cdots \overline{W}_{i, x, x_n}^{(2)} \Delta \phi_i^{(1)}(x_1) \Delta \phi_i^{(1)}(x_2) \cdots \Delta \phi_i^{(1)}(x_n). \tag{2.1.21}
\]

Equation (2.1.21) can also be derived by a similar procedure as in the case of the proof of tree theorem in field theory. To see this, let us write (2.1.3) explicitly and solve it in $\Delta \phi_i(x)$:

\[
0 = \Gamma_{i, x}^{(1)} = \frac{\delta \Gamma^{(1)}}{\delta \phi_i(x)}
= \Gamma_{i, x, y}^{(2)} \Delta \phi_j(y) + \frac{1}{2!} \Gamma_{i, x, y, h, k}^{(3)} \Delta \phi_j(y) \Delta \phi_k(z) + \cdots. \tag{2.1.22}
\]

The solution is given as

\[
\Delta \phi_i(x) = \Delta \phi_i^{(1)}(x) + W_{i, x, y}^{(2)} \left( \frac{1}{2!} \Gamma_{y, h, k, l}^{(3)} \Delta \phi_k(z) \Delta \phi_l(w) + \cdots \right), \tag{2.1.23}
\]

where $\Delta \phi_i^{(1)}(x)$ is the solution of the homogeneous equation (2.1.5) so that we can set $\Delta \phi_i^{(0)}(x) = \Delta \phi_i^{(1)}(x)$. The iterative solution of (2.1.23) is known to produce all the "tree diagrams", but in our case the bare vertex is replaced by full 1PI vertices $\Gamma^{(3)}$, $\Gamma^{(4)}$, \ldots, and bare propagator by full propagator $W^{(2)}$. Since all the "tree diagrams" exhaust all one-particle-reducible diagrams, we have proved (2.1.21).

Now Eq. (2.1.21) is well defined since $\overline{W}^{(2)}$ cancels the pole of $W^{(n+1)}$ and we are just taking the residue of the pole of $W^{(n+1)}$. Therefore our expansion formalism is expected to be related to S-matrix elements. However, there is one difference: the channel specified by $x$ is off the mass-shell, while the remaining $n$ channels are projected onto the mass-shell by $\Delta \phi^{(1)}$. S-matrix elements appear when we discuss $\Gamma$ itself.

In the classical mechanical case, the higher-order terms in $\Delta q$ represent the effects due to the unharmonicity of the model Lagrangian or the non-linear interactions among the modes (see Table 1.1). In the field theoretical case, on the other hand, the higher-order part of the variation $\Delta \phi$, when it is inserted into $\Gamma$, is directly related to the S-matrix elements among the modes determined by the lowest order condition (2.1.4a). This will be shown below in two different ways. The way of reverse use of LSZ reduction formula is presented in § 2.2 and the same problem is discussed in § 2.3 by introducing sources at remote past and future.

§ 2.2. On-shell variation, coherent state and connected S-matrix element

Here we examine the relation between the effective action and the S-matrix element by paying particular attention to the change of the boundary condition which specifies the effective action in field theory. At the same time we can solve the problem of how to construct Fock space from the effective action.

For this purpose, we first investigate the physical meaning of $\Delta \phi$, which leads us to the concept of on-shell variation by a straightforward analogy with physical
variation $\Delta q$ introduced in (1.1.4) in classical mechanical case.\(^2\)\(^,5\) On the basis of this novel use of the variation, the relation between the effective action and the scattering among physical modes is then clarified. In the following, we first consider a single component field case for simplicity. The generalization to the other cases is discussed later on.

Recall that the variable $\phi(x)$ of $\Gamma[\phi]$ represents the vacuum expectation value of the field operator under the existence of the external source $J(x)$. In the usual argument, a small deviation of $\phi(x)$ means the corresponding change in the source $J(x)$, i.e., $\phi^{(0)}(x) + \delta \phi(x) = \langle 0 | \tilde{\phi}(x) | 0 \rangle_{J+\delta J}$. In the present case, however, both $\phi^{(0)}(x)$ and $\phi^{(0)}(x) + \Delta \phi(x)$ are defined to satisfy $J = 0$. Therefore it is expected that the non-zero variation $\Delta \phi(x)$ should change the state $| 0 \rangle$ specified by a chosen solution $\phi^{(0)}(x) = \langle 0 | \tilde{\phi}(x) | 0 \rangle_{J=0}$. Recall here that the boundary state is the only freedom left to be varied under the condition of the vanishing external source. This is analogous to the classical mechanical case discussed in Chapter I. The "boundary conditions" used there are now replaced by the "boundary states". That this is the case can be shown explicitly as follows.

In order to examine the physical meaning of the variation $\Delta \phi(x)$, it is convenient to use the asymptotic field,\(^6\)

$$\tilde{\phi}_{\text{in(out)}}(x) = \int \frac{d^3 p}{(2 \pi)^3} \frac{1}{2 p^0} \left[ \tilde{a}_{\text{in(out)}}(p) e^{- i p \cdot x} + \tilde{a}^*_{\text{in(out)}}(p) e^{i p \cdot x} \right], \quad (2.2.1)$$

where $p^0 = (p^2 + m^2)^{1/2}$. This is defined under the limit,

$$\tilde{\phi}(x) \rightarrow Z^{1/2} \tilde{\phi}_{\text{in(out)}}(x) + \phi^{(0)}(x), \quad (t \rightarrow -\infty (+\infty)) \quad (2.2.2)$$

with $Z$ being the renormalization factor. We utilize LSZ original proof of their well-known reduction formula.\(^6\) Following steps just correspond to the reverse process of their approach.

Now, consider the second order variation $\Delta \phi^{(2)}(x)$ as an example. We assume first $\phi^{(0)}(x) = 0$ for simplicity by a proper redefinition of the field operator. The case $\phi^{(0)}(x) \neq 0$ is discussed separately below.

From (2.1.18), $\Delta \phi^{(2)}(x)$ can be written as follows,

$$\Delta \phi^{(2)}(x) = \frac{1}{2!} \int d^4 x_1 d^4 x_2 i Z^{-1} \Delta \phi^{(1)}(x_1)(\Box x_1 + m^2) i Z^{-1} \Delta \phi^{(1)}(x_2)(\Box x_2 + m^2) \times \langle 0 | T \tilde{\phi}(x_1) \tilde{\phi}(x_2) | 0 \rangle_c, \quad (2.2.3)$$

where subscript $c$ means the connected part of the Green's function as required by $W^{(3)}$. Since $W^{(3)}$ is multiplied by $\Delta \phi^{(1)}(x)$ we have used the mass shell form of $W^{(2)}$:

$$W^{(2)}_{x,y} = i Z^{-1}(\Box x + m^2) \delta^4(x - y). \quad \text{(on the mass-shell)} \quad (2.2.4)$$

$Z$ is the residue of mass-shell pole, or the renormalization factor of the corresponding field. Equation (2.2.3) is then transformed in the following way by using (2.1.15), (2.1.16) or (2.1.17). First the integration over $x_1$ is carried out;
\[ iZ^{-1} \int d^4x_1 \Delta \phi^{(1)}(x_1)(\square x_1 + m^2) \langle 0| \bar{\phi}(x) \phi(x_1) \phi(x_2)|0\rangle_c \]
\[ = iZ^{-1} \sum_{\delta = \pm} \int d^3k \int d^4x_1 \bar{C}^\delta(k) \partial x_1^\delta [e^{-i\hbar k \cdot x_1} \partial x_1^\delta \langle 0| \bar{\phi}(x) \phi(x_1) \phi(x_2)|0\rangle_c ] \]
\[ = iZ^{-1} \sum_{\delta = \pm} \int d^3k \int d^4x_1 x_1^\delta \lim_{x_1^\delta \to \infty} \bar{C}^\delta(k) e^{-i\hbar k \cdot x_1} \partial x_1^\delta \langle 0| \bar{\phi}(x) T[\phi(x_1) \phi(x_2)]|0\rangle_c \]
\[ - \lim_{x_1^\delta \to -\infty} \bar{C}^\delta(k) e^{-i\hbar k \cdot x_1} \partial x_1^\delta \langle 0| T[\bar{\phi}(x_2) \phi(x)]\phi(x_1)|0\rangle_c \]
\[ = Z^{-1/2} \int d^3k \left\{ \bar{C}^-(k) \langle 0| \bar{a}_{\text{out}}(k) T[\phi(x) \phi(x_2)]|0\rangle_c + \bar{C}^+(k) \langle 0| T[\phi(x) \phi(x_2)] \bar{a}_{\text{in}}(k)|0\rangle_c \right\} \]
\[ , \quad (2.2.5) \]

where we have used (2.1.17), (2.2.1) and (2.2.2). The notation $f^\delta \partial \equiv f(\partial y) - (\partial f) g$ is also introduced and $x_1^\delta$ is the time component of $x_1$ and $\partial x_1^\delta \equiv \partial / \partial x_1^\delta$. It is tacitly assumed as usual that $\Delta \phi^{(1)}(x)$ vanishes at spatial infinity by taking a wave packet regularization in the intermediate steps. The second integration for $x_2$ can be done in the same way and we get

\[ \Delta \phi^{(2)}(x) = \frac{1}{2!} (Z^{-1/2})^2 \int d^3k d^3l \left[ \bar{C}^-(k) \bar{C}^-(l) \langle 0| \bar{a}_{\text{out}}(k) \bar{a}_{\text{out}}(l) \phi(x)|0\rangle_c \right. \]
\[ + 2 \bar{C}^-(k) \bar{C}^+(l) \langle 0| \bar{a}_{\text{out}}(k) \bar{a}_{\text{in}}(l) \phi(x)|0\rangle_c \]
\[ + \bar{C}^+(k) \bar{C}^+(l) \langle 0| \phi(x) \bar{a}_{\text{in}}(k) \bar{a}_{\text{in}}(l)|0\rangle_c \right] \]
\[ , \quad (2.2.6) \]

(2.2.7)

The new states introduced in (2.2.7) are defined as

\[ |1^{(+)}\rangle = Z^{-1/2} \int d^3k \bar{a}_{\text{in}}(k)|0\rangle_c \]
\[ , \quad (2.2.8) \]

\[ |2^{(+)}\rangle = \frac{1}{2!} (Z^{-1/2})^2 \int d^3k \int d^3l \bar{a}_{\text{in}}(k) \bar{a}_{\text{in}}(l)|0\rangle \]
\[ , \quad (2.2.9) \]

with notations $\bar{a}_{\text{out}}(k) \equiv \bar{C}^-(k) \bar{a}_{\text{out}}(k)$ and $\bar{a}_{\text{in}}(k) \equiv \bar{C}^+(k) \bar{a}_{\text{in}}(k)$. In the general case, the following state will be used for $n = 0, 1, 2, \cdots$

\[ |n^{(+)}\rangle = \frac{1}{n!} (Z^{-1/2})^n \int d^3k_1 \cdots d^3k_n \bar{a}_{\text{in}}(k_1) \cdots \bar{a}_{\text{in}}(k_n)|0\rangle \]
\[ , \quad (2.2.10) \]

In these equations, we have assumed the uniqueness of the vacuum.

Back to the case $n = 1$, we can easily check the following relation by using (2.2.8) and (A.8),

\[ \Delta \phi^{(1)}(x) = - \Delta \phi^{(1)}(x) \Gamma^{(2)}(x, y) W^{(2)}(y, x) \]
\[ = iZ^{-1} \int d^4y \Delta \phi^{(1)}(y)(\Box_y + m^2) \langle 0 | T \dot{\phi}(y) \dot{\phi}(x) | 0 \rangle_c \]
\[ = \langle 1^- | \dot{\phi}(x) | 0 \rangle_c + \langle 0 | \dot{\phi}(x) | 1^+ \rangle_c. \quad (2.2.11) \]

The lowest order variation \( \Delta \phi^{(1)}(x) \) is thus the wave function of the corresponding field \( \dot{\phi}(x) \). The general term \( \Delta \phi^{(n)}(x) \) is similarly obtained by a straightforward mathematical induction, which can be summed up to get the total form of \( \Delta \phi(x) \),
\[ \Delta \phi(x) = [\langle \theta^- | \dot{\phi}(x) | \theta^+ \rangle + \text{(disconnected terms)}]_c, \quad (2.2.12) \]
\[ |\theta^{(+)}\rangle = \sum_{n=0}^\infty |n^{(+)}\rangle = \exp \left[ Z^{-1/2} \int d^3k \tilde{a}^+_k \right] |0\rangle. \quad (2.2.13) \]

The “disconnected terms” in (2.2.12) represent the situations where at least one particle is not affected by the collision process except for the one referring to the channel \( x \) that is still off the mass shell. These contributions come from the terms which include the product \( \tilde{a}_{\text{out}} \tilde{a}_{\text{out}}^\dagger \) or \( \tilde{a}_{\text{in}} \tilde{a}_{\text{in}}^\dagger \) which is not of normal ordered form. Recall that the corresponding terms are absent in (2.2.6) because of the condition \( \phi^{(0)}(x) = \langle 0 | \dot{\phi}(x) | 0 \rangle \equiv 0 \). For \( \Delta \phi^{(n)}(x) \) with \( n \geq 3 \), however, such terms appear. On the other hand, when we calculate \( \langle \theta^- | \dot{\phi}(x) | \theta^+ \rangle \) by using the LSZ reduction formula, the same disconnected contributions appear with the minus sign — the “disconnected terms” in (2.2.12) just play the role of cancelling them to get the correct \( \Delta \phi^{(n)}(x) \). So the result can simply be written as follows,
\[ \Delta \phi(x) = \langle \theta^- | \dot{\phi}(x) | \theta^+ \rangle_{(c)} = \frac{\langle \theta^- | \dot{\phi}(x) | \theta^+ \rangle}{\langle \theta^- | \theta^+ \rangle}. \quad (2.2.14) \]

We notice that the symbol “(c)” in (2.2.14) implies the situation which coincides with the one used the usual definition of connected S-matrix element.\(^7\)

It has thus been shown that the variational process implied by \( \Delta \) changes the initial and final states into the form of coherent state (2.2.13). In particular, the particle number is changed. Namely the non-trivial variation \( \Delta \phi(x) \) defined under the condition \( J = 0 \) clearly has a physical meaning of creating the on-shell modes. This is the reason why we call it on-shell variation and is in sharp contrast to the conventional off-shell variation \( \delta \phi \), which leads to the off-shell (IPI) Green's functions as in (1.2.11).

Let us study the relation between (2.2.14) and (1.2.7). For this purpose we further introduce new generating functional \( W_{\theta^+}[J] \),
\[ \exp(iW_{\theta^+}[J]) = \langle \theta^- | \text{Exp}(i \int_0^{+\infty} d^4x J(x) \dot{\phi}(x)) | \theta^+ \rangle, \quad (2.2.15) \]
whose boundary states are selected to satisfy the equation
\[ \left( \frac{\delta W_{\theta^+}[J]}{\delta J(x)} \right)_{J=0} = \langle \theta^- | \dot{\phi}(x) | \theta^+ \rangle_{(c)}. \quad (2.2.16) \]

For \( \theta^- = \theta^+ = 0 \), \( W_{\theta^+} \) reduces to \( W[J] \) of (1.2.7),
\[ W_{00}[J] = W[J]. \]
Since $W_{\theta^*}$ is inside the exponential we can forget the restriction (c) in (2.2.15). From this expression we find that looking for another solution of (2.1.2) around the vacuum solution can be interpreted as changing the initial and final states into the form of coherent states (2.2.13). One thing is to be noted here. In order to get non-vanishing value for (2.2.15), we have to limit the region of time integration to be finite as $\int_{t^*}^{t_f} dt$ and after evaluating the matrix element between $|\theta^*\rangle$ and $|\theta^+\rangle$ the limit $t_f \to \infty$, $t_i \to -\infty$ is taken. Otherwise, with Feynman prescription (Appendix B) only the vacuum state is selected. This point will be made clear in the next section where the problem is discussed from a different point of view.

We define the following effective action by using $W_{\theta^*}[J]$:

$$\Gamma_{\theta^*}[\phi^*] = W_{\theta^*}[J] - \int d^4x J(x) \phi^*(x), \quad (2.2.17)$$

$$\phi^*(x) = \frac{\delta W_{\theta^*}[J]}{\delta J(x)} . \quad (2.2.18)$$

We remark that $\phi^*$ satisfies

$$\phi^*(x)_{J=0} = \left[ \frac{\delta W_{\theta^*}}{\delta J(x)} \right]_{J=0} = \Delta \phi(x). \quad (2.2.19)$$

If we set $J=0$ in (2.2.17), then we find the relation

$$\Gamma_{\theta^*}[\Delta \phi]$$

$$= W_{\theta^*}[J=0]$$

$$= -i \langle \theta^- | \theta^+ \rangle (c)$$

$$= \Gamma[\phi^{(0)}=0] - i \langle 1^- | 1^+ \rangle + \sum_{n=3}^{\infty} \frac{1}{n!} (\bar{W}^{(n)})_{x_1, \ldots, x_n} \Delta \phi^{(1)}(x_1) \cdots \Delta \phi^{(1)}(x_n), \quad (2.2.20)$$

where $\bar{W}^{(n)}$ denotes $W^{(n)}$ with its external legs amputated by $W^{(2)-1}$. In the final step of (2.2.20), the reduction formula has been used together with the fact $\langle 1^- | 0 \rangle = \langle 0 | 1^+ \rangle = 0$. We note here that $\Gamma[\phi^{(0)}=0]$ in (2.2.20) vanishes since $\Gamma[\phi^{(0)}=0] = -i \ln \langle 0 | 0 \rangle = 0$. By assuming the stability of one-particle state we get $\langle 1^- | 1^+ \rangle = Z^{-1} \int d^4k 2k^0(2\pi)^3 \tilde{C}^-(\mathbf{k}) \tilde{C}^*(\mathbf{k})$. The remaining terms in (2.2.20) are just $S$-matrix elements.

Equation (2.2.20) is the on-shell expansion of the effective action in the sense that all terms in (2.2.20) are projected onto the mass shell by the $\Delta \phi^{(1)}$. It is $\Gamma_{\theta^*}[\Delta \phi]$ that corresponds to the generating functional of the connected $S$-matrix elements, which we denote by $S^{(c)}(\tilde{C}^-, \tilde{C}^+)$. 

### § 2.3. Source at the boundary $t = t_i, t_f$

As has been stated in § 1.2 and in Appendix B, in the functional-integral formulation for the infinite time interval $t_i = -\infty$, $t_f = \infty$, the boundary states are naturally taken as the vacuum by use of Feynman prescription. In this section we show that our conclusions in the previous section can be obtained by sticking to the vacuum as
boundary state. For this purpose we define new effective action whose boundary states are the vacuum, not the coherent states. The essential point is that we introduce a δ-function like source at initial \( t = t_i \) and final time \( t = t_F \) which plays the role of changing the vacuum state into the desired coherently excited state.\(^9\) The effective action can be calculated under the presence of this type of source while the boundary state is the vacuum.

Let us introduce new generating functional \( W_{e \cdot \theta}[J] \) defined for finite time interval,

\[
\exp(iW_{e \cdot \theta}[J]) = \langle \theta^- | T \exp(i \int_{x^0 = t_i}^{x^0 = t_F} d^4x J(x) \hat{\phi}(x)) | \theta^+ \rangle.
\]

Here the limits \( t_i \to -\infty \) and \( t_F \to \infty \) are assumed to be taken in the end. If we trivially set \( \bar{C}^\pm \) in \( | \theta^\pm \rangle \) equal to zero, Eq. (2.3.1) is nothing but the operator expression of (1.2.1) (up to the normalization constant) under Feynman prescription (Appendix B). Using \( W_{e \cdot \theta}[J] \), we introduce new effective action \( \Gamma_{e \cdot \theta}[\phi^*] \) defined in the same way as (2.2.17), (2.2.18). Hereafter, the presence of \( t_i \) or \( t_F \) is understood although it is not explicitly written.

Then we find that, for the case \( J = 0 \), newly defined \( i\Gamma_{e \cdot \theta}[\phi^*] \) itself becomes the generating functional \( S^{(0)}(\bar{C}^-, \bar{C}^+) \) of the connected S-matrix element.

We note here the following crucial relation,

\[
\langle \theta^- | T e^{i J \cdot \hat{\phi}} | \theta^+ \rangle = \exp \left[ Z^{-1} \int d^3 p 2\theta^0 (2\pi)^3 \bar{C}^-(p) \bar{C}^+(p) \right] \langle 0 | T e^{i J \cdot \hat{\phi}} | 0 \rangle,
\]

\[
K(x) = \lim_{t_i(t_F \rightarrow -\infty, +\infty)} Z^{-1} \int_{t_i}^{t_F} d^4y \Delta \phi^{(1)}(y)(\Box + m^2) \delta^4(y-x).
\]  

This is straightforwardly obtained by applying the LSZ reduction formula for the coherent state \( | \theta^\pm \rangle \):

\[
\exp \left[ -Z^{-1} \int d^3 k 2\theta^0 (2\pi)^3 \bar{C}^-(k) \bar{C}^+(k) \right] \langle \theta^- | T e^{i J \cdot \hat{\phi}} | \theta^+ \rangle
\]

\[
= \exp \left[ -Z^{-1} \int d^3 k 2\theta^0 (2\pi)^3 \bar{C}^-(k) \bar{C}^+(k) \right] \times \langle 0 | \exp \left[ Z^{-1/2} \int d^3 k \bar{C}^-(k) \bar{a}_{\text{out}}(k) \right] T e^{i J \cdot \hat{\phi}} \exp \left[ Z^{-1/2} \int d^3 p \bar{C}^+(p) \bar{a}_{\text{in}}(p) \right] | 0 \rangle
\]

\[
= \langle 0 | \exp \left[ Z^{-1/2} \int d^3 k [\bar{C}^-(k) \bar{a}_{\text{out}}(k) - \bar{C}^+(k) \bar{a}_{\text{out}}^*(k)] \right] \times T e^{i J \cdot \hat{\phi}} \exp \left[ Z^{-1/2} \int d^3 p [\bar{C}^+(p) \bar{a}_{\text{in}}^*(p) - \bar{C}^-(p) \bar{a}_{\text{in}}(p)] \right] | 0 \rangle
\]

\[
= \langle 0 | T e^{i J \cdot \hat{\phi}} \exp \left[ i Z^{-1} \int d^4 x \Delta \phi^{(1)}(x)(\Box + m^2) \hat{\phi}(x) \right] | 0 \rangle.
\]

In (2.3.4) we have used the assumption that \( \phi^{(0)}(x) = 0 \) and also the formula

\[
\exp(\hat{X} + \hat{Y}) = \exp \left( -\frac{1}{2} [\hat{X}, \hat{Y}] \right) \exp(\hat{X}) \exp(\hat{Y}),
\]

where \( [\hat{X}, \hat{Y}] \) commutes with \( \hat{X} \) and \( \hat{Y} \).
The above formula shows that changing the boundary states into coherent states \( |\theta^{\pm}\rangle \) is equivalent to introduce an artificial source \( K(x) \). Note that \( K(x) \) in (2·3·3) is non-zero only at the boundaries \( x^r = t_1 \) and \( t_f \) as can be seen by partial integration.

Recall here that the variation \( \delta \phi(x) \) satisfies in its lowest order,

\[
\delta \phi(x) = \int d^4y \delta J(y) \left( \frac{\partial \phi(x)}{\partial J(y)} \right) = \int d^4y \delta J(y) \left( \frac{\delta W}{\delta J(y)} \right) \left( \frac{\delta J(x)}{\delta J(y)} \right).
\]  

(2·3·5)

Therefore on-shell variation \( \Delta \phi^{(1)}(x) \) is also expected to satisfy

\[
\Delta \phi^{(1)}(x) = \int d^4y \Delta J(y) \left( \frac{\delta W}{\delta J(y)} \right) \left( \frac{\delta J(x)}{\delta J(y)} \right) _0,
\]

(2·3·6)

but, since the variational process \( \Delta \) is defined on the trajectory \( J = 0 \), the non-trivial change \( \Delta J \) of the external source is allowed only at the boundary of the region \( t_1 \leq t \leq t_f \) we are examining. In fact, by using the identity (A·8), we find from (2·3·6) that

\[
\Delta J(x) = -\int d^4y \Delta \phi^{(1)}(y) \left( \frac{\delta}{\delta \phi(y)} \right) \left( \frac{\delta \phi(x)}{\delta \phi(y)} \right) _0 = K(x).
\]  

(2·3·7)

Now coming back to (2·3·2)~(2·3·4), we get, by setting \( J = 0 \) and using (2·2·17) and (2·2·19),

\[
i \Gamma_0^{(1)}[\Delta \phi] = Z^{-1} \int d^3 p \theta(2\pi)^3 c^\nu(p) c^{\nu}(-p) + i W[J = Z^{-1} \Delta \phi^{(1)}(\square + m^2)].
\]

(2·3·8)

This is seen to agree with (2·2·20) by noting that the last term just generates the connected \( S \)-matrix elements:

\[
i \Gamma_0^{(1)}[\Delta \phi] = S^{(c)}(c^\nu, c^{\nu}).
\]

(2·3·9)

The \( S \)-matrix element is generated by

\[
(Z^{1/2})^{n+m} \left[ \frac{\delta^{n+m} i \Gamma_0^{(1)}[\Delta \phi]}{\delta c^\nu(p_1) \cdots \delta c^\nu(p_n) \delta c^{\nu}(q_1) \cdots \delta c^{\nu}(q_m) | c^\nu = c^{\nu} = 0} \right] c^{\nu} = c^{\nu} = 0
\]

(2·3·10)

where the normalization factor \( Z \) can be absorbed by a proper renormalization of the field, \( \phi^r = Z^{-1/2} \phi \). Let us transform these relations involving \( \Gamma_0^{(1)} \) into the one for original \( \Gamma \).

Using (2·3·2) and (2·2·17), the following relation between \( \Gamma_0^{(1)} \) and original effective action \( \Gamma_1 \) (1·2·5), defined by using the vacuum \( |0\rangle \) not by \( |\theta^{\pm}\rangle \), is derived;

\[
\Gamma_0^{(1)}[\phi^*] = \left\{ W[J + K] - \int d^4x (J + K)(x) \frac{\delta W[J + K]}{\delta (J + K)(x)} \right\}
\]

\[+ i Z^{-1} \int d^3 k 2k^0(2\pi)^3 \bar{c}^\nu(k) c^{\nu}(k) + \int d^4x K(x) \phi^*(x)\]

\[= \Gamma[\phi^*] - i Z^{-1} \int d^3 k 2k^0(2\pi)^3 \bar{c}^\nu(k) c^{\nu}(k)\]

\[+ Z^{-1} \int d^4x \Delta \phi^{(1)}(x)(\square + m^2) \phi^*(x).\]  

(2·3·11)
Chapter II. On-Shell Expansion of Effective Action

By setting $J=0$, and by using \((2.2.19)\) and \((2.3.8)\), Eq. \((2.3.11)\) becomes

$$i\Gamma[\Delta \phi] = iW[K] - iZ^{-1}\int d^4x \Delta \phi^{(1)}(x)(\Box_x + m^2)\Delta \phi(x)$$

or equivalently,

$$i\Gamma[\Delta \phi] + iZ^{-1}\int d^4x \Delta \phi^{(1)}(x)(\Box_x + m^2)\Delta \phi(x) = iT^{(c)}(\bar{C}^-, \bar{C}^+)$$

where $T^{(c)}(\bar{C}^-, \bar{C}^+)$ is the generating functional of connected $T$-matrix element defined as

$$S^{(c)}(\bar{C}^-, \bar{C}^+) = Z^{-1}\int d^3p 2\phi^0(2\pi)^3 \bar{C}^-(p)\bar{C}^+(p) + iT^{(c)}(\bar{C}^-, \bar{C}^+)$$

The left-hand side of \((2.3.13)\) can be expressed in another way. Define $\Gamma[\phi^*, K] \equiv \Gamma[\phi^*] + i\int d^4x K(x)\phi^*(x)$ evaluated at $J=0$. Then we get

$$\Gamma[\Delta \phi, K] = T^{(c)}(\bar{C}^-, \bar{C}^+)$$

Note that $\Gamma[\phi^*, K]$ is effective action with original action having extra boundary term $\int d^4x K(x)\tilde{\phi}(x)$.

Equation \((2.3.15)\) summarizes our results in a compact way. We remark that Eq. \((2.3.12)\) is formally derived by setting $J(x) = K(x)$ (and $\phi(x) = \Delta \phi(x)$) in the original definition \((1.2.5)\) of the effective action $\Gamma[\phi]$, assuming that $\Delta \phi^{(1)}$ in $K(x)$ is a given quantity. This is essentially the conventional approach of deriving $S$-matrix element from the effective action.\(^{8}\) The present method, on the other hand, clarifies the physical role of boundary states in terms of on-shell variation $\Delta \phi$. Our on-shell expansion, as stated at the beginning of this chapter, permits a systematic study of $S$-matrix elements where the vacuum and excited modes are also determined within the formalism.

For the general case $\phi^{(0)}(x) \neq 0$, Eq. \((2.3.12)\) is replaced by

$$i\Gamma'[\Delta \phi] = iW'[J = -\Delta \phi^{(1)}(\Gamma^{(2)}_{\phi=\phi^{(0)}}) + i\Delta \phi^{(1)}(x)(\Gamma^{(2)}_{\phi=\phi^{(0)}} - 0)\Delta \phi(y)]$$

where $W'$ is defined for the shifted field $\bar{\phi} = \phi - \phi^{(0)}$. Note here that $\Delta \phi' = \Delta \phi$. According to LSZ reduction process, the on-shell projections by the $\Delta \phi^{(1)}$ in \((2.3.16)\) are assumed to be taken at the end of calculations. Now by using the following relations,

$$i\Gamma'[\Delta \phi] = i\Gamma[\phi^{(0)} + \Delta \phi]$$

$$\Gamma^{(2)}_{\phi=\phi^{(0)}}(\phi^{(0)}(x) + \Delta \phi(y)) = iW[\phi^{(0)}(x) + \Delta \phi(y)]$$

Eq. \((2.3.16)\) can be written as

$$i\Gamma[\phi^{(0)} + \Delta \phi] - i\Delta \phi^{(1)}(x)(\Gamma^{(2)}_{\phi=\phi^{(0)}}) = iW[J = -\Delta \phi^{(1)}(\Gamma^{(2)}_{\phi=\phi^{(0)}})]$$
Then we get, as a generalization of (2.3.13) or (2.3.15),
\[ i\Gamma[\phi^{(0)} + \Delta\phi] = i\Delta\phi^{(1)}(x)(\Gamma^{(2)})_{\phi = \phi^{(0)}} \Delta\phi(y) = i\Gamma^{(1)}(\tilde{C}^-, \tilde{C}^+) \]
(2.3.19)
where the following relation has been used
\[ iW[J = -\Delta\phi^{(1)}(\Gamma^{(2)})_{\phi = \phi^{(0)}}] = i\left(\frac{\delta W}{\delta J}\right)_{\phi = \phi^{(0)}} \Delta\phi^{(1)}(\Gamma^{(2)})_{\phi = \phi^{(0)}} + i\Gamma^{(1)}(\tilde{C}^-, \tilde{C}^+) \]
(2.3.20)
with \(\delta W/\delta J\)\(\phi = \phi^{(0)}\) = \(\delta W/\delta J\)\(\phi = \phi^{(0)}\). The subscript \(\phi = \phi^{(0)}\) implies that \(J = -\Delta\phi^{(1)}(\Gamma^{(2)})\) is evaluated at \(\phi = \phi^{(0)}\). In (2.3.20) we have isolated from \(W[J]\) the term which is linear in \(J\).

### § 2.4. Generalization to composite field case

The above formalism can be generalized to composite field case and as a byproduct we get a new solution to the normalization problem of BS amplitude. Let us examine two-body channel through non-local field operator \(\bar{\phi}(x) \bar{\phi}(y)\). We will see that the Legendre transformation automatically leads to the proper vertex of composite fields as defined by Ref. 9) and on-shell expansion brings us the S-matrix elements of composite particles. There are several off-shell approaches to the related subjects; see Ref. 10).

The generating functional \(W[J]\) in this case is defined with the source term,
\[ \frac{1}{2!} \int d^4xd^4yJ(x, y) \langle \bar{\phi}(x) \bar{\phi}(y) \rangle -|0 \rangle \langle T \bar{\phi}(x) \bar{\phi}(y) |0 \rangle_{J=0} \]
(2.4.1)
where the subtraction of the vacuum expectation value has been made so as to set the stationary solution of shifted variable conveniently equal to zero. The effective action is then introduced as follows,
\[ \Gamma[G] = W[J] - \frac{1}{2!} \int d^4xd^4yJ(x, y)G(x, y) \]
(2.4.2)
\[ G(x, y) \equiv 2! \frac{\delta W[J]}{\delta J(x, y)} \]
(2.4.3)
We have to solve the zero eigenvalue equation of the second derivative of \(\Gamma\) which has four variables now,
\[ \Gamma^{(2)}(x, y; x', y') \Delta G(x', y') = 0 \]

In order to make a parallel argument as in the previous case, here we write \(G(x, y) \equiv G(x)\) with the relative coordinate \(i \equiv x - y\) and the center coordinate \(X \equiv (x + y)/2\). We also write \(\Gamma^{(2)}(x, y; x', y') = \Gamma^{(2)}(X, X')\) where \(j = x' - y'\), \(X' = (x' + y')/2\). In this way the relative coordinate is regarded as the index specifying the component of \(G(X)\). This makes things transparent since we can use the same formulation as in the case of multicomponent Klein-Gordon field we have already discussed. The mode determining equation is then symbolically written in the (total) momentum space as
\[ (\Gamma^{(2)}(P))_{\phi} \Delta G_{\phi}^{(1)}(P) = 0 \]
(2.4.4)
where $P$ is the total momentum of two body channel specified by $(x, y)$ or $(x', y')$.

Let us study the symmetry property of $\Gamma^{(3)}(P)$ under $i \leftrightarrow j$ with $P$ fixed. Now we write original variables explicitly as $\Gamma^{(3)}(P) = \Gamma^{(3)}(\xi, \xi', P)$, where $\xi = x - y$, $\xi' = x' - y'$. From Lorentz invariance $\Gamma^{(3)}(\xi, \xi', P)$ is a function of $P^2$, $P \cdot \xi$, $P \cdot \xi'$, $\xi^2$, $\xi'^2$, $\xi \cdot \xi'$ with $\xi = \xi \pm \xi'$. Since $\Gamma^{(3)}$ is obtained from the second derivative $\delta^2/\delta \phi(\xi, X) \delta \phi(\xi', X')$ of $\Gamma$, $\Gamma^{(3)}(\xi, \xi', P)$ is symmetric under $P \leftrightarrow -P$, $\xi \leftrightarrow \xi'$, thus it is an even function of $P \cdot \xi$, $P \cdot \xi'$ since these terms change sign under this operation. We further use the obvious symmetry of $\Gamma^{(3)}(\xi, \xi', P)$ under $\xi \leftrightarrow -\xi$, $\xi' \leftrightarrow -\xi'$ which leads to the fact that $\Gamma^{(3)}(\xi, \xi', P)$ is also even in $P \cdot \xi'$. These two symmetries imply that $\Gamma^{(3)}(\xi, \xi', P)$ is symmetric under $\xi \leftrightarrow \xi'$: $\Gamma^{(3)}_\xi(P) = \Gamma^{(3)}_{\xi'}(P)$.

The left-hand side of (2.4.4) is then transformed into a diagonalized form,

$$O \tilde{G}^i(P)(\Gamma^{(3)}_\xi(P))_i O^i_\xi(P)O \tilde{G}^j(P) \Delta G^{(3)}_\xi(P) = \gamma_i(P^2) \Delta \tilde{G}^{(3)}_i(P)$$  (2.4.5)

with an appropriate orthogonal matrix $O$. In order for $O$ to be real orthogonal $\Gamma^{(3)}_\xi$ has to be real symmetric. To assure this we assume that the Wick rotation has been performed and after all the calculations we rotate back to the Lorentz metric. The following discussions rely on this assumption and we work in the Euclidian metric below. Then we can assume that $\gamma_i(P^2)$ in (2.4.5) is explicitly given by

$$\gamma_i(P^2) = Z_i^{-1}(P^2 - m_i^2),$$  (2.4.6)

near its mass-shell pole $P^2 = m_i^2$. Each $m_i^2$ represents the physical mass squared. If $\gamma_i(P^2)$ has two or more zeros, we can discuss them separately. The continuum levels are assumed to be discretized properly by using a system frame with large but finite volume, while we concentrate below only on the bound state solutions.

The lowest order on-shell variation for the $i$th mode $\Delta \tilde{G}_i(1)(X)$ is given by Fourier transform of $O \tilde{G}^i(P) \Delta G^{(3)}_i(P)$ which is written similarly as in (2.1.16),

$$\Delta \tilde{G}_i(1)(X) = \int d^3 P [\tilde{G}_i^+(P)e^{-ip \cdot x} + \tilde{G}_i^-(P)e^{ip \cdot x}],$$  (2.4.7)

where $P^2 = m_i^2$ and $P^0$ satisfies $P^0 = (P^2 + m_i^2)^{1/2}$. The asymptotic field for $\tilde{\phi}(x)/\tilde{\phi}(y) = \tilde{G}(X)$ is also introduced for the bound state mode after taking the same orthogonal transformation used in (2.4.5),

$$\tilde{G}_i(X)_{\text{in(out)}} = \int \frac{d^3 P}{(2\pi)^3} \frac{1}{2P^0} \left[ \tilde{a}_{i \text{in(out)}}(P)e^{-ip \cdot x} + \tilde{a}_{i \text{in(out)}}(P)e^{ip \cdot x} \right],$$  (2.4.8)

$$\tilde{G}_i(X) \rightarrow Z_i^{1/2} \tilde{G}_i(X)_{\text{in(out)}}, \quad (X^0 \rightarrow -\infty(+\infty))$$  (2.4.9)

where $\tilde{G}_i$ is given in momentum space as

$$\tilde{G}_i(P) = O \tilde{G}^i(P) \tilde{G}_i(P) = \tilde{G}_i(P)O_{\text{ii}}(P).$$  (2.4.10)

The reduction process for the bound state mode $i$ is essentially the same as in the case of elementary field. Each step of the reduction is considered within a large but finite time interval and the bound state is expected to be localized in its relative coordinate of constituent fields. Therefore, if the bounded mode exists at all, the result can be written in terms of coherent states again. $|\theta^+\rangle$ and $|\theta^-\rangle$ introduced in (2.2.13) are
now replaced by
\[
|\bar{\theta}^+\rangle = \exp \left[ \sum_j d^3P Z_j^{-1/2} \tilde{C}_j^+(P) \bar{a}_{j,\text{in}}(P) \right] |0\rangle ,
\]
\[
\langle \bar{\theta}^-| = \langle 0| \exp \left[ - \sum_j d^3P Z_j^{-1/2} \tilde{C}_j^-(P) \bar{a}_{j,\text{out}}(P) \right].
\]

The normalization for the one-particle bound state is fixed to be
\[
\langle 0| a_{i,\text{in(out)}}(P) \bar{a}_{j,\text{in(out)}}(Q)|0\rangle = (2\pi)^3 2P^0 \delta_{ij} \delta^3(P - Q).
\]

The connected S-matrix element among bound state modes, each labeled by \(i_\theta\), is then generated from the effective action as follows,
\[
\frac{\delta^n m_i}{\delta \tilde{C}_{i,\text{in}}(P_1) \cdots \delta \tilde{C}_{i,\text{in}}(P_n) \delta \tilde{C}_{i,\text{in}}(Q_1) \cdots \delta \tilde{C}_{i,\text{out}}(Q_m)} \langle \bar{C}^+ - \bar{C}^- = 0 \rangle
\]
\[
= \langle 0| a_{i,\text{in}}(P_1) \cdots a_{i,\text{out}}(P_n) \bar{a}_{i,\text{in}}(Q_1) \cdots \bar{a}_{i,\text{out}}(Q_m)|0\rangle_{(c)} .
\]

The subscript \((c)\) indicates the connected part. The renormalization constant in \((2.4.13)\) has been included in each coefficient \(\tilde{C}_{i,\text{in}} \) as \(Z_i^{-1/2} \tilde{C}_{i,\text{in}} = \tilde{C}_{i,\text{in}} \). After renormalizing field variable as \(\tilde{G}^\prime_i = Z_i^{-1/2} \tilde{G}_i\), on-shell variation \(\Delta G^{\prime(1)}(x, y)\) can be written in the form
\[
\Delta G^{\prime(1)}(x = -y, X = (x+y)/2)
\]
\[
= \int d^3P [O(P)_{ij} \tilde{G}^\prime_j(P) e^{-ip \cdot x} + O(P)_{ij} \tilde{G}_j(P) e^{ip \cdot x}] .
\]

The operation \(\delta / \delta \tilde{C}_{i,\text{in}}\) now properly generates the bound state wave function or \(\phi(x)\phi(y)\)-component of the corresponding state \(|B\rangle\) for each pair of legs in the scattering diagrams. We see also from (2.4.14) that it is given by
\[
\langle 0| T \phi(x) \phi(y)|B\rangle = O(P)_{x-y,ij} e^{-ip \cdot (x+y)/2} .
\]

**Normalization problem:** Recall that the wave function obtained above, or the Bethe-Salpeter amplitude, is written as a plane wave times a matrix element of an orthogonal (unitary after the reverse Wick rotation) matrix and thus it is automatically normalized which is of course in accordance with the condition (2.4.12). Note moreover that the present normalization condition is given only by using the on-shell quantities compared with the conventional methods\(^{11}\) where the derivative of the Green's function around the mass-shell pole is utilized.

By a straightforward extension of the above procedure, the same argument can be made also for higher composite channels, of course.

### § 2.5. Grassmann number case

#### 2.5.1. Legendre transformation in Grassmann number channel

Here we study the Legendre transformation in Grassmann number channel\(^{12,13}\) in general terms. The detailed discussions on Grassmann number are inevitable for the
application of our formalism to fermionic problem. The argument is essentially the same as in the previous cases except for the sign factors appearing because of the anticommutativity of variables. For mathematical manipulation of Grassmann number, see for example Refs. 14 and 15).

Let us consider the generating functional $W[J]$ defined by the action $I[\psi]$ with the vector notation $\psi = [\psi_1, \psi_2] = [\psi, \bar{\psi}]$ denoting any fermion annihilation or creation operator respectively. For relativistic case we have in mind the Dirac field but they can be a non-relativistic electron field, in which case $\bar{\psi}$ is replaced by $\psi^\dagger$. We start from $W[J]$ defined by

$$\exp(iW[J]) = \int [d\psi] \exp{i(I[\psi] + J_a \psi_a)}, \tag{2.5.1}$$

where $\psi_a$ and $J_a$ are Grassmann number variables. The subscript $a$ indicates, besides $\psi$ or $\bar{\psi}$, the species of component-field as well as the other degrees of freedom including space-time coordinate. Like bosonic case, $W[J]$ is given by, in the operator formalism,

$$\exp(iW[J]) = \langle 0 | \exp(iJ_a \bar{\psi}_a) | 0 \rangle \tag{2.5.2}$$

with Heisenberg field operator $\bar{\psi}$. The effective action $I[\psi]$ is then introduced as follows,

$$I[\psi] = W[J] - J_a \psi_a, \tag{2.5.3}$$

$$\psi_a = \frac{\delta W[J]}{\delta J_a}, \tag{2.5.4}$$

where the functional left (and right) derivative is defined as$^{12,14}$

$$F[J + \delta J] - F[J] = \delta J \frac{\delta}{\delta J} F[J] \equiv F[J] \frac{\delta}{\delta J} F[J]. \tag{2.5.5}$$

The use of $\delta / \delta J$ is convenient in actual calculations because of our choice of source term $J_a \psi_a$ in (2.5.1). (If we take the source term as $\psi_a J_a$, the right derivative $\delta / \delta J$ will be used instead.) We have to invert (2.5.4) to get $I[\psi]$, which is done formally as follows. Since $W[J]$ is the ordinary (non-Grassmann) quantity $W[J]$ and $\psi_a$ has the following expansion,

$$W[J] = \sum_{n=0,2,\ldots} C_{a_0, a_2, \ldots, a_n} J_{a_0} J_{a_2} \cdots J_{a_n}, \tag{2.5.6a}$$

$$\psi_a = \sum_{n=2,4,\ldots} n C_{a_2, a_4, \ldots, a_n} J_{a_2} J_{a_4} \cdots J_{a_n}, \tag{2.5.6b}$$

where we have used complete antisymmetry of the coefficient $C_{a_0, a_2, \ldots, a_n}$. The inverted series of (2.5.6b) has the form

$$J_a = \sum_{n=2,4,\ldots} D_{a_2, a_4, \ldots, a_n} \psi_{a_2} \psi_{a_4} \psi_{a_n}. \tag{2.5.6c}$$

Here $J_a$ is given by the sum of terms which are odd in $\psi_a$'s. The coefficient $D_{a_0, a_2, \ldots, a_n}$ is determined by requiring that, when (2.5.6c) is inserted into (2.5.6b), we get an identity. Now consider $I[\psi]$ and take the right derivative of (2.5.3),
\[
\Gamma[\phi] \frac{\delta}{\delta \phi_a} = W[J] \frac{\delta}{\delta \phi_a} + J_b \frac{\delta}{\delta \phi_a} \phi_b - J_a.
\]

Now, using (2.5.6a) and the fact that \( J \) contains odd number of \( \phi \),
\[
W[J] \frac{\delta}{\delta \phi_a} = \left( W[J] \frac{\delta}{\delta J_b} \right) J_b \frac{\delta}{\delta \phi_a} = - \left( \frac{\delta}{\delta J_b} W[J] \right) J_b \frac{\delta}{\delta \phi_a}.
\]

Thus we arrive at
\[
\Gamma[\phi] \frac{\delta}{\delta \phi_a} = -J_a. \quad (2.5.7)
\]

We also use the notation \( \Gamma[\phi] \frac{\delta}{\delta \phi_a} = \frac{\delta}{\delta \phi_a} \Gamma[\phi] / \delta \phi_a \) in the following. The information of the ground state is determined by the solution \( \phi_a^{(0)} \) of (2.5.7) with \( J_a = 0 \). In the following, \( \phi_a^{(0)} \) is supposed to be selected as a fermion number conserving solution \( \phi_a^{(0)} = 0 \).

Let us operate \( (\delta J_a \cdot \frac{\delta}{\delta J_a})^n \) on both sides of (2.5.7). Under the variation \( J_a \to J_a + \delta J_a \), the following relation holds for arbitrary functional \( F[\phi] \),
\[
F \left[ \phi_a(J) + \delta J_b \frac{\delta}{\delta J_b} \phi_a(J) \right] - F[\phi_a(J)] = F[\phi] \frac{\delta}{\delta \phi_a} \delta J_b \frac{\delta}{\delta J_b} \phi_a(J)
\]
\[
= F[\phi] \frac{\delta}{\delta \phi_a} \delta J_b \frac{\delta}{\delta J_b} \left( \frac{\delta}{\delta J_a} W \right). \quad (2.5.8)
\]

It is therefore convenient to use the operator \( \frac{\delta}{\delta \phi_a} \cdot \frac{\delta}{\delta J_a} \cdot (\frac{\delta}{\delta J_a} W / \delta J_a) \) for the functional of \( \phi \), while \( \delta J_a \cdot \frac{\delta}{\delta J_a} \) for the functional of \( J \). Since they both are ordinary number operators, the identities are then obtained without an extra sign factor as follows,
\[
\Gamma \frac{\delta}{\delta \phi_a} \left[ \frac{\delta}{\delta \phi_a} \cdot \delta J_b \frac{\delta}{\delta J_b} \left( \frac{\delta}{\delta J_a} W \right) \right] = - \delta J_b \delta \phi_a, \quad (2.5.9a)
\]
\[
\Gamma \frac{\delta}{\delta \phi_a} \left[ \frac{\delta}{\delta \phi_a} \cdot \delta J_b \frac{\delta}{\delta J_b} \left( \frac{\delta}{\delta J_a} W \right) \right] \frac{\delta}{\delta \phi_a} \frac{\delta}{\delta J_c} \frac{\delta}{\delta J_c} \left( \frac{\delta}{\delta J_a} W \right) \]
\[
+ \Gamma \frac{\delta}{\delta \phi_a} \left[ \frac{\delta}{\delta \phi_a} \cdot \delta J_b \frac{\delta}{\delta J_b} \left( \frac{\delta}{\delta J_a} W \right) \right] \frac{\delta}{\delta \phi_a} \frac{\delta}{\delta J_d} \frac{\delta}{\delta J_d} \left( \frac{\delta}{\delta J_a} W \right) = 0, \quad (2.5.9b)
\]
\[
\Gamma \frac{\delta}{\delta \phi_a} \left[ \frac{\delta}{\delta \phi_a} \cdot \delta J_b \frac{\delta}{\delta J_b} \left( \frac{\delta}{\delta J_a} W \right) \right] \frac{\delta}{\delta \phi_a} \frac{\delta}{\delta J_c} \frac{\delta}{\delta J_c} \left( \frac{\delta}{\delta J_a} W \right) \]
\[
+ 3 \Gamma \frac{\delta}{\delta \phi_a} \left[ \frac{\delta}{\delta \phi_a} \cdot \delta J_b \frac{\delta}{\delta J_b} \left( \frac{\delta}{\delta J_a} W \right) \right] \frac{\delta}{\delta \phi_a} \frac{\delta}{\delta J_d} \frac{\delta}{\delta J_d} \left( \frac{\delta}{\delta J_a} W \right) \]
\[
+ \Gamma \frac{\delta}{\delta \phi_a} \left[ \frac{\delta}{\delta \phi_a} \cdot \delta J_b \frac{\delta}{\delta J_b} \delta J_c \frac{\delta}{\delta J_c} \delta J_d \frac{\delta}{\delta J_d} \left( \frac{\delta}{\delta J_a} W \right) \right] = 0, \quad (2.5.9c)
\]

etc. By convention, the symbol \( [\frac{\delta}{\delta \phi}\cdot] \)s in (2.5.9) are assumed to operate only on \( \Gamma[\phi] \) so that they commute with each other. Especially from the lowest order identity (2.5.9a), we get
\[
\left( \frac{\delta}{\delta \phi_a} - \frac{\delta}{\delta \phi_c} \right) \left( \frac{\delta}{\delta J_a} - \frac{\delta}{\delta J_c} W \right) = - \epsilon_{a-b} \epsilon_{c-b} \delta_{ab},
\]

where \( \epsilon_{a-b} \) denotes the sign factor caused by the interchange of components \( a \) and \( b \). For Grassmann variables, \( \epsilon_{a-b} = -1 \). Here we notice that Eq. (2.5.10) is also applicable when the ordinary number components are further included. In such cases, the components of \( \Gamma \frac{\delta}{\delta \phi_a} \frac{\delta}{\delta \phi_c} \frac{\delta}{\delta J_a} \frac{\delta}{\delta J_c} W \) which are of Grassmannian character vanish by setting \( \phi = \phi^{(0)} \) (\( J = 0 \)) because of our choice of the vacuum \( \phi^{(0)} = 0 \). By this assumption, Eq. (2.5.10) simply becomes

\[
\left( \frac{\delta}{\delta \phi_a} - \frac{\delta}{\delta \phi_c} \right) \left( \frac{\delta}{\delta J_a} - \frac{\delta}{\delta J_c} W \right) = - \delta_{ab},
\]

where \((\cdots)_0\) implies the value evaluated at \( \phi_{a}^{(0)} \). Henceforth we use the notation

\[
\Gamma \frac{\delta}{\delta \phi_a} \frac{\delta}{\delta \phi_c} = \frac{\delta}{\delta \phi_a} \left( \frac{\delta}{\delta \phi_c} \right),
\]

then

\[
\frac{\delta}{\delta J_a} \left( \frac{\delta}{\delta J_c} W \right) \bigg|_{0} = \frac{\delta}{\delta \phi_a} \left( \frac{\delta}{\delta \phi_c} \right) \bigg|_{0} = \frac{\delta}{\delta \phi_a} \left( \frac{\delta}{\delta \phi_c} \right) \bigg|_{0} = - \delta_{ab}.
\]

In changing the order of operations, we have used the fact that components \( a, b \) and \( c \) in (2.5.13) should be chosen so that all of them are Grassmann or ordinary number variables. Other combinations vanish for \( J = 0 \).

When the variable \( \phi \) in (2.5.13) is replaced by composite one whose indices satisfy for example \( \phi_i = \phi_{ji} \) or \( - \phi_{ji} \), the delta function on the right-hand side will be replaced by the symmetric part \( \delta_{ii}^{(s)} \equiv (1/2!) (\delta_{ii} \delta_{jj} + \delta_{jj} \delta_{ii}) \) or the anti-symmetric part \( \delta_{ii}^{(as)} \equiv (1/2!) (\delta_{ii} \delta_{jj} - \delta_{jj} \delta_{ii}) \) of unit tensor, respectively. In general cases, a properly mixed symmetry will be taken into account in the identity (2.5.13).

### 2.5.2. On-shell expansion in Grassmann number channel

We now apply the above formulas to on-shell expansion in fermionic channel. Let us look for another solution of (2.5.7) for \( J_a = 0 \) in the form \( \phi_a = \phi_{a}^{(0)} + \Delta \phi_a \) where \( \Delta \phi_a \) is written as in (2.1.1),

\[
\Delta \phi_a = \Delta \phi_a^{(1)} + \Delta \phi_a^{(2)} + \Delta \phi_a^{(3)} + \cdots.
\]

The variation \( \Delta \phi_a \) is to be determined by the condition,

\[
0 = \Gamma[\phi] \frac{\delta}{\delta \phi_a} \bigg|_{\phi = \phi^{(0)} + \Delta \phi} = \left( \Gamma[\phi] \frac{\delta}{\delta \phi_a} \right) \frac{\delta}{\delta \phi_b} \Delta \phi_b \bigg|_{\phi^{(0)}} + \frac{1}{2!} \left( \Gamma[\phi] \frac{\delta}{\delta \phi_a} \right) \frac{\delta}{\delta \phi_b} \Delta \phi_b \frac{\delta}{\delta \phi_c} \Delta \phi_c \bigg|_{\phi^{(0)}} + \cdots,
\]

where \( \frac{\delta}{\delta \phi_c} \) operates to the left and the following set of equations are obtained in each order of \( (\Delta \phi_a^{(1)})^n \),

\[
\left( \Gamma[\phi] \frac{\delta}{\delta \phi_a} \right) \frac{\delta}{\delta \phi_b} \Delta \phi_b^{(1)} = 0,
\]

(2.5.16a)
\[
\left( \Gamma[\phi] - \frac{\delta}{\delta \phi_a} \frac{\partial}{\partial \phi_b} \Delta \phi_b^{(2)}(1) \right)_{0} + \frac{1}{2} \left( \Gamma[\phi] - \frac{\delta}{\delta \phi_a} \frac{\partial}{\partial \phi_b} \Delta \phi_b^{(1)}(1) \frac{\delta}{\delta \phi_c} \Delta \phi_c^{(1)}(2) \right)_{0} = 0 ,
\]
\[
\left( \Gamma[\phi] - \frac{\delta}{\delta \phi_a} \frac{\partial}{\partial \phi_b} \Delta \phi_b^{(3)}(1) \right)_{0} + 2 \times \frac{1}{2!} \left( \Gamma[\phi] - \frac{\delta}{\delta \phi_a} \frac{\partial}{\partial \phi_b} \Delta \phi_b^{(1)}(1) \frac{\delta}{\delta \phi_c} \Delta \phi_c^{(1)}(2) \right)_{0} + \frac{1}{3!} \left( \Gamma[\phi] - \frac{\delta}{\delta \phi_a} \frac{\partial}{\partial \phi_b} \Delta \phi_b^{(1)}(1) \frac{\delta}{\delta \phi_c} \Delta \phi_c^{(1)}(2) \right)_{0} = 0 ,
\]

etc. The notation \( \mid_0 \) implies that the quantity is evaluated at \( \phi_a = \phi_a^{(0)} (=0) \).

First we consider the lowest order equation (2.5.16a), which determines the particle modes. We assume here that \( \phi \) is the Dirac field. Other non-relativistic cases can similarly be studied. Writing the component of \( \phi_a \) as \( \langle \psi, \bar{\psi} \rangle \) (we omit the hat for the operator), Eq. (2.5.16a) is given by the following matrix form,

\[
\Delta \phi^{(1)} - \frac{\delta}{\delta \phi_b} \left( \frac{\delta \Gamma}{\delta \phi_a} \right)_{0} = \begin{bmatrix}
0 & -Z_2^{-1} (i \partial_x - m) \psi \delta (x-y) \\
Z_2^{-1} (i \partial_y - m) \bar{\psi} \delta (y-x) & 0
\end{bmatrix} = 0 .
\]

\( Z_2 \) is the renormalization factor of \( \phi \)-field and \( m \) denotes the observed mass. The solutions \( \Delta \phi^{(1)} \) and \( \Delta \bar{\phi}^{(1)} \) of (2.5.17) are now represented using arbitrary Grassmann variables \( \tilde{C}^{\pm} \) as follows,

\[
\Delta \phi^{(1)} = \int \frac{d^3p}{(2\pi)^3} \frac{m}{p_0} \left[ C^+(p, \sigma) u(p, \sigma) e^{-ip \cdot x} + C^-(p, \sigma) \bar{u}(p, \sigma) e^{ip \cdot x} \right]
\]

\[
= \int \frac{d^3p}{(2\pi)^3} \frac{m}{p_0} \left[ \tilde{C}^+(p, \sigma) u(p, \sigma) e^{-ip \cdot x} + \tilde{C}^-(p, \sigma) \bar{u}(p, \sigma) e^{ip \cdot x} \right] ,
\]

\[
\Delta \bar{\phi}^{(1)} = \int \frac{d^3p}{(2\pi)^3} \frac{m}{p_0} \left[ C^{\ast+}(p, \sigma) \bar{u}(p, \sigma) e^{ip \cdot x} + C^{\ast-}(p, \sigma) \bar{u}(p, \sigma) e^{-ip \cdot x} \right]
\]

\[
= \int \frac{d^3p}{(2\pi)^3} \frac{m}{p_0} \left[ \tilde{C}^{\ast+}(p, \sigma) \bar{u}(p, \sigma) e^{ip \cdot x} + \tilde{C}^{\ast-}(p, \sigma) \bar{u}(p, \sigma) e^{-ip \cdot x} \right] ,
\]

where \( p_0 = (p^2 + m^2)^{1/2} \), \( \tilde{C}^{\pm}(p, \sigma) = (m/(2\pi)^3)^{1/2} C^{\pm}(p, \sigma) \), and \( u(p, \sigma) \) or \( \bar{u}(p, \sigma) \) is the Dirac spinor with fixed helicity \( \sigma \) satisfying \( (\vec{p} - m) u(p, \sigma) = 0 \) or \( (\vec{p} + m) \bar{u}(p, \sigma) = 0 \), respectively. (Summation over \( \sigma \) has been assumed in (2.5.18a, b).)

In order to write higher-order variations \( \Delta \phi^{(n)} \) in the form of (2.1.21), the relations (2.5.9b), (2.5.9c), etc., are used under the condition of \( J_a = 0 \) (or \( \psi_a = \psi_a^{(0)} = 0 \)). In this case, \( \delta J_a \) is replaced by \( \Delta J_a \), or \( K_a \), as in (2.3.7). Since \( K_a \) is given by

\[
K_a = - \Delta \phi^{(1)} \frac{\delta}{\delta \phi_a} \left( \frac{\delta \Gamma}{\delta \phi_a} \right)_{0} ,
\]

we find that \( (\delta / \delta \phi_a) \Delta \phi^{(1)} \) appearing in (2.5.16b, c) can be written as

\[
\frac{\delta}{\delta \phi_a} \Delta J_a \frac{\delta}{\delta \phi_b} \left( \frac{\delta W}{\delta J_a} \right)_{0} = \frac{\delta}{\delta \phi_a} \Delta \phi^{(1)} .
\]

(2.5.20)
From (2.5.16b), (2.5.16c), etc., and comparing them with (2.5.9b), (2.5.9c), etc., with the replacement \( \delta f \to \Delta f \), the following formula is obtained:

\[
\Delta \phi_a^{(n)} = \frac{1}{n!} \left[ \left( -\Delta \phi_a^{(1)} \frac{\delta}{\delta \phi_{a_1}} \frac{\delta}{\delta \phi_{a_1}} \right) \cdots \left( -\Delta \phi_a^{(n)} \frac{\delta}{\delta \phi_{a_n}} \frac{\delta}{\delta \phi_{a_n}} \right) \frac{\delta}{\delta J_{a_1}} \cdots \frac{\delta}{\delta J_{a_n}} \right] \frac{\delta W}{\delta J_a} \right]_0.
\]

(2.5.21)

Here we have used the notation (2.5.12) and the fact that, except for the fixed order of variables and operators, all the coefficients in (2.5.16) and (2.5.9) are the same as in boson field case. The result (2.5.21) is, of course, available also when the ordinary number variables are included as some of the components of \( \phi \).

Let us check the physical meaning of on-shell variation \( \Delta \phi_a \). For this purpose, the following asymptotic fields are introduced:

\[
\tilde{\phi}_{(\text{in/out})}(x) = \int \frac{d^3p}{(2\pi)^3} \frac{p}{\hat{p}^0} \left[ \bar{b}_{(\text{in/out})}(\hat{p}, \sigma) u(\hat{p}, \sigma) e^{-i\hat{p} \cdot x} + \bar{a}_{(\text{in/out})}(\hat{p}, \sigma) v(\hat{p}, \sigma) e^{i\hat{p} \cdot x} \right],
\]

(2.5.22a)

\[
\tilde{\phi}_{(\text{in/out})}(x) = \int \frac{d^3p}{(2\pi)^3} \frac{m}{\hat{p}^0} \left[ \bar{b}_{(\text{in/out})}(\hat{p}, \sigma) \bar{u}(\hat{p}, \sigma) e^{i\hat{p} \cdot x} + \bar{a}_{(\text{in/out})}(\hat{p}, \sigma) \bar{v}(\hat{p}, \sigma) e^{-i\hat{p} \cdot x} \right],
\]

(2.5.22b)

where \( \hat{p}^0 = (\hat{p}^2 + m^2)^{1/2} \). They are asymptotic fields of \( \tilde{\phi}(x) \),

\[
\tilde{\phi}(x) \longrightarrow Z_{1/2} \tilde{\phi}_{(\text{in/out})}(x). \quad (x^0 \longrightarrow -\infty (+\infty))
\]

(2.5.23)

Let us examine the lowest order variation \( \Delta \phi_a^{(1)} \). Equation (2.5.21) for the trivial case \( n=1 \) can be transformed as follows,

\[
\Delta \phi_a^{(1)} = -\Delta \phi_b^{(1)} \frac{\delta}{\delta \phi_b} \left( \frac{\delta \Gamma}{\delta \phi_c} \right) \frac{\delta}{\delta J_c} \left( \frac{\delta W}{\delta J_a} \right) \left|_0 \right.
\]

\[
= i \left\langle 0 \right| T \left[ -\Delta \phi_b^{(1)} \frac{\delta}{\delta \phi_b} \left( \frac{\delta \Gamma}{\delta \phi_c} \right) \frac{\delta}{\delta J_c} \left( \frac{\delta W}{\delta J_a} \right) \right] \left| 0 \rightangle
\]

\[
= \left\langle 0 \right| T \left[ -iZ_2^{-1} \int d^4x \left( \Delta \tilde{\phi}_c(x) \right)^{(1)} \left( i \bar{J}_x - m \right) \tilde{\phi}_a(x) + \tilde{\phi}_a(x) \left( -i \bar{J}_x - m \right) \Delta \tilde{\phi}_c(x) \right] \left| 0 \right\rangle,
\]

(2.5.24)

where we have used (2.5.17) and the relation,

\[
\frac{\delta}{\delta J_c} \left( \frac{\delta W}{\delta J_a} \right) \left|_0 \right. = i \left\langle 0 \right| T \left( \tilde{\phi}_c \tilde{\phi}_a \right) \left| 0 \right\rangle_{j=0}.
\]

(2.5.25)

Each term of (2.5.24) is further transformed in the following ways,

\[
-iZ_2^{-1} \int d^4x \Delta \left( \tilde{\phi}_c(x) \right)^{(1)} \left( i \bar{J}_x - m \right) \tilde{\phi}_a(x)
\]

\[
= -iZ_2^{-1} \int d^4x i \partial_x \left[ \Delta \left( \tilde{\phi}_c(x) \right)^{(1)} \gamma_5 \tilde{\phi}_a(x) \right]
\]
\[= Z_s^{-1} \int d^3 x (\lim_{x^0 \to -\infty} - \lim_{x^0 \to +\infty} \left[ \int d^3 p \left( \bar{C}^{+*}(p, \sigma) \bar{u}(p, \sigma) e^{ip \cdot x} + \bar{C}^{-*}(p, \sigma) \bar{v}(p, \sigma) e^{-ip \cdot x} \right) \gamma_0 \tilde{\psi}(x) \right] \]

\[= Z_s^{-1/2} \int d^3 p \left[ \bar{C}^{+*}(p, \sigma) \left( \bar{b}_{\text{out}}(p, \sigma) - \bar{b}_{\text{in}}(p, \sigma) \right) + \bar{C}^{-*}(p, \sigma) \left( \bar{d}^*_\text{out}(p, \sigma) - \bar{d}^*_\text{in}(p, \sigma) \right) \right], \tag{2.5.26a} \]

\[-iZ_s^{-1} \int d^4 x \tilde{\psi}(x) (-i \gamma_5 - m) \Delta \langle \psi(x) \rangle^{(1)} \]

\[= -iZ_s^{-1} \int d^4 x (-i \partial_5) [\tilde{\psi}(x) \gamma_0 \Delta \langle \psi(x) \rangle^{(1)}] \]

\[= -Z_s^{-1} \int d^3 x (\lim_{x^0 \to -\infty} - \lim_{x^0 \to +\infty} \left[ \tilde{\psi}(x) \gamma_0 \int d^3 p \left( \bar{C}^{+}(p, \sigma) u(p, \sigma) e^{-ip \cdot x} + \bar{C}^{-}(p, \sigma) v(p, \sigma) e^{ip \cdot x} \right) \right] \]

\[= Z_s^{-1/2} \int d^3 p \left[ \bar{C}^{+}(p, \sigma) \left( \bar{b}_{\text{out}}(p, \sigma) - \bar{b}_{\text{in}}(p, \sigma) \right) + \bar{C}^{-}(p, \sigma) \left( \bar{d}^*_\text{out}(p, \sigma) - \bar{d}^*_\text{in}(p, \sigma) \right) \right]. \tag{2.5.26b} \]

Then we find, after taking proper time ordering, that

\[\Delta \psi_a^{(1)}(x) = Z_s^{-1/2} \int d^3 p \left\langle 0 \left| \left( \bar{C}^{+*}(p, \sigma) \bar{b}_{\text{out}}(p, \sigma) + \bar{C}^{-*}(p, \sigma) \bar{d}^*_\text{out}(p, \sigma) \right) \tilde{\psi}_a \right| 0 \right\rangle \]

\[+ Z_s^{-1/2} \int d^3 p \left\langle 0 \left| \tilde{\psi}_a \left( \bar{b}_{\text{in}}(p, \sigma) \bar{C}^{+}(p, \sigma) + \bar{d}^*_\text{in}(p, \sigma) \bar{C}^{-}(p, \sigma) \right) \right| 0 \right\rangle \]

\[\equiv |1_f \tilde{\psi}_a|0\rangle + |0| \tilde{\psi}_a|1_f^\rangle, \tag{2.5.27} \]

which is a general representation of the wave function of the Dirac field \( \tilde{\psi} = [\tilde{\psi}, \tilde{\psi}^\dagger] \).

In this way, by using asymptotic states, the total form of \( \Delta \psi_a \) can be summed up into

\[\Delta \psi_a = \frac{\langle \theta_f^- | \tilde{\psi}_a | \theta_f^+ \rangle}{\langle \theta_f^- | \theta_f^+ \rangle}, \tag{2.5.28} \]

where \(|\theta_{f}^\pm\rangle\) are the coherent states of the form

\[|\theta_{f}^+\rangle = \exp \left[ Z_s^{-1/2} \int d^3 p \left( \bar{b}_{\text{in}}(p, \sigma) C^{+}(p, \sigma) + \bar{d}^*_\text{in}(p, \sigma) \bar{C}^{-}(p, \sigma) \right) \right] |0\rangle, \tag{2.5.29a} \]

\[\langle \theta_{f}^- | = \langle 0 | \exp \left[ Z_s^{-1/2} \int d^3 p \left( C^{+*}(p, \sigma) \bar{b}_{\text{out}}(p, \sigma) + \bar{C}^{-*}(p, \sigma) \bar{d}^*_\text{out}(p, \sigma) \right) \right]. \tag{2.5.29b} \]

Let us introduce the generating functional \( W_{\theta_f}[J] \) in finite time interval,

\[\exp(iW_{\theta_f}[J]) \equiv \langle \theta_f^- | \text{Exp} \left( i \int_{x^0=t_f}^{x^0=t_i} d^4 x f(x) \cdot \tilde{\psi}(x) \right) | \theta_f^+ \rangle, \tag{2.5.30} \]
and also the effective action $\Gamma^{\sigma_j \sigma_j}[\phi]$ as in boson field case,

$$\Gamma^{\sigma_j \sigma_j}[\phi^*] = W^{\sigma_j \sigma_j}[J] - J_a \phi_a^*,$$  \hspace{2cm} (2.5.31)

$$\phi_a^* = \frac{\delta W^{\sigma_j \sigma_j}[J]}{\delta J_a}. \quad ((\phi_a^*)_{J=0} = \Delta \phi_a)$$  \hspace{2cm} (2.5.32)

Then we utilize the following relation instead of (2.3.2),

$$\langle \theta^- | T e^{\int J_a \phi_a} | \theta^+ \rangle = e^{i\langle \phi_0 \rangle} \langle 0 | T e^{\int (J_a + I_a) \phi_a} | 0 \rangle,$$  \hspace{2cm} (2.5.33)

$$\langle 1_\tau | 1_\tau \rangle = Z_\tau^{-1} \int d^3p \frac{e^{0}}{m} (2\pi)^4 \left( \bar{\psi}^+(\mathbf{p}, \sigma) \psi(\mathbf{p}, \sigma) + \bar{\psi}^-(\mathbf{p}, \sigma) \psi(\mathbf{p}, \sigma) \right),$$  \hspace{2cm} (2.5.34)

to find that, by setting $J = 0$, $i\Gamma^{\sigma_j \sigma_j}$ becomes the generating functional of connected $S$-matrix element among the modes created by on-shell variation $\Delta \phi$,

$$i\Gamma^{\sigma_j \sigma_j}[\Delta \phi] = \langle 1_\tau | 1_\tau \rangle + iW[J_a = \Delta \phi] = S^{(c)}(\bar{\psi}^+, \bar{\psi}^-; \bar{\psi}^+, \bar{\psi}^-).$$  \hspace{2cm} (2.5.35)

By (2.5.33) and (2.5.35), the effective action $\Gamma[\phi]$ originally defined in (2.5.3) using the vacuum state $|0\rangle$ not $|\theta^+\rangle$ is now related to the generating functional of connected $T$-matrix element, or equivalently $iW[J_a = \Delta \phi]$, in the following way,

$$i\Gamma[\Delta \phi] + i\bar{\psi}^+ \Delta \phi \bar{\psi} = iT^{(c)}(\bar{\psi}^+, \bar{\psi}^-; \bar{\psi}^+, \bar{\psi}^-).$$  \hspace{2cm} (2.5.36)

When we calculate the scattering matrix elements, $\bar{\psi}^{\pm(*)}$-derivatives are to be taken in an appropriate order. The result just corresponds to (2.3.10) in boson field case.

**References**

1) See, for example, the textbook by N. N. Bogoliubov, A. A. Logunov and I. T. Todorov, *Introduction to Axiomatic Field Theory* (Benjamin/Cummings Pub. Comp. Inc., 1975).
7) As a textbook, see for example, C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, 1980).
15) For textbooks, see for example:
Chapter III. Applications of On-Shell Equation

We discuss in this chapter some applications of the lowest order equation of the on-shell expansion (2·1·4a). As has been discussed in § 2.1, it takes various forms depending on the situations.

On the basis of the properties of the kernel $I^{(2)}$ together with the natural appearance of the wave function $\Delta \phi^{(1)}$, our on-shell condition presents a general framework for deriving the wave equation both in relativistic and non-relativistic quantum field theory.

Below we first exemplify the derivation of the equation which takes the form of Bethe-Salpeter (BS) type wave equation, for one-, two- and three-body channels. Although BS equation is used mainly in relativistic theory, it holds for the non-relativistic problems also. The extension to the general $N$-body channel will be discussed in Chapter V from a different point of view. Then the correct criterion of the stability of the state is given and the role of the self-energy in the ladder type BS equation is discussed. Other applications of the on-shell equation, such as the on-shell BS equation and the formal proof of the existence of Goldstone mode in the case of symmetry breaking are also studied. The last result will be used in Chapters X and XIV.

§ 3.1. 1, 2, 3-body Bethe-Salpeter equations

Let us first examine Hermite boson field case and start with the generating functional $W$ of the form,

$$\exp(iW[v_\nu]) = \int [d\phi] \exp i \int dt L[\phi]$$

$$= \int [d\phi] \exp i \left[ \nu_j(\phi_j) + \frac{1}{2i} \nu_k(j, k) \phi_j \phi_k + \frac{1}{3!} \nu_\ell(j, k, l) \phi_j \phi_k \phi_\ell + \frac{1}{4!} \nu_m(j, k, l, m) \phi_j \phi_k \phi_\ell \phi_m \right], \quad (3·1·1)$$

where $L[\phi]$ is the Lagrangian of the system and subscripts $j, k, \cdots$ represent the space-time as well as other internal degrees of freedom. (Summations or integrations over repeated indices are implied.) Each $\nu_\nu (\nu = 1, \cdots, 4)$ is completely symmetrized with respect to its arguments. The artificial external source $J_\nu$, which will be set equal to zero after calculations, is included in $v_\nu (\nu = 1, 2, 3)$ in (3·1·1); $v_\nu = v_\nu^0 + J_\nu$ where $v_\nu^0$ is assumed to be present in the original Lagrangian density. The rules for deriving the effective action of the elementary field variables$^{1,2}$ and two-body composite variables$^{3,3,4}$ are summarised in Appendix C together with three-body case.$^1$ In Appendix C, we present the derivation by using De Dominicis-Martin's graphical rule of the Legendre transformation.$^1$ Following their notations, here we introduce $G_\nu (\nu = 1, 2, 3)$ as the variable of the effective action,
\[ G_\nu(j, k, \ldots) = \nu^1 \frac{\delta W[v_\nu]}{\delta v_\nu(j, k, \ldots)}. \]  

(3.1.2)

The connected part of \( G_\nu \) is denoted by \( \tilde{G}_\nu \),

\[ G_\nu(j) = \tilde{G}_\nu(j), \]

\[ G_\nu(j, k) = \tilde{G}_\nu(j, k) + G_1(j)G_1(k), \]

\[ G_\nu(j, k, l) = \tilde{G}_\nu(j, k, l) + G_1(j)\tilde{G}_\nu(k, l) + G_1(k)\tilde{G}_\nu(l, j) + G_1(l)\tilde{G}_\nu(j, k) \]

\[ + G_1(j)G_1(k)G_1(l). \]  

(3.1.3)

For convenience of graphical representation, \( C_3 \)-vertex is further introduced as the amputated part of \( \tilde{G}_\nu \),

\[ \tilde{G}_\nu(j, k, l) = C_3(j', k', l', j')\tilde{G}_\nu(j', j)\tilde{G}_\nu(k', k)\tilde{G}_\nu(l', l). \]  

(3.1.4)

The Legendre transformations for 1-, 2- and 3-body channels are then carried out step by step and we obtain the effective action explicitly as follows (Appendix C):

\[ \Gamma'[G_1, J_2, J_3] = W[v_\nu] - J_1(j)G_1(j) \]

\[ = v_1^0(j)G_1(j) + \frac{1}{2} G_1(j)ig_{g^0}^{-1}(j, j')G_1(j') - i\kappa^{(1)}(G_1, J_2, J_3), \]  

(3.1.5a)

\[ \Gamma'[G_1, \tilde{G}_2, J_3] = W[v_\nu] - J_1(j)G_1(j) - \frac{1}{2i} J_2(j, k)G_2(j, k) \]

\[ = v_1^0(j)G_1(j) + \frac{1}{2i} \nu_2^0(j, k)G_2(j, k) - \frac{i}{2} \text{Tr} \ln \tilde{G}_2 - i\kappa^{(2)}(G_1, \tilde{G}_2, J_3), \]  

(3.1.5b)

\[ \Gamma'[G_1, \tilde{G}_2, C_3] = W[v_\nu] - J_1(j)G_1(j) - \frac{1}{2i} J_2(j, k)G_2(j, k) - \frac{1}{3i} J_3(j, k, l)G_3(j, k, l) \]

\[ = v_1^0(j)G_1(j) + \frac{1}{2i} \nu_2^0(j, k)G_2(j, k) + \frac{1}{3i} \nu_3^0(j, k, l)G_3(j, k, l) \]

\[ - \frac{i}{2} \text{Tr} \ln \tilde{G}_2 + \frac{i}{2} \frac{1}{3i} C_3(i, j, k)\tilde{G}_2(i, i')\tilde{G}_2(j, j')\tilde{G}_2(k, k')C_3(i', j', k') \]

\[- i\kappa^{(3)}(G_1, \tilde{G}_2, C_3), \]  

(3.1.5c)

where \( G_2^0 \) is defined from \( \nu_2 \) as \( iG_2^0^{-1}(j, k) = \nu_2(j, k) \). We have introduced \( \kappa^{(1)}(G_1, J_2, J_3) \), \( \kappa^{(2)}(G_1, \tilde{G}_2, J_3) \) and \( \kappa^{(3)}(G_1, \tilde{G}_2, C_3) \), which represent the one-particle irreducible (1PI), one- and two-particle irreducible (1, 2PI), and one-, two- and three-particle irreducible (1, 2, 3PI) vacuum diagrams constructed in terms of their arguments, respectively. The term "three-particle irreducible (3PI)" usually means the graphs which cannot be disconnected by cutting any three internal lines. But even when the graph is disconnected by this process, here we call it 3PI diagram if one (and only one) of disconnected parts is \( C_3 \)-vertex itself. Also we note that \( \kappa^{(3)} \) does not include the vacuum diagrams made up of a single \( C_3 \)-vertex. These are the conventions employed by De Dominicis and Martin."
3.1.1. 1-body channel

Now it is straightforward to derive the mode-determining equation in the form of (3.1.4a). Consider (3.1.5a) and set $J_2=J_3=0$ there since we are interested only in 1-body channel. Writing $I'[G_1, 0, 0]=I'[G_1]$ we first solve $J_1(\nu)=\delta I'[G_1]/\delta G_1(\nu)=0$ and assume that the solution is given by $G_1(\nu)=G_1^{(0)}(\nu)$. Then after calculating the second derivative of the effective action, on-shell condition for $G_1$-channel becomes

$$
\left( G_2^{\nu^{-1}}(i,j)-\frac{\delta^2 \kappa^{(1)}(i)}{\delta G_1(\nu) \delta G_1(j)} \right)_0 \Delta G_1^{(1)}(j)=0, \tag{3.1.6}
$$

where $(\cdots)_0$ means the value evaluated at $G_1^{(0)}(\nu)$, i.e., at $J_\nu=0$ ($\nu=1, 2, 3$). Since $\kappa^{(1)}$ includes all the one-particle irreducible diagrams, the second derivative of $\kappa^{(1)}$ in (3.1.6) coincides with the full self-energy correction terms. Equation (3.1.6) determines one-particle modes defined above the vacuum characterized by a chosen stationary solution $G_1^{(0)}(\nu)$. For relativistic field theory it is the Klein-Gordon equation including the quantum corrections.

3.1.2. 2-body channel

On-shell condition for $\tilde{G}_2$-channel is obtained from (3.1.5b).\textsuperscript{5} We will see that it coincides with the familiar Bethe-Salpeter (BS) equation\textsuperscript{6,7}

\begin{equation}
J_1(\nu)=\frac{\delta I'[G_1, \tilde{G}_2]}{\delta G_1(\nu)}, \quad J_2(\nu)=\frac{\delta I'[G_1, \tilde{G}_2]}{\delta \tilde{G}_2(\nu, j)} \tag{3.1.7}
\end{equation}

with the solution $G_1^{(0)}, \tilde{G}_2^{(0)}$. Note that the condition $J_2=0$ is nothing but the Schwinger-Dyson equation,

$$
\frac{i}{2} \tilde{G}_2^{-1}(j, i)-\frac{1}{2} \nu_{2}^{\nu}(i, j) + i \frac{\delta \kappa^{(2)}(i, j)}{\delta G_2(\nu, j)} = 0, \tag{3.1.7}
$$

where $\kappa^{(2)}=\kappa^{(2)}[G_1, \tilde{G}_2, J_3=0]$. The second derivative of $\kappa^{(2)}$ represents the BS kernel because it is just $2\Pi$ four point function since $\kappa^{(2)}$ is $2\Pi$, and on-shell variation $\Delta \tilde{G}_2^{(1)}$ plays the role of BS amplitude. Now on-shell condition can also be represented in the following matrix form,

$$
\begin{bmatrix}
I_{11} & I_{12} \\
I_{21} & I_{22}
\end{bmatrix}
\begin{bmatrix}
\Delta G_1^{(1)} \\
\Delta \tilde{G}_2^{(1)}
\end{bmatrix} = 0, \tag{3.1.8}
$$

where we have defined $I_{11}=\delta^2 I/\delta G_1 \delta G_1, \ I_{12}=\delta^2 I/\delta \tilde{G}_2 \delta G_1, \ I_{21}=\delta^2 I/\delta G_1 \delta \tilde{G}_2, \ I_{22}=\delta^2 I/\delta \tilde{G}_2 \delta \tilde{G}_2$. This is our BS equation which is necessarily a coupled equation in 1- and 2-body channels because these channels have the same quantum number. The conventional two-body BS equation\textsuperscript{6,7} is reproduced as follows.

First consider the case where the original Lagrangian $L[\phi]$ of (3.1.1) is symmetric under $\phi \leftrightarrow -\phi$ (in particular $\nu_{i}^{\theta}=\nu_{i}^{0}=0$). Then $I'[G_1, \tilde{G}_2]$ is also symmetric under $G_1 \leftrightarrow -G_1$. This implies that there is a solution $G_1^{(0)}=0$, which implies $(I_{12})_{\theta}=(I_{21})_{0}=0$. We thus have two decoupled equations:
Chapter III. Applications of On-Shell Equation

\[ 0 = (\Gamma_{11})_0 \Delta G_{1}^{(1)} = \left( i \frac{\delta^2 \kappa^{(2)}}{\delta G_{1}(j) \delta G_{1}(k)} \right)_0 \Delta G_{1}^{(1)}(k), \quad (3.1.9) \]

\[ 0 = (\Gamma_{22})_0 \Delta \tilde{G}_{2}^{(1)} = \left( i \frac{\delta^2 \kappa^{(2)}}{\delta \tilde{G}_{2}(j) \delta \tilde{G}_{2}(k)} \right)_0 \Delta \tilde{G}_{2}^{(1)}(l, m). \quad (3.1.10) \]

In (3.1.9) and (3.1.10) we have used the second line of (3.1.5b). It is easy to see that Eq. (3.1.9) coincides with (3.1.6) when the solution \( \tilde{G}_{2}^{(0)} \) in its perturbative form is inserted into \( \tilde{G}_{2} \) appearing in \( \kappa^{(2)} \) of (3.1.9). With this substitution \( \kappa^{(2)} \) becomes \( \kappa^{(1)} \) which contains two-particle reducible diagrams written by using the bare propagator. Equation (3.1.10) is nothing but the BS equation of 2-body channel.5)

The above argument implies the following important fact. Equation (3.1.6) is obtained by the Legendre transformation of 1-body channel only since \( J_2 = 0 \) from the start. On the other hand Eq. (3.1.9) is obtained first by the Legendre transformation in both 1-, 2-body channel and then by substituting the perturbative solution \( \tilde{G}_{2}^{(0)} \). This means that if we do not introduce the probe source in some channel we are studying that channel perturbatively. Such an observation applies to any channel.

Second we discuss the general case. Eliminating \( \Delta G_{1}^{(1)} \) or \( \Delta \tilde{G}_{2}^{(1)} \) by using one of (3.1.8), as \( \Delta G_{1}^{(1)} = - \Gamma_{11}^{-1} \Gamma_{12} \Delta \tilde{G}_{2}^{(1)} \), for instance, we get

\[ (\Gamma_{22} - \Gamma_{21} \Gamma_{11}^{-1} \Gamma_{12} \Gamma_{21})_0 \Delta \tilde{G}_{2}^{(1)} = 0. \quad (3.1.11) \]

In order to see the precise meaning of the subtracted term let us introduce \( W[J_1, \tilde{G}_2] \) which is defined as

\[ W[J_1, \tilde{G}_2] = \Gamma[G_1, \tilde{G}_2] - \Gamma_1(G_1) \frac{\delta \Gamma[G_1, \tilde{G}_2]}{\delta G_1(j)}, \]

\[ -J_1(j) = \frac{\delta \Gamma[G_1, \tilde{G}_2]}{\delta G_1(j)} \cdot (3.1.12) \]

Then we have, using the formula (A.8),

\[ \Gamma_1^{-1} = -\frac{\delta^2 W[J_1, \tilde{G}_2]}{\delta J_1(i) \delta J_1(j)} = - W_{11}, \]

therefore, suppressing the indices,

\[ \Gamma_{22} - \Gamma_{21} \Gamma_{11}^{-1} \Gamma_{12} = \Gamma_{22} + \Gamma_{21} W_{11} \Gamma_{12} \]

\[ = i \frac{1}{2} \tilde{G}_2^{-1} \tilde{G}_2^{-1} - i \frac{\delta^2 \kappa^{(2)}}{\delta \tilde{G}_2 \delta \tilde{G}_2} + \Gamma_{21} W_{11} \Gamma_{12} \]

\[ = i \frac{1}{2} \tilde{G}_2^{-1} \tilde{G}_2^{-1} - i \kappa_4. \]

We observe that \( W_{11} \) is the propagator of \( \phi \) field regarding \( \tilde{G}_2 \) a fixed quantity so that the role of the term \( \Gamma_{11} W_{11} \Gamma_{12} \) is to supply \( \Gamma_{22} \) with the one-particle reducible part. This is due to the mixing of 2-body channel with 1-body channel. In this case we have to use \( \kappa_4 \) (defined above) as the BS kernel.
If we eliminate $\Delta \tilde{G}_2^{(1)}$ by inserting $\Delta \tilde{G}_2^{(1)} = -\Gamma_{22}^{-1} \Gamma_{21} \Delta G_1^{(1)}$, we get

$$0 = (\Gamma_{11} - \Gamma_{12} \Gamma_{22}^{-1} \Gamma_{21})_0 \Delta G_1^{(1)} = (\Gamma_{11} + \Gamma_{12} W_{22} \Gamma_{21})_0 \Delta G_1^{(1)}$$

$$= \left( iG_2^{(1)} - i \frac{\delta \kappa^{(2)}}{\delta G_1} + \Gamma_{12} W_{22} \Gamma_{21} \right)_0 \Delta G_1^{(1)}$$

$$\equiv (iG_2^{(1)} - \kappa_2)_0 \Delta G_1^{(1)} ,$$

(3.1.13)

where $W_{22}$ is the second derivative of $\Gamma[G_1, J_2, J_3=0]$ defined in (3.1.5a),

$$(W_{22})_{ij} = \left( \frac{\delta^2 \Gamma[G_1, J_2, J_3=0]}{\delta f_i(\bar{f}) \delta f_j(j)} \right)_0 .$$

It can be shown that Eq. (3.1.13) coincides with (3.1.6) when we insert the perturbative solution of $\tilde{G}_2^{(0)}$ into (3.1.13). Note that in (3.1.11) or in (3.1.13), $\Gamma_{11}$ or $\Gamma_{22}^{-1}$ has to be regular respectively, which implies that 1-particle or 2-particle channel is off the mass shell. Upon this assumption we are looking for the mass shell condition of 2-particle or 1-particle channel respectively.

3.1.3. 3-body channel

Using $\Gamma[G_1, \tilde{G}_2, C_3]$ of (3.1.5c), and defining $\Gamma_{23} = \delta^2 \Gamma/\delta \tilde{G}_2 \delta C_3$, etc., the BS equation takes the $3 \times 3$ form,

$$\begin{bmatrix} \Gamma_{11} & \Gamma_{12} & \Gamma_{13} \\ \Gamma_{21} & \Gamma_{22} & \Gamma_{23} \\ \Gamma_{31} & \Gamma_{32} & \Gamma_{33} \end{bmatrix} \begin{bmatrix} \Delta G_1^{(1)} \\ \Delta \tilde{G}_2^{(1)} \\ \Delta C_3^{(1)} \end{bmatrix} = 0 ,$$

(3.1.14)

where $[\cdots]_0$ is evaluated at the solution $G_1^{(0)}$, $\tilde{G}_2^{(0)}$, $C_3^{(0)}$ of $\delta \Gamma/\delta G_1 = \delta \Gamma/\delta \tilde{G}_2 = \delta \Gamma/\delta C_3 = 0$. This is the most general BS equation of 3-body channel. Reduction to the equation for $\Delta C_3^{(1)}$ only in general case proceeds step by step. After eliminating $\Delta G_1^{(1)}$, we get

$$\begin{bmatrix} \tilde{\Gamma}_{22} & \tilde{\Gamma}_{23} \\ \tilde{\Gamma}_{32} & \tilde{\Gamma}_{33} \end{bmatrix} \begin{bmatrix} \Delta \tilde{G}_2^{(1)} \\ \Delta C_3^{(1)} \end{bmatrix} = 0 ,$$

$$\tilde{\Gamma}_{jk} = \Gamma_{jk} - \Gamma_{j1} \Gamma_{11}^{-1} \Gamma_{1k} , \quad (j, k=2, 3)$$

(3.1.15)

which brings about the one-particle reducible graphs. Further elimination of $\Delta \tilde{G}_2^{(1)}$ gives the BS equation in 3-body channel.

$$(\tilde{\Gamma}_{33})_0 \Delta C_3^{(1)} = 0 ,$$

$$\tilde{\Gamma}_{33} = \tilde{\Gamma}_{33} - \tilde{\Gamma}_{32} \tilde{\Gamma}_{22}^{-1} \tilde{\Gamma}_{23} .$$

(3.1.16)

Now let us compare (3.1.16) with the conventional form of the 3-body BS equation. As has been stated, if we do not probe 1- and 2-body channel by setting $J_1 = J_2 = 0$ from the start and make the Legendre transformation in $J_3$ only, we are discussing 1- and 2-body channel perturbatively.

This process leads us to define new $\tilde{\Gamma}[C_3]$ which includes one, two particle reducible vacuum graphs denoted by $\kappa^{(0)}$, and has the form
\[
\tilde{\Gamma}[C_3] = -\frac{i}{2} \frac{1}{3!} C_3 \tilde{G}_2 \tilde{G}_2 \tilde{G}_2 C_3 - i \tilde{\kappa}^{(3)}(C_3),
\]  
(3.1.17)

where \( \tilde{G}_2 \) is now that part of perturbative connected propagator which is independent of \( C_3 \). The \( C_3 \)-dependent part is included in \( \tilde{\kappa}^{(3)}(C_3) \) which contains two particle reducible diagrams. In this form, usual 3-body BS equation is obtained as \( \langle \delta^2 \tilde{\Gamma}[C_3] / \delta C_3 \delta C_3 \rangle \delta C_3^{(1)} = 0 \), which reads explicitly as
\[
\left[ \frac{1}{3!} \tilde{G}_2(j, j') \tilde{G}_2(k, k') \tilde{G}_2(l, l') - \frac{\delta^2 \tilde{\kappa}^{(3)}(C_3)}{\delta C_3(j, k, l) \delta C_3(j', k', l')} \right] \delta C_3^{(1)}(j', k', l') = 0.
\]  
(3.1.18)

On the other hand, the route to arrive at (3.1.18) from \( \Gamma'[G_1, \tilde{G}_2, C_3] \) is as follows. Suppose \(- J_1 = \delta \Gamma / \delta G_1 = 0, - J_2 = \delta \Gamma / \delta \tilde{G}_2 = 0 \) is solved perturbatively with fixed \( C_3 \) and we express the solution \( G_1^{(0)} \) and \( \tilde{G}_2^{(0)} \) in terms of \( C_3 \) and then they are inserted into \( \Gamma'[G_1, \tilde{G}_2, C_3] \) to get \( \Gamma'[C_3] = \Gamma'[G_1^{(0)}(C_3), \tilde{G}_2^{(0)}(C_3), C_3] \). This is \( \tilde{\Gamma}[C_3] \) defined in (3.1.17). Therefore \( \tilde{\Gamma}_{33} \) of (3.1.16) is given in this case by \( \tilde{\Gamma}_{33} = \delta^2 \tilde{\Gamma}[C_3] / \delta C_3 \delta C_3 \).

However in general case where non-perturbative effect is essential in 1- and 2-body channel, we have to use (3.1.14) or (3.1.16) without using perturbative solutions for \( G_1^{(0)}, \tilde{G}_2^{(0)} \). We remark finally that all the above results can be given using \( \tilde{G}_3 \) of (3.1.4) instead of \( C_3 \) but the results become slightly complicated.

For the application to fermion system, especially to the equation of atomic energy levels in QED, see Ref. 9. Instead, in Chapter VIII (§ 8.1), we discuss the non-relativistic atomic system by our formalism.

§ 3.2. Role of self-energy in ladder approximation

The energy levels in 1-, 2-, 3-body channel can be determined by the Bethe-Salpeter equation discussed in the previous section but in practical calculations, we have to make approximations. Consider (3.1.10). The simplest one, which is the usually accepted ladder approximation, is to replace the inverse of the full propagator \( G_2 \) by its free part and to take the lowest term as the second derivatives of the kernel \( \kappa^{(2)} \).

However this contradicts with our observations since energy levels are determined by zeros of the second derivative of \( \Gamma \) so that we have to retain all the terms appearing in the perturbative expansion of (the second derivative of) the whole \( \Gamma \). Ladder approximation neglects the self-energy correction to the propagator which is expected to lead to the incorrect energy eigenvalue of excited state. We present explicit calculations in Chapter XIII (§ 13.1), where energy level in quantum mechanical system is studied. There we find that our expectation is correct in fact and that inclusion of self-energy term reproduces the correct value.

It is well-known that the ladder calculation has several diseases such as the abnormal solution or the appearance of negative metric state. The value of energy eigenvalue is no doubt a primary quantity, more fundamental than these diseases, and the above hitherto unobserved fact about the ladder approximation has to be kept in mind.
§ 3.3. Criterion for stability of quantum system

One of the direct consequences of on-shell expansion is that we automatically obtain the correct criterion of the stability of the chosen solution denoted in general by $\phi^{(0)}$. Since $\phi^{(0)}$ is the ground state expectation value, the criterion is the one for the stability of the ground state. As is easily convinced we have to study the solution of small oscillation around $\phi^{(0)}$ which is written as $\Delta\phi^{(1)}$.

The problem is whether such a picture can be transformed into the familiar language of the sign of the second derivative of the potential which is defined by the time-independent stationary part of action functional. Recall here that such a familiar criterion holds only for classical mechanical systems and for quantum system we will see that in general it is not a correct statement of the stability of ground state. Indeed there are much debates about the stability criterion of the stationary solution of the effective action. In fact the second derivative of the effective potential defined below evaluated at the stationary solution is not unique and it depends on how one calculates the effective potential. It has been found00 moreover that in some cases the effective potential is not bounded from below. There is also a case where the chosen solution corresponds to the state of the lowest energy yet the second derivative of the effective potential at the solution is not positive definite.

The purpose of this section is to answer these problems using the formula (2.1.4a). On the basis of this equation the general correct criterion for the stability has been given in Refs. 5 and 12). The crucial observations which constitute the starting point are summarized in (i)~(iii) below. For this purpose, we need a relation between the effective potential $V(\phi)$ and the effective action $\Gamma[\phi]$, which is obtained by the local expansion of $\Gamma[\phi]$:

$$\Gamma[\phi]=\int d^4x\left[-V(\phi_1(x))+\frac{1}{2}Z(\phi_1(x))\partial_\mu\phi_1(x)\partial^\mu\phi_1(x)+\cdots\right].$$

We have assumed relativistic case but the arguments hold for non-relativistic case also. Now we state our observations.

(i) The stability problem is essentially a time-dependent phenomenon and it cannot be discussed by the effective potential. In order to make clear this point, let us take a classical-mechanical system (1.1.16). Let one of the static solution to the equation of motion be $q_i^{(0)}$ and write as in (1.1.4) $q_i(t)=q_i^{(0)}+\Delta q_i(t)$. Then Eq. (1.1.17) takes the form,

$$m\ddot{q}_i(t)=-V_\phi\Delta q_i(t).$$

Here $V_\phi$ is the second derivative matrix of $V$ evaluated at the solution $q_i^{(0)}$. The requirement that $\Delta q_i(t)$ does not contain a blowing-up solution is equivalent to positive definiteness of the matrix $V_\phi$, which is the well-known stability condition of the solution $q^{(0)}$. Note that such a criterion follows because the kinetic-energy term is known to be $(1/2)m\dot{q}_i^2$, which is positive definite. Recall here that the stability depends on the relative sign of the kinetic energy and $V_\phi$. In any quantum system,
however, we have to calculate \( Z(\phi_i(x)) \) of (3.3.1) and also all the terms with higher
derivatives for the discussion of the (space-) time dependence of the solution. The
condition of the positive definiteness of \( V_\nu \) is not necessarily the stability criterion.

(ii) The original theory is recovered only at \( J_i(x) = 0 \) so that we have always to
satisfy \( J_i(x) = 0 \) in order to discuss the physical quantities. Remember that the
stability is of course a property of the physical process. The second derivative of the
effective potential is, however, an off-shell quantity in general (except for the case
where it has the vanishing second derivative) so that it involves the information of the
theory with \( J_i(x) \neq 0 \).

(iii) The stability of a given solution is a physical statement and it is determined
once the theory is fixed. It follows that the stability criterion should not depend on
(1) the gauge we have chosen in the case of the gauge theory, on (2) the renormalization
scheme, or on (3) the operator we have chosen to study the stability. The last
statement needs clarification. Suppose we choose the operator \( \tilde{O} \) to study the ground
state which might have finite expectation value of \( \tilde{O} \). But we can equally utilize
another \( \tilde{O}' \) and should get the same physical results (such as the energy of the
condensed state and the stability) as long as \( \tilde{O} \) and \( \tilde{O}' \) have the same quantum number
and therefore they mix. The fact that we get different answers to the stability
problem for different operators is related to the ambiguity problem stated above.

Now we state our stability criterion\(^{5,12}\) which clarifies the points (i)~(iii) above:
any solution to (2.1.4a) does not blow up for large \( t \). If \( \phi_i^{(0)}(x) \) is space-time
independent, \( \phi_i^{(0)}(x) = \phi_i^{(0)} \), then we have the solution (2.1.13). In \( x \)-space, we see
from (2.1.17) that the stability condition of our solution \( \phi_i^{(0)} \) is that there do not exist
any poles of \( W^{(2)} \) [evaluated at \( \phi_i(x) = \phi_i^{(0)} \)] in the spacelike region \( m^2 < 0 \); the
absence of the tachyonic pole. Otherwise \( \Delta \phi_i^{(1)}(t, p) \) for \( p^2 < -m^2 \) blows up for large
\( t \), as \( \exp(\pm i(p^2 + m^2)^{1/2}t) \).

Our criterion naturally answers the questions (i)~(iii) since it is the position of
the pole of the Green's function which determines the stability. Several examples of
both local and non-local operator case have been given in Refs. 5) and 12).

\section*{§ 3.4. On-shell bound state equation}

In this section, we present a novel approach to the bound state problem which
utilizes the on-shell quantity only.\(^{13}\) It is one of the applications of on-shell equation
(2.1.4a) for composite bound state.

Let us first consider the bound state wave function defined by

\[
\Delta G_i^{(1)}(X) = \langle 0 | T \tilde{\Phi}(x) \tilde{\Phi}(y) | B \rangle,
\]

where \( i = x - y \), \( X = (x + y)/2 \). This wave function is defined of course on the mass-
shell of \( B \)-state but off-shell in two constituent channels specified by \( x \) and \( y \).

Our program here is to project out on to the mass shell of these two constituent
particles and obtain bound state equation where all channels involved are on the mass
shell. However, once two constituent particles become on-shell particles, bound state
appears in the unphysical region in the composite channel so that our approach has
to be combined with the analytic continuation in the variable $s = E^2$. This variable is defined, in the center of mass (CM) frame, to be the square of total energy $E$ of the physical, i.e., on-shell, two constituent particles. Our starting observations are the following two points:

1. Any state, which appears as a pole of the off-shell Green's function, also contributes to a pole of the $S$-matrix element if it is a physical state lying in the physical Hilbert space. Therefore if we find an eigenvalue equation corresponding to the pole of the $S$-matrix element, or $T$-matrix element defined by $S = 1 + iT$, then it can equally be used as a bound state equation.

2. From the practical point of view, we have to find some calculable scheme of the equation obtained above. Since the pole of the $T$-matrix element is equivalent to the zero of $T^{-1}$, the perturbative expansion of $T^{-1}$ gives the solution to the equation successively in the coupling constant.

By applying the above two observations we get the on-shell BS equation which has several remarkable features listed below. We believe that they are all essential to the bound state problem both conceptually and technically:

(A) Decomposing two-particle scattering amplitude into the partial wave with the total angular momentum $J$ in the relevant $s$-channel, our equation takes the form $T^{-1}(s, J) = 0$. The problem is simply to find a zero of the ordinary analytic function $T^{-1}(s, J)$, while the conventional off-shell BS equation is an integral equation.

(B) Off-shell BS equation refers to the pole of the Green's function, so that there arises a problem about whether it appears in the physical $S$-matrix elements or not. This is a difficult problem to answer, which however is bypassed in our formalism since we are looking for the pole of the $S$-matrix element from the start.

(C) For the case of the gauge theory, on-shell BS equation is gauge invariant even if it is solved approximately by making the perturbation in the coupling constant. Recall here that it has been a long-standing problem to get the bound state equation which gives us the gauge invariant numerical value for the energy. This was in fact our starting motivation.

(D) Since the off-shell BS equation is an integral equation, the perturbative approximation to the kernel sometimes produces ultraviolet divergences in the solution since the equation involves the off-shell integration in the momentum. This divergence cannot be absorbed by the usual perturbative renormalization. The appearance of the bound state, however, is the low energy phenomenon and should not be affected by the integral in the ultraviolet region, so that the above is one of the shortcomings of the conventional formalism. Our equation is not an integral equation and $T(s, J)$ is renormalized order by order in the coupling constant, so the solution to $T^{-1}(s, J) = 0$ is finite and expressed by the renormalized parameters. This is due to the fact that the off-shell integration in the off-shell formalism is replaced by the analytic continuation in the $s$-variable in our on-shell formalism.

(E) For more than two-particle bound state equation, our on-shell BS equation takes a nontrivial form of integral equation. But the ultraviolet divergences never
appear in this integration process since we are using physical scattering matrix elements only. We point out furthermore that the number of variables coming into this integral equation is smaller than the usual off-shell approach because of the on-shell restrictions on the constituent channels.

3.4.1. On-shell BS equation

The projection on to the mass-shell in $x$ and $y$ channels can be done as follows. Take the source term $J(x, y)$ of (2.4.1) in the following way,

$$J(x, y) = Z^{-1} \int d^3 p_1 d^3 p_2 \left[ J_1(p_1, p_2) f_{p_1}^*(x) K_x f_{p_2}^*(y) K_y + J_2(p_1, p_2) f_{p_1}^*(x) K_x f_{p_2}^*(y) K_y \right].$$

(3.4.1)

We take in this section the relativistic scalar field (Klein-Gordon field $\phi(x)$) and $Z$ is the field renormalization constant of $\phi$. $J_i(p_1, p_2)$ ($i=1, 2$) are the new sources which can be assumed to satisfy $J_1^* = J_1$ but here $J_1$ and $J_2$ are taken as independent sources. The symbol $K_x$ denotes the Klein-Gordon operator ($\Box_x + m^2$) and $f_{p}(x) = \exp(-ip_0 x_0 + ip \cdot x)$ is proportional to the wave function of asymptotic state with 3-momentum $p$. It satisfies the wave equation $K_x f_{p}(x) = 0$, therefore $p_0 = \sqrt{p^2 + m^2}$. The mass $m$ is supposed to include the effect of the self-energy correction. The effective action $\Gamma[\phi]$ in this case is given by

$$\Gamma[\phi] = W - \sum_{i=1,2} \int d^3 p_1 d^3 p_2 \phi_i(p_1, p_2) J_i(p_1, p_2),$$

(3.4.2)

$$\phi_i(p_1, p_2) \equiv W_i(p_1, p_2) \equiv \frac{\delta W}{\delta J_i(p_1, p_2)},$$

(3.4.3)

where explicit $J_i$ dependence is eliminated from $\Gamma$ by inverting (3.4.3). By these definitions, we have the identities $\Gamma_i(p_1, p_2) = \delta \Gamma / \delta \phi_i(p_1, p_2) = -J_i(p_1, p_2)$ and

$$\sum_{j=1,2} \int d^3 p'_1 d^3 p'_2 \Gamma_{ij}(p_1, p_2; p'_1, p'_2) W_{ijk}(p'_1, p'_2; p''_1, p''_2)$$

$$= \sum_{j=1,2} \int d^3 p'_1 d^3 p'_2 W_{ij}(p_1, p_2; p'_1, p'_2) \Gamma_{jk}(p'_1, p'_2; p''_1, p''_2)$$

$$= -\frac{1}{2} \delta_{ik} \left[ \delta^3(p_1 - p'_1) \delta^3(p_2 - p''_2) + \delta^3(p_1 - p''_2) \delta^3(p_2 - p'_1) \right],$$

(3.4.4)

where $\Gamma_{ij}(p_1, p_2; p'_1, p'_2)$ implies $\delta^3 \Gamma / \delta \phi_i(p_1, p_2) \delta \phi_j(p'_1, p'_2)$. $W_{ij}(p_1, p_2; p'_1, p'_2)$ is defined in the same way.

The equation of motion $\Gamma_i(p_1, p_2) = 0$ determines $\phi_i$ to be zero,

$$\phi_1(p_1, p_2) = Z^{-1} \int d^4 x d^4 y f_{p_1}^*(x) K_x f_{p_2}^*(y) \phi_0(x) \phi(y) 0 = 0,$$

(3.4.5)

$$\phi_2(p_1, p_2) = Z^{-1} \int d^4 x d^4 y f_{p_1}^*(x) K_x f_{p_2}^*(y) \phi_0(x) \phi(y) 0 = 0,$$

(3.4.6)

as is seen by using the LSZ reduction formula. Following the scheme of on-shell expansion, we now discuss another solutions which are slightly shifted from these
trivial solutions. Substituting $\phi_i = \Delta \phi_i$ into the equation $\Gamma_i(p_1, p_2) = 0$ and ignoring higher order terms in $\Delta \phi_i$, we get our on-shell BS equation

$$\sum_{j=1,2} \int d^3p_1 d^3p_2 \Gamma_j(p_1, p_2; p'_1, p'_2) \mid_{\phi_i = 0} = 0. \quad (3.4.7)$$

The LSZ formula tells us that $W_i(p_1, p_2; p'_1, p'_2) \mid_{j=0} = W_1(p'_1, p'_2; p_1, p_2) \mid_{j=0}$ equals to the $T$-matrix elements defined by $S=1+iT$,

$$W_1(p_1, p_2; p'_1, p'_2) \mid_{j=0} = W_2(p'_1, p'_2; p_1, p_2) \mid_{j=0} = \langle i | a^\text{out}_{p_1} a^{\text{out}\dagger}_{p'_1} a^{\text{in}}_{p_2} a^{\text{in}\dagger}_{p'_2} | 0 \rangle = -T(p_1, p_2; p'_1, p'_2), \quad (3.4.8)$$

while $W_1(p_1, p_2; p'_1, p'_2) \mid_{j=0} = W_2(p'_1, p'_2; p_1, p_2) \mid_{j=0}$ vanishes. Here, $a^\text{in(out)}_p$ or $a^\text{in(out)}_{p'}$ denotes the annihilation or creation operator of the in(out) asymptotic field of $\tilde{\phi}_i$, respectively. From these equations and the identity $(3.4.4)$, Eq. $(3.4.7)$ is reduced to the following two decoupled equations,

$$\int d^3p_1 d^3p_2 \Gamma_{12}(p_1, p_2; p'_1, p'_2) \Delta \phi_2(p'_1, p'_2)$$

$$= \int d^3p_1 d^3p_2 \Delta \phi_2(p'_1, p'_2) T^{-1}(p'_1, p'_2; p_1, p_2) = 0, \quad (3.4.9)$$

$$\int d^3p_1 d^3p_2 \Gamma_{21}(p_1, p_2; p'_1, p'_2) \Delta \phi_1(p'_1, p'_2)$$

$$= \int d^3p_1 d^3p_2 T^{-1}(p_1, p_2; p'_1, p'_2) \Delta \phi_1(p'_1, p'_2) = 0, \quad (3.4.10)$$

where we have defined $T^{-1}(p_1, p_2; p'_1, p'_2)$ as

$$\int d^3p_1 d^3p_2 T(p_1, p_2; p'_1, p'_2) T^{-1}(p'_1, p'_2; p_1, p_2)$$

$$= \frac{1}{2} \left[ \delta^3(p_1 - p'_1) \delta^3(p_2 - p'_2) + \delta^3(p_1 - p'_2) \delta^3(p_2 - p'_1) \right]. \quad (3.4.11)$$

The translational invariance of the theory implies the form of $T(p'_1, p'_2; p_1, p_2)$ in the CM frame as

$$T(p'_1, p'_2; p_1, p_2) = \delta^4(P' - P) T(s; \theta', \varphi'; \theta, \varphi) \frac{v}{q^2}. \quad (3.4.12)$$

Here $P$ or $P'$ is the total 4-momentum of the incoming or outgoing particles, respectively and $s = P^2 = P'^2$. Explicitly, $P$ is given by $P = (P^0, \mathbf{P}) = (2\sqrt{q^2 + m^2}, 0)$. We have introduced the relative 3-momentum $q$ or $q'$ of each pair of particles, $q = p_1 = -p_2$, $q' = p'_1 = -p'_2$. The polar angle of $q$ or $q'$ is denoted by $(\theta, \varphi)$ or $(\theta', \varphi')$, respectively. The normalization factor $v/q^2$ has been inserted in order to simplify the following equations, where $v = 2|q|/\sqrt{q^2 + m^2}$ is the magnitude of the relative velocity in the CM frame. Similarly for $T^{-1}$, we write

$$T^{-1}(p'_1, p'_2; p_1, p_2) = \delta^4(P' - P) T^{-1}(s; \theta', \varphi'; \theta, \varphi) \frac{v}{q^2}. \quad (3.4.13)$$
then, after the change of the integration variables Eq. (3.4.11) takes the form,

$$\int d\Omega' T(s; \theta'', \varphi''; \theta', \varphi') T^{-1}(s; \theta', \varphi'; \theta, \varphi) = \frac{1}{2} \left[ \delta(\Omega''-\Omega) + \delta(\Omega''+\Omega) \right],$$

(3.4.14)

where \( d\Omega' = d(\cos \theta') d\varphi' \), \( \delta(\Omega''-\Omega) = \delta(\cos \theta''-\cos \theta) \delta(\varphi''-\varphi) \) and \( \delta(\Omega''+\Omega) = \delta(\cos \theta''+\cos \theta) \delta(\varphi''-\varphi-\pi) \). Thus, in the CM frame we can rewrite the on-shell BS equations (3.4.9) and (3.4.10) as

$$\int d\Omega' \Delta \phi_2(s; \theta', \varphi') T^{-1}(s; \theta', \varphi'; \theta, \varphi) = 0,$$

(3.4.15)

$$\int d\Omega T^{-1}(s; \theta', \varphi'; \theta, \varphi) \Delta \phi_1(s; \theta, \varphi) = 0.$$ 

(3.4.16)

These equations determine the eigenvalues of the bound state energy by regarding \( T^{-1}(s; \theta', \varphi'; \theta, \varphi) \) as an analytic function of the Lorentz invariant variable \( s \) which is analytically continued to the region \( s<4m^2 \). It is of course the forbidden region of the physical scattering, but it is well-known that the pole corresponding to the bound state definitely appears in \( T \) at the correct position in the \( s \) variable.

Now we decompose the on-shell BS equation into the sectors specified by the total angular momentum \( J \) of the bound state. Since \( J \) and \( J_z=\pm M \) are conserved, the on-shell BS equation (3.4.15) or (3.4.16) is decoupled in each channel of \((J, M)\), so we consider \( T \) or \( T^{-1} \) in one of these channels. The formulas necessary to get these decoupled equations are

$$\chi(s, J, M) = \int d\Omega Y^*_m(\theta, \varphi) \Delta \phi_1(\theta, \varphi),$$

(3.4.17)

$$\bar{\chi}(s, J, M) = \int d\Omega Y^*_m(\theta, \varphi) \Delta \phi_2(\theta, \varphi)$$

(3.4.18)

for the BS amplitudes, \( T(s, J) = \int d\Omega T(s; \theta, \varphi; 0, 0) P_J(\cos \theta) \) for the \( T \)-matrix element, and the same for \( T^{-1}(s, J) \). The identity (3.4.14) is also reduced to \( T(s, J) T^{-1}(s, J) = 1 \) for even \( J \), while odd \( J \) is absent because we are considering the scattering of the identical particles. Then the on-shell BS equations (3.4.16) and (3.4.15) read \( T^{-1}(s, J) \chi(s, J, M) = 0 \) and \( \bar{\chi}(s, J, M) T^{-1}(s, J) = 0 \), respectively. These equations imply

$$T^{-1}(s, J) = 0$$

(3.4.19)

for the nontrivial solution of \( \chi \) or \( \bar{\chi} \). This is a simple equation to determine \( s \) as a zero of the ordinary function, and it is not the differential or the integral equation, or the matrix equation as in the case of the conventional BS equation.

### 3.4.2. Perturbative calculation of \( T^{-1} \)

In order to get the perturbative expansion of \( T^{-1}(s, J) \), we use essentially the same process of inversion method which will be explained in Chapter VII below. It is originally introduced to compute the nonperturbative quantity in a perturbative way. However, for the present purpose we can do the calculation without using
explicit inversion formulas and proceed as follows.

First of all, we expand $T(s, J)$ and $T^{-1}(s, J)$ into the perturbative series of the coupling constant $\lambda$,

$$T = \lambda T_1 + \lambda^2 T_2 + \lambda^3 T_3 + \cdots, \tag{3.4.20}$$

$$T^{-1} = \lambda^{-1} V_{-1} + V_0 + \lambda V_1 + \cdots. \tag{3.4.21}$$

Substituting them into the identity $T(s, J)T^{-1}(s, J) = 1$, and comparing the terms in the same order of the coupling constant $\lambda$, we get the set of the equations, $T_1 V_{-1} = 0$, $T_1 V_0 + T_2 V_{-1} = 0$, $T_1 V_1 + T_2 V_0 + T_3 V_{-1} = 0$, etc. This can be solved successively as $V_{-1} = T_1^{-1}$, $V_0 = -T_1^{-1} T_2 T_1^{-1}$, $V_1 = -T_1^{-1} T_3 T_1^{-1} + T_1^{-1} T_2 T_1^{-1} - T_2 T_1^{-1}$, etc.

The on-shell amplitude for the scattering of particles with any spin is most elegantly described by the Jacob-Wick helicity formalism.\(^{10}\) Let us consider the CM $T$-matrix element in helicity representation $T_{\frac{1}{2} \frac{1}{2} 1; \frac{1}{2} \frac{1}{2} 1}(s; \theta, \varphi)$. Using partial wave amplitude $T_{\frac{1}{2} \frac{1}{2} 1; \frac{1}{2} \frac{1}{2} 1}(s, J)$, let us introduce $T^{-1}_{\frac{1}{2} \frac{1}{2} 1; \frac{1}{2} \frac{1}{2} 1}$ which is the inverse matrix of $T_{\frac{1}{2} \frac{1}{2} 1; \frac{1}{2} \frac{1}{2} 1}$ in helicity space. Then our on-shell BS equation for arbitrary spin is given by $T^{-1}_{\frac{1}{2} \frac{1}{2} 1; \frac{1}{2} \frac{1}{2} 1}(s, J) = 0$. The bound state energy $\sqrt{s(J)}$ is obtained for any fixed value of helicity by the zero of this ordinary function. (Whether the zero in $s$ lies on the desirable sheet in the complex $s$-plane has to be carefully analyzed by looking into the analytic property of $T_{\frac{1}{2} \frac{1}{2} 1; \frac{1}{2} \frac{1}{2} 1}(s, J)$.)\(^{10}\)

We have shown a novel method of obtaining the energy eigenvalue of the bound state. The wave function of the bound state in the usual formalism, $\Delta \phi(x, y)$ is the off-shell quantity. It is missing in our formalism. Does this mean that we have lost the information on the bound state? It seems to be the case but remember that the wave function itself is not an observable. Only the $S$-matrix element is the real observable quantity so that it is possible that by our formalism we can calculate all the physical observables about the bound states.

The essence of the inversion method is that although we discard in the expansion of $T^{-1}$ the higher-order terms than some finite order, the non-perturbative solution, such as the existence of the bound state, is not lost in the series

$$T^{-1} = \lambda^{-1} V_{-1} + V_0 + \lambda V_1 + \cdots + \lambda^n V_n. \tag{3.4.22}$$

This can be seen from the fact that the full re-inversion of $T^{-1}$ given in (3.4.22) to the original $T$ contains the infinitely many terms, which can elucidate the non-perturbative effects. A sharp contrast with the conventional BS equation exists when we solve (3.4.19) perturbatively. In the usual off-shell BS equation,\(^{6, 7}\) the perturbative expansion of $\Gamma(x, y; x', y')$ starts from the zeroth order of $\lambda$; $\Gamma(x, y; x', y') = V_0 + \lambda V_1 + \cdots$. However, for the on-shell BS equation here, the perturbative expansion of $T$ starts from $O(\lambda)$ since the real scattering occurs due to the interaction between the on-shell particles.

3.4.3. Examples of $\lambda \phi^4$ theory

Let us illustrate the above idea taking $\lambda \phi^4$ as a simple example. We will study (3.4.19) taking $V_{-1}$ and $V_0$ into account. In order to calculate $V_{-1}$ and $V_0$ we need $T_1$ and $T_2$. They have the expressions in momentum space given by
Chapter III. Applications of On-Shell Equation

\[ T_1(p', p'; p, p) = -(2\pi)^4 \delta^4(P' - P)Z^2, \quad (3.4.23) \]

\[ T_2(p', p'; p, p) = (2\pi)^4 \delta^4(P' - P)Z^2 \left[ A(s) + A(t) + A(u) \right], \quad (3.4.24) \]

where \( t = (p_1 - p_1)^2, \ u = (p_2 - p_2)^2, \)

\[ A(s) = \frac{1}{(4\pi)^2} \left[ 1 + \ln \frac{m^2 - s}{m^2} - 2\sqrt{\frac{4m^2 - s}{s}} \arctan \sqrt{\frac{s}{4m^2 - s}} \right], \quad (3.4.25) \]

and \( \Lambda \) is the ultraviolet momentum cutoff. The renormalization can easily be performed as usual. For simplicity, we take the symmetric point as the subtraction point, \( s = t = u = 4m^2/3 \) since \( s + t + u = 4m^2 \). Then the renormalized coupling constant \( \lambda_r \) is given by \( \lambda_r = \lambda - (3/2)\lambda^2 A(4m^2/3) \). If we expand \( T \) in \( \lambda_r, T_2 \) now becomes finite and is given by (3.4.24) with \( A(s) \) etc. replaced by \( A(s) \) etc. where

\[ \tilde{A}(s) = \frac{2}{(4\pi)^2} \left[ \sqrt{2} \arctan \frac{1}{\sqrt{2}} - \sqrt{\frac{4m^2 - s}{s}} \arctan \sqrt{\frac{s}{4m^2 - s}} \right]. \quad (3.4.26) \]

Next, we evaluate the angular momentum representation of \( T_1 \) and \( T_2 \). Since \( T_1 \) contains only the \( s \)-wave scattering, \( T_1(s, J) = -(2\pi)^4 \delta_0(2\pi)^4 Z^2 q^2 / v \), we project out only the \( J = 0 \) part of \( T_2 \) (in order to discuss \( J \neq 0 \) mode, we have to calculate \( T_3 \) or higher). \( T_3(s, J = 0) \) is calculated as

\[ T_2(s, J = 0) = 4\pi(2\pi)^4 Z^2 q^2 / v \left[ \tilde{A}(s) + 2\tilde{A}(s) \right], \quad (3.4.27) \]

\[ \tilde{A}(s) = \frac{1}{4\pi} \int d\Omega \tilde{A}((4m^2 - s)(1 - \cos \theta)/2) \]

\[ = \frac{1}{(4\pi)^2} \left[ 2\sqrt{2} \arctan \frac{1}{\sqrt{2}} \left( 1 + \frac{1}{x^2} \right) \arctan x - \frac{2}{x} \arctan x + 1 \right] \quad (3.4.28) \]

with \( x = \sqrt{(4m^2 - s)/s} \). Then after the inversion of \( T_1 \) and \( T_2 \) to get \( V_1 \) and \( V_6 \), Eq. (3.4.19) leads to \( 1/\lambda_r + [\tilde{A}(s) + 2\tilde{A}(s)]/2 = 0 \). In the weakly binding region, i.e., \( 0 < x < 1 \), this equation becomes \( -(4\pi)^2/\lambda_r = C - (\pi/2)x + O(x^2) \), where \( C = 3\sqrt{2} \arctan(1/\sqrt{2}) - 2 \). It has the solution \( s(\lambda_r) \) below the critical value \( \lambda_r^c = -(4\pi)^2/C < 0 \). Recall here that negative \( \lambda \) corresponds to the attractive force. Near the threshold \( \lambda_r \approx \lambda_r^c \) the binding energy \( B = 2m - \sqrt{s} \) behaves as \( B \approx m[C^4/(2\pi)^6](\lambda_r^c - \lambda_r)^2 \), so that as \( |\lambda_r| \) increases the binding energy gets large as expected.

Now compare the above result with the conventional off-shell BS equation in the lowest order. It is given in momentum space as

\[ G_0 \left( \frac{P}{2} + p \right) G_0 \left( \frac{P}{2} - p \right) \Delta \phi(P, p) + i \frac{\lambda}{2} \int \frac{d^4k}{(2\pi)^4} \Delta \phi(P, k) = 0, \quad (3.4.29) \]

where \( P \) or \( p \) is the total or the relative momentum of the particles, respectively, and \( G_0(p) = i/(p^2 - m^2) \). It is easy to see that this equation gives us the well-known eigenvalue equation \( -1/\lambda = A(s)/2 \). The integral equation is reduced to the ordinary functional equation but this is limited to the lowest order in the off-shell case. Here
$A(s)$ includes the momentum cutoff $\Lambda$, and diverges as $\Lambda$ becomes infinity. However this equation can *not* be renormalized by the ordinary perturbative renormalization scheme, $\lambda \rightarrow \lambda r - (3/2)\alpha^2 A(4m^2/3)$. If we assume $\Lambda$ to be finite, the bound state solution to (3.4.29) exists for $\lambda < \lambda_c < 0$, where the critical coupling $\lambda_c$ is given by $\lambda_c = -(4\pi)^2/C$, $C = [1 + \ln(\Lambda^2/m^2)]/2$. Near the threshold $\lambda \approx \lambda_c$, the binding energy behaves as above $B$ with $C, \lambda r$, and $\lambda r^2$ replaced by $C, \lambda$, and $\lambda_c$, respectively. These results are qualitatively similar to ours in the on-shell BS formalism.

Although we have taken a very simple model, these results serve as an illustration of the statement (D) above.

§ 3.5. Symmetry breaking and Goldstone mode

When the symmetry of the Hamiltonian or the Lagrangian is broken by the ground state, on-shell equation tells us about the existence of the Goldstone mode and its explicit form of wave function. The presence of the Goldstone state has been proven in Ref. 17) by the same technique as shown below. Let the Lagrangian density $L(\phi) = L(\phi_i(x), \partial_x \phi_i(x))$ be invariant under a continuous global transformation of the field whose infinitesimal version is given as

$$\phi_i(x) \rightarrow \phi_i(x) + \sum_j a_{i,j} \phi_j(x) \equiv \phi_i(x) + \Delta \phi_i(x), \quad (3.5.1)$$

where $a_{i,j}$ is an infinitesimal transformation parameter independent of $x$. Consider the generating functional $W[J]$ defined by functional integral as

$$e^{(i/h)W[J]} = \int [d\phi] \exp \frac{i}{\hbar} \int d^4 x L(\phi) , \quad (3.5.2)$$

$$L(\phi) = L(\phi) + \sum_i J_i(x) \phi_i(x) . \quad (3.5.3)$$

Then $W[J]$ is invariant under an infinitesimal transformation of $J$,

$$J_i(x) \rightarrow J_i(x) - \sum_j J_j(x) a_{j,i} . \quad (3.5.4)$$

The invariance is inherited by the effective action $\Gamma[\phi]$ which is defined as

$$\Gamma[\phi] = W[J] - \int d^4 x \sum_i \frac{\delta W[J]}{\delta J_i(x)} J_i(x) ,$$

$$\phi_i(x) = \frac{\delta W[J]}{\delta J_i(x)} . \quad (3.5.5)$$

$\Gamma[\phi]$ is invariant under (3.5.1),

$$\Gamma[\phi] = \Gamma[\phi + \Delta \phi] .$$

Up to linear term in $a_{i,i}$, this gives us an identity,

$$\int d^4 x \sum_i \frac{\delta \Gamma[\phi]}{\delta \phi_i(x)} a_{i,i} \phi_i(x) = 0 . \quad (3.5.6)$$
Now differentiate (3.5.6) with respect to $\phi_n(y)$ and set $\phi_i(x)$ to a symmetry breaking solution $\phi_i^{(0)}$ of stationary equation,

$$\frac{\delta \Gamma[\phi]}{\delta \phi_i(x)} = 0.$$

We assume that $\phi_i^{(0)}$ is space-time independent. Then we get

$$\int d^4y \sum_j \left( \frac{\delta \Gamma[\phi]}{\delta \phi_i(x) \delta \phi_j(y)} \right) a_{i,j} \phi_k^{(0)} = 0, \quad (3.5.7)$$

where $(\cdots)_0$ implies that $(\cdots)$ is evaluated at $\phi_i^{(0)}$ and we have changed the notations of summation or integration variables.

Equation (3.5.7) just takes the form of on-shell equation (2.1.4a). Since $\int d^4x$ picks out zero energy and zero momentum we conclude that there is a four momentum zero mode $|G\rangle$, i.e., Goldstone mode, when $\phi_i^{(0)} \neq 0$ and the value of its wave function at zero four momentum is given by

$$\langle 0| \hat{\phi}_i(x)|G\rangle + \langle G| \hat{\phi}_i(x)|0\rangle = \sum_j a_{i,j} \phi_j^{(0)}. \quad (3.5.8)$$

These well-known results are thus simply derived by on-shell equation. We can look at the Goldstone state from the channel other than $\hat{\phi}_i(x)$ by introducing into the original Lagrangian a source term which is different from (3.5.3). If we choose $J(x) \hat{O}(x)$ then the wave function $\langle 0| \hat{O}(x)|G\rangle + \langle G| \hat{O}(x)|0\rangle$ is determined. Application of these facts will be given in Chapters X and XIV where we discuss the Hubbard model and superfluidity by our method.

References

6) E. E. Salpeter and H. A. Bethe, Phys. Rev. 84 (1951), 1232.
Chapter IV. S-Matrix and Condensed Vacuum

The main purpose of this chapter is to apply higher-order relations of on-shell expansion scheme to the problem of particle scattering above non-perturbatively condensed vacuum. The salient feature of the scheme is the clear separation of the diagrams into three elements,

(I) the diagrams representing the interaction with the particles which condense in the vacuum,

(II) the diagrams making up the wave function of the bound states,

(III) the diagrams responsible for the scattering among the bound states determined in (II).

The elucidation of these different aspects of the effective action constitutes our formalism to study the particle scattering including the case where the ground state realizes the condensation. However, less attention seems so far to have been paid to this possibility but now, with on-shell expansion scheme of the effective action at hand as a total framework to the problem, we exemplify the above approach through the construction of two-body hadronic scattering diagrams by starting from the explicit form of the effective action for quantum chromodynamics (QCD)\(^{1,2}\). Effective action is expected to be an ideal tool for the problem since the ground state of QCD is expected to be a condensed one which is determined by the stationary condition and effective action is directly related to S-matrix element among hadrons whose spectrum is in turn determined by the scheme of on-shell expansion. It is shown below that the lowest order approximation reproduces the conventional constituent rearrangement diagrams (CRD) of quark-line physics.\(^{3}\) Here the precise mathematical expression of these diagrams is automatically obtained. For previous attempts at the related problems, see Refs. 2) and 4).

§ 4.1. QCD and quark-line physics

The Lagrangian density of QCD theory takes the form,

\[
L_{\text{QCD}} = \frac{1}{2} A^{\mu \nu} D_{\sigma \rho}^{-1 \mu \nu} A_{\rho \sigma} + \bar{q} i \gamma^\mu D_\mu q^\nu + \bar{\eta} i \gamma^\rho D_\rho \eta^\sigma
\]

\[
- \frac{1}{2} g f_{\alpha \beta \gamma} (\partial_\mu A_{\alpha \nu} - \partial_\nu A_{\alpha \mu}) A^{\mu \rho} A^{\nu \rho} - \frac{1}{4} g^2 f_{\alpha \beta \gamma} f_{\delta \epsilon \sigma} A_{\alpha \beta} A_{\gamma \delta} A_{\epsilon \sigma}
\]

\[
+ g \bar{q} i \gamma^\alpha A_{\mu} (\frac{\lambda_\alpha}{2})_{AB} q^B + g f_{\alpha \beta \gamma} \bar{\eta} A_\mu A_\nu \eta^\mu \eta^\nu ,
\]

where \(q, A\) and \(\eta\) indicate quark field, gluon field and ghost field, respectively. Furthermore \(\alpha, \beta \cdots\) represent the color of the gauge field and ghost field and \(g\) is the gauge coupling constant, \(\lambda^a (a=1, \cdots, 8)\) is the Gell-Mann matrix satisfying the Lie algebra \([\lambda_a/2, \lambda_b/2] = i f_{\alpha \beta \gamma} \lambda_\gamma/2\), and the index \(A\) or \(B\) represents the color of quarks.
The flavour indices are suppressed in (4.1.1).

Exact calculation of the non-perturbative quantities of QCD is, of course, out of question but it is not necessary if one wants to see how the physical variables defined by the Legendre transformation appear in scattering diagrams. As a practical use the vacuum solutions can be taken as given parameters to be determined by experiments. The effective form of the lowest-order on-shell variations, or the wave function of hadrons, can also be assumed in the actual calculations. Apart from these non-perturbative quantities, the scattering matrix element among hadrons is diagrammatically expanded in a systematic way by higher-order terms of on-shell expansion. In this respect, the present formalism will also be a useful basis for the approximate numerical evaluation of high-energy hadronic scatterings. Recall here that the perturbative scattering diagrams can be a good description for high-energy scattering but we have to keep the vacuum parameters and the wave functions of hadrons to be fixed since the energy scale characterizing these parameters does not become large.

We first construct the effective action \( \Gamma[\phi] \),

\[
\Gamma[\phi] = \Gamma[\langle q_\mu q_{\mu}, \bar{q}, \bar{q} j \bar{q} j, \bar{q} \bar{q} \bar{q} \bar{q}, \bar{q} i A_{\mu} A_{\rho}, \bar{q} \bar{q} i A_{\mu} q_j, \bar{q} i A_{\mu} q_j, \bar{q} i A_{\mu} j, \bar{q} i A_{\mu} j \rangle]. \tag{4.1.2}
\]

The subscripts are assumed to represent all the attributes of the field including space-time, Lorentz, color and flavour indices. Here the variables are introduced for two- and three-body channels of baryon, meson-glueball sectors and the symbol \( \sim \) to denote the operator is not written for simplicity. For convenience we have introduced the variables which cover all the possible color and flavour channels, not only the color singlet combination. The effective action (4.1.2) can be obtained again by using the De-Dominicis and Martin graphical approach,\(^5\) see Appendix C. We start from writing the bare QCD action with external sources \( J_\nu (\nu = 1, 2, 3) \) in the form,

\[
I_{\text{QCD}}[\Psi, J] = I_1(a) \Psi(a) + \frac{1}{2!} \left[ I_2(a, b) + \nu_2^b(a, b) \right] \Psi(a) \Psi(b) + \frac{1}{3!} \left[ I_3(a, b, c) + \nu_3^b(a, b, c) \right] \Psi(a) \Psi(b) \Psi(c) + \frac{1}{4!} \nu_4^b(a, b, c, d) \Psi(a) \Psi(b) \Psi(c) \Psi(d), \tag{4.1.3}
\]

where \( \Psi = [\bar{q}, q, \bar{q}, \eta, A] \) and \( \nu_\nu^b (\nu = 2, 3, 4) \) come from the original QCD action. The external sources in (4.1.3) are introduced for all the combinations of the fields up to three-body channels. (The sources are assumed to be anti-symmetric for the Grassmann components and symmetric for the others.) Then we find (see Ref. 5) and Appendix C),

\[
\Gamma[G_1, G_2, G_3] = W[J] - \sum_{\nu=1}^4 \frac{1}{\nu!} J_\nu(a, b, \cdots) G_\nu(a, b, \cdots)
\]
\[ \frac{1}{2!} \nu_2^0(a, b)G_2(a, b) + \frac{1}{3!} \nu_3^0(a, b, c)G_3(a, b, c) + \frac{i}{2} \text{STrln} \tilde{G}_2 \]

\[ + \frac{i}{2 \cdot 3!} \sum \epsilon^{\rho(a,b,c';a',b',c')} C_3(a, b, c) \tilde{G}_2(a, a') \tilde{G}_2(b, b') \tilde{G}_2(c, c') C_3(a', b', c') - i \kappa^{(3)}, \]

(4.1.4)

where \( \text{STr} \) is the supertrace and \( \sum \) implies the summation over \( a, b, c, a', b', c' \) and the symbol \( G_\nu \) is used including \( \langle a \rangle \equiv G_1(a) \) for fermionic field \( a \),

\[ G_\nu(a, b, \ldots) \equiv \nu! \frac{\delta \mathcal{W}[J]}{\delta J_\nu(a, b, \ldots)}. \quad (\nu = 1, 2, 3) \]  

(4.1.5)

In (4.1.4), \( \kappa^{(3)} \) denotes the sum of all possible 1, 2, 3PI vacuum diagrams including tree diagrams constructed out of \( G_1, \tilde{G}_2 \) (connected part of the propagator), \( C_3 \) (amputated connected three-point vertex), and the original gluon four-point vertex \( i \nu_4^0 \) \( (A, A, A, A) \) (see Fig. 4.1). The sign factor \( \epsilon^\rho \) is defined by

\[ \Psi(a') \Psi(b') \Psi(c') \Psi(a) \Psi(b) \Psi(c) = \epsilon^\rho(a', b', c'; a, b, c) \Psi(a') \Psi(a) \Psi(b') \Psi(b) \Psi(c') \Psi(c). \]

The problem simplifies if we assume the color singlet nature of the vacuum and excited states. This fact implies that among \( G_\nu(a, b, \ldots) \), the color non-singlet component can be set equal to zero. Indeed the vacuum expectation value \( G_\nu^{(0)}(a, b, \ldots) \) (which is a solution to \( \delta I/\delta G_\nu = 0 \)) is zero and the first variation \( \Delta G_\nu^{(1)}(a, b, \ldots) \) also does not exist since, for any hadronic states \( |B\rangle, \langle 0| \tilde{\Psi}(a) \tilde{\Psi}(b) \ldots |B\rangle = 0 \) if the operator \( \tilde{\Psi}(a) \tilde{\Psi}(b) \ldots \) is not color singlet. Thus we can set \( G_\nu(a, b, \ldots) = 0 \) for color non-singlet channel in the DeDominicis and Martin rule \( (G_1(A) = 0 \) as an example). These assumptions correspond to the situation where the external sources are not introduced from the start for the corresponding channels in (4.1.3). The remaining part of the effective action is explicitly written in terms of the quark, gluon, and ghost fields as in (4.1.2). It is, however, technically convenient to keep all the color channel in these variables without color singlet projection. Then \( \Gamma \) is given as

\[ \kappa^{(3)} = \]

\[ \text{Fig. 4.1. Graphical representation of } \kappa^{(3)} \text{part of QCD effective action (4.1.6). Solid line denotes } \tilde{S} \text{ and wavy line } \tilde{D}. \text{ They are the quark and the gluon full propagator in the presence of external sources, respectively. Each three point vertex is given by an appropriate component of } C_3(a, b, c). \]

A four-point vertex represents the original four-gluon vertex \( i \nu_4^0 (A, A, A, A) \).
\[ \Gamma[G_1, \tilde{G}_2, C_3] \]
\[ = \frac{1}{2} iD_0^{-1} \mu \tilde{D}^{\mu} - iS_0^{-1} \xi_\mu \tilde{S}_{\mu} - iD_0^{-1} \xi_\mu \tilde{A}_{\mu} \]
\[ + \frac{1}{3!} \left( v_3^0(A_\mu, A_\nu, A_\rho) + i\frac{1}{2} C_3(A_\mu, A_\nu, A_\rho) \right) \tilde{D}^{\mu \nu} \tilde{D}^{\nu \rho} C_3(A_{\mu'}, A_{\nu'}, A_{\rho'}) \]
\[ - \left( v_3^0(\tilde{q}_i, A_\mu, q_\nu) + i\frac{1}{2} C_3(\tilde{q}_i, A_\mu, q_\nu) \right) \tilde{S}_{\mu \nu} \tilde{S}_{\nu \rho} C_3(\tilde{q}_{\mu'}, \tilde{q}_{\nu'}, \tilde{q}_{\rho'}) \]
\[ - \left( v_3^0(\tilde{\eta}_i, A_\mu, \eta_\nu) + i\frac{1}{2} C_3(\tilde{\eta}_i, A_\mu, \eta_\nu) \right) \tilde{A}_{\mu \nu} \tilde{A}_{\nu \rho} C_3(\tilde{\eta}_{\mu'}, \tilde{\eta}_{\nu'}, \tilde{\eta}_{\rho'}) \]
\[ + i\text{Trln} \tilde{D} - \frac{i}{2} \text{Trln} \tilde{D} + i\text{Trln} \tilde{S} - i \quad \text{(corresponding part of } k^{(3)}) \] 
\[ \quad = 0. \]

where we have employed the simplified notations \( \tilde{D} \equiv \tilde{G}_{2}(A, A), \tilde{S} \equiv \tilde{G}_{2}(q, \bar{q}), \) \( \tilde{A} \equiv \tilde{G}_{3}(\eta, \bar{\eta}) \).

The vacuum expectation values are now determined by the stationary condition of the effective action
\[ \frac{\delta \Gamma}{\delta \langle q_i q_j q_k \rangle} = \frac{\delta \Gamma}{\delta \langle q_i \bar{q}_j \bar{q}_k \rangle} = \ldots \frac{\delta \Gamma}{\delta \langle \eta_i \bar{\eta}_j \rangle} = 0. \]
\[ \quad = 0. \]

The solutions for meson-like and glueball-like channel \( \langle A_\mu A_\nu \rangle^{(0)}, \langle q_i \bar{q}_j \rangle^{(0)}, \) etc., are expected to include the effects of chiral and gluon condensations in the color singlet channel. For baryon and anti-baryon-like channel, we get \( \langle q_i q_j q_k \rangle^{(0)} = \langle q_i \bar{q}_j \bar{q}_k \rangle^{(0)} = 0 \) for all the color flavour combinations.

Possible physical modes of baryon, meson and glueball are examined next in terms of the generalized on-shell condition which is given in matrix form,\(^6\)
\[ \begin{bmatrix} \text{Baryon} \\ \text{part} \end{bmatrix} \begin{bmatrix} \Delta \langle q qq \rangle^{(1)} \\ \Delta \langle q \bar{q} \bar{q} \rangle^{(1)} \end{bmatrix} = 0. \]
\[ \begin{bmatrix} \Delta \langle A A A \rangle^{(1)} \\ \Delta \langle q A q \rangle^{(1)} \\ \Delta \langle \bar{q} A \bar{q} \rangle^{(1)} \\ \Delta \langle \tilde{\eta} A \eta \rangle^{(1)} \\ \Delta \langle A A \rangle^{(1)} \\ \Delta \langle q \bar{q} \rangle^{(1)} \\ \Delta \langle \tilde{\eta} \tilde{\eta} \rangle^{(1)} \end{bmatrix} \]
\[ = 0. \]

The subscript 0 means the substitution of the selected (condensed) vacuum solutions. Due to the assumed color confinement, the non-trivial solution to (4.1.8) is expected only for the color singlet combinations \( \Delta \langle q A B C \rangle^{(1)} \propto e_{ABC}, \Delta \langle q A \bar{q} B \rangle^{(1)} \propto \delta_{AB}, \Delta \langle A A A \rangle^{(1)} \propto \delta_{AB}, \Delta \langle q A q \rangle^{(1)} \propto e_{AB}, \) etc., where \( A, B, \ldots \) or \( \alpha, \beta, \ldots \) imply the color index of each field.

The baryonic part of (4.1.8) is given by the three-body bound state equations,\(^6\)
\[ \int d^4x' d^4y' d^4z' \left( \frac{1}{3!} \tilde{S}^{(9-1)}_{ij}(x, x') \tilde{S}^{(9-1)}_{kl}(y, y') \tilde{S}^{(9-1)}_{m'n'}(z, z') \right) \\
- \left[ \frac{-i}{\delta^2 \tilde{\kappa}^{(3)}} \delta \langle q_i(x) \bar{q}_j(y) \bar{q}_k(z) \rangle \delta \langle q_{k'}(x') \bar{q}_{l'}(y') \bar{q}_{m'}(z') \rangle \right] \Delta \langle q_{l'} q_{k'} q_{m'}(z') \rangle \right] = 0, \tag{4.1.9} \]

\[ \int d^4x' d^4y' d^4z' \left( \frac{1}{3!} \tilde{S}^{(9-1)}_{ij}(x, x') \tilde{S}^{(9-1)}_{kl}(y, y') \tilde{S}^{(9-1)}_{m'n'}(z, z') \right) \\
+ \left[ \frac{-i}{\delta^2 \tilde{\kappa}^{(3)}} \delta \langle q_i(x) q_j(y) q_k(z) \rangle \delta \langle \bar{q}_{k'}(x') \bar{q}_{l'}(y') \bar{q}_{m'}(z') \rangle \right] \Delta \langle \bar{q}_{l'} \bar{q}_{k'} \bar{q}_{m'}(z') \rangle = 0. \tag{4.1.10} \]

The interaction kernel consists of six-point diagrams which are 3PI with respect to quark line. This is due to the topological property of \( \kappa^{(3)} \). The result of course coincides with the one obtained by the intuitive graphical expansion approach.

Note here that the color singlet solution of \( \Delta \langle q_{l'} q_{k'} q_{m'} \rangle \) in (4.1.9) is obtained by taking the color singlet projection from the left: we simply multiply \( \epsilon_{ABC} \) from the left then the coefficient kernel of \( \Delta \langle q_{l'} q_{k'} q_{m'} \rangle \) given in the parenthesis \( \cdots \) becomes proportional to \( \epsilon_{k'l'k''} \). The process automatically brings us on-shell equation for color singlet channel.

The meson-glueball channel of (4.1.8) presents a set of coupled equations. For massless quarks, only the flavour singlet channel of meson and glueball will mix with each other. The mixing in the pseudo-scalar channel is related to the \( U(1) \) problem.\(^7\)\(^8\) To see the formal relation between the channel mixing and on-shell variation, let us examine the simplified model given by the following 2\( \times \)2 on-shell condition,

\[ \begin{bmatrix} \Gamma_{11}^{(2)} & \Gamma_{12}^{(2)} \\ \Gamma_{21}^{(2)} & \Gamma_{22}^{(2)} \end{bmatrix} \begin{bmatrix} \Delta \langle \phi_1 \rangle \rangle^{(1)} \\ \Delta \langle \phi_2 \rangle \rangle^{(1)} \end{bmatrix} = 0, \tag{4.1.11} \]

where the subscripts 1 and 2 denote the species of the ordinary number field and the second derivative \( \Gamma^{(2)} \) of \( \Gamma \) is assumed to have been evaluated at the vacuum solutions. The above example is sufficient to handle the actual mixing problems. From (4.1.11), we get

\[ \Delta \langle \phi_1 \rangle \rangle^{(1)} = - \Gamma_{11}^{(2)-1} \Gamma_{12}^{(2)} \Delta \langle \phi_2 \rangle \rangle^{(1)}, \tag{4.1.12a} \]

\[ \Delta \langle \phi_2 \rangle \rangle^{(1)} = - \Gamma_{22}^{(2)-1} \Gamma_{21}^{(2)} \Delta \langle \phi_1 \rangle \rangle^{(1)}. \tag{4.1.12b} \]

On the other hand, the matrix \( \Gamma^{(2)} \) satisfies the identity,

\[ \begin{bmatrix} \Gamma_{11}^{(2)} & \Gamma_{12}^{(2)} \\ \Gamma_{21}^{(2)} & \Gamma_{22}^{(2)} \end{bmatrix} \begin{bmatrix} W_{11}^{(2)} & W_{12}^{(2)} \\ W_{21}^{(2)} & W_{22}^{(2)} \end{bmatrix} = -1. \tag{4.1.13} \]

By eliminating \( \Delta \langle \phi_1 \rangle \rangle^{(1)} \) or \( \Delta \langle \phi_2 \rangle \rangle^{(1)} \) with (4.1.12) and (4.1.13), one finds that

\[ (\Gamma_{12}^{(2)} \Gamma_{21}^{(2)} - \Gamma_{11}^{(2)} \Gamma_{22}^{(2)}) \Delta \langle \phi_1 \rangle \rangle^{(1)} = (W_{12}^{(2)})^{-1} \Delta \langle \phi_1 \rangle \rangle^{(1)} = 0, \tag{4.1.14a} \]
\[(\Gamma_{21}^{(2)} - \Gamma_{12}^{(2)} - \Gamma_{22}^{(2)}) \Delta \langle \psi_2 \rangle^{(1)} = (W_{22}^{(2)})^{-1} \Delta \langle \psi_2 \rangle^{(1)} = 0. \]  
\hspace{10cm} (4\cdot1\cdot14b)

Thus the non-trivial eigenstates \( \Delta \langle \psi_1 \rangle^{(1)} \) and \( \Delta \langle \psi_2 \rangle^{(1)} \) of (4\cdot1\cdot14) are really shown to be determined by the pole structure of the corresponding Green’s functions. The solutions may be written in Fourier space as

\begin{align*}
\Delta \langle \phi_1(p) \rangle^{(1)} &= f_a(p) \delta(p^2 - m_a^2) + f_b(p) \delta(p^2 - m_b^2) + \cdots, \hspace{10cm} (4\cdot1\cdot15a) \\
\Delta \langle \phi_2(p) \rangle^{(1)} &= g_a(p) \delta(p^2 - m_a^2) + g_b(p) \delta(p^2 - m_b^2) + \cdots \hspace{10cm} (4\cdot1\cdot15b)
\end{align*}

with some functions \( f_{a,b}(p) \) and \( g_{a,b}(p) \). Let us assume that

\[ |f_a(m_a)| > |f_b(m_b)| \quad \text{and} \quad |g_a(m_a)| < |g_b(m_b)|. \hspace{10cm} (4\cdot1\cdot16)\]

In this case, the modes \( a \) and \( b \) in (4\cdot1\cdot15) will be identified practically with the particle corresponding to the field 1 and 2, respectively. We call \( \Delta \langle \phi_1(p) \rangle^{(1)} \) the proper wave function of mode \( a \). The \( S \)-matrix element among the \( a \)-modes is now given as follows. Perform on-shell expansion for \( \Delta \langle \psi_{1,2} \rangle^{(1)} \) and eliminate \( \Delta \langle \psi_2 \rangle^{(1)} \) by using (4\cdot1\cdot12b). In this way the proper wave function graphically appears in each external leg. Then take the derivative of (2\cdot3\cdot19) (with \( \Gamma[\phi] \) of this model) in terms of \( \tilde{C}_a \) defined from \( f_a(p) \) in this case. Alternatively, \( \Delta \langle \psi_1 \rangle^{(1)} \) can be eliminated instead of \( \Delta \langle \psi_2 \rangle^{(1)} \) or both can be used without eliminating either of them. The correct \( S \)-matrix element appears in all cases of course if we take the on-shell projection corresponding to the \( a \)-mode. The situation is straightforwardly generalized to the present case.

**Meson-meson scattering**

Let us consider the meson-meson two-body scattering. Expanding the left-hand side of (2\cdot3\cdot19) or (2\cdot5\cdot36) with the effective action (4\cdot1\cdot6) around the vacuum solutions for each component, we find that the corresponding \( S \)-matrix element appears in

\[\left[ \frac{1}{4!} \Gamma \frac{\delta}{\delta \phi_x} \Delta \phi_x^{(1)} \frac{\delta}{\delta \phi_y} \Delta \phi_y^{(1)} \frac{\delta}{\delta \phi_z} \Delta \phi_z^{(1)} \frac{\delta}{\delta \phi_w} \Delta \phi_w^{(1)} + \frac{3}{3!} \Gamma \frac{\delta}{\delta \phi_x} \Delta \phi_x^{(1)} \frac{\delta}{\delta \phi_y} \Delta \phi_y^{(1)} \frac{\delta}{\delta \phi_z} \Delta \phi_z^{(1)} + \frac{1}{2!} \Gamma \frac{\delta}{\delta \phi_x} \Delta \phi_x^{(2)} \frac{\delta}{\delta \phi_y} \Delta \phi_y^{(2)} \right]_0, \hspace{10cm} (4\cdot1\cdot17)\]

where we have used the abbreviated notations as \( \Delta \phi_x^{(1)} \) for \( \Delta \langle \psi_x \rangle^{(1)} \) and the subscripts \( X, Y, \cdots \) imply the components which couple to meson and glueball channels. (The left and right derivatives are the same in this case). We then pick up the terms which are proportional to the fourth order of proper wave function of mesons, \( \Delta S^{(1)} \). The colour indices of \( \Delta S^{(1)} \) are supposed to be chosen in their singlet channel. Other degrees of freedom, such as flavour combinations and total spin of the wave function, are to be determined when we project out the proper mode of the observed mesons. The second order variation \( \Delta \phi_x^{(2)} \) of (4\cdot1\cdot17) is explicitly given by its definition,

\[ \Delta \phi_x^{(2)} = \frac{1}{2!} \left( \frac{\delta}{\delta f_x} \frac{\delta}{\delta W} \right)_0 \left( \Gamma \frac{\delta}{\delta \phi_Y} \frac{\delta}{\delta \phi_x} \Delta \phi_x^{(1)} \frac{\delta}{\delta \phi_Y} \Delta \phi_Y^{(1)} \right)_0, \hspace{10cm} (4\cdot1\cdot17)\]
where we have conveniently used the notation \( \langle \delta / \delta J \cdot \delta W / \delta J \rangle \) instead of writing it as the inverse of \( (-\Gamma \partial \delta / \partial \psi \cdot \partial \delta / \partial \psi) \). (Recall that the source \( J_o \) here symbolically represents \( J_o, J_{13} \) and \( J_{13} / 3! \) in (4.1.3).)

The variation \( \Delta \psi_{a}^{(1)} \) for meson and glueball channel mix with each other in their mode-determining equation (4.1.8). So we write

\[
\frac{\delta}{\delta \psi^a} \Delta \psi_{x}^{(1)} = \frac{\delta}{\delta \psi^a} \tilde{\gamma}_{x,\bar{s}} \tilde{\gamma}_{x,\bar{s}} \Delta S^{(1)},
\]

(4.1.19)

where \( \tilde{\gamma}_{x,\bar{s}} \) represents a unit tensor. This is a natural generalization of (4.1.12). It is convenient to suppose that the mixing matrix \( \tilde{\gamma}_{x,\bar{s}} \) itself is also a given quantity. Such mixing problem, however, does not appear in the lowest order diagrams or the quark line graphs which dominate the high energy scattering of QCD. Combining (4.1.17) with (4.1.18) and (4.1.19), the general full order expression of the S-matrix element of the meson-meson scattering is obtained as follows,

\[
\left[ \frac{1}{4!} \Gamma_{x,\bar{s},\bar{s},s} \Delta S^{(1)} - \frac{\delta}{\delta \psi^a} \tilde{\gamma}_{x,\bar{s}} \tilde{\gamma}_{x,\bar{s}} \Delta S^{(1)} \right] \times \left( \frac{\delta}{\delta \psi^a} \tilde{\gamma}_{x,\bar{s}} \tilde{\gamma}_{x,\bar{s}} \Delta S^{(1)} \right) \times \left( \frac{\delta}{\delta \psi^a} \tilde{\gamma}_{x,\bar{s}} \tilde{\gamma}_{x,\bar{s}} \Delta S^{(1)} \right)
\]

(4.1.20)

Here \( \frac{\delta}{\delta \psi^a} \), etc., operate only on the effective action \( \Gamma \). Graphically \( \Gamma_{x,\bar{s},\bar{s},s}^{(1)} \) or \( \Gamma_{x,\bar{s},\bar{s},s}^{(2)} \) part of (4.1.20) does not have a set of internal propagators which connect their adjacent external lines. Such corrections have already been included in the second step of on-shell expansion scheme since they are the interactions making up the bound state. Some of these interactions are restored in the scattering diagram through \( \gamma_{x,\bar{s}} \) to have the proper mesonic wave functions in the external legs. The mixing in meson-glueball channel automatically appears in the result. Recall that they are all represented by the non-trivial variables defined by Legendre transformation.

Let us calculate the lowest order term of (4.1.20), which produces the quark line diagram. It is given by keeping only the term \( i Tr ln S \) in (4.1.6). The result (4.1.20) then becomes non-zero only for \( X = Y = \cdots = Y' = \bar{S} \). Since

\[
(i Tr ln S) \frac{\delta}{\delta S_{ij}} \frac{\delta}{\delta S_{kl}} = -i \bar{S}_{ij} \bar{S}_{kl},
\]

(4.1.21)

the symbolical notation \( \frac{\delta}{\delta S_{ij}} (\delta W / \delta S_{ij}) \) can be replaced by \( -i \bar{S}_{ij} \bar{S}_{kl} \) owing to the
identity (2.5.11), which reads in this case,

$$
\left( \frac{\delta}{\delta \tilde{S}_{ij}} \frac{\delta}{\delta \tilde{S}_{mn}} \right) = \left( \frac{\delta}{\delta \tilde{J}_{ik}} \frac{\delta}{\delta \tilde{J}_{lm}} \right) \left( \frac{\delta}{\delta \tilde{S}_{kl}} \frac{\delta}{\delta \tilde{S}_{mn}} \right) = \left( \frac{\delta}{\delta \tilde{J}_{ik}} \frac{\delta}{\delta \tilde{J}_{lm}} \right) \left( \frac{\delta}{\delta \tilde{S}_{kl}} \frac{\delta}{\delta \tilde{S}_{mn}} \right) = - \delta_{ik} \delta_{jl},
$$

(4.1.22)

The result now simply becomes

$$
i \frac{\delta}{4!} \left( \tilde{S}_{jk}^{(0)-1} \tilde{S}_{im}^{(0)-1} \tilde{S}_{n0}^{(0)-1} \tilde{S}_{pl}^{(0)-1} \Delta \langle q_k \bar{q}_l \rangle^{(1)} \Delta \langle q_m \bar{q}_n \rangle^{(1)} \Delta \langle q_o \bar{q}_p \rangle^{(1)} \Delta \langle q_i \bar{q}_j \rangle^{(1)} \right),
$$

(4.1.23)

where $\Delta \langle q_i \bar{q}_j \rangle^{(1)} = \Delta \tilde{S}_{ij}^{(1)}$ and $\tilde{S}^{(0)}$ is the stationary solution of $\tilde{S}$. In the present approach, each line naturally represents the full propagator $\tilde{S}^{(0)}$. This includes the effect of the chiral and gluon condensation. If we try to calculate $\tilde{S}^{(0)}$ itself directly from the effective action after some approximations, not only $i \text{Tr} \ln \tilde{S}$, but also the remaining terms of (4.1.6) should properly be taken into account of course, since the higher-order diagrams cannot be neglected any more for the correct estimation of the non-perturbative ground state or the low energy behavior of QCD.

The scattering matrix element is extracted as follows. Consider, for instance, the mesons $A$, $B$ and $C$, $D$ in the initial and final states, respectively. $S$-matrix element is given by operating $\delta/\delta \tilde{C}\tilde{A}^{+} \circ \delta/\delta \tilde{C}\tilde{B}^{+} \circ \delta/\delta \tilde{C}\tilde{C}^{-} \circ \delta/\delta \tilde{C}\tilde{D}^{-}$ to (4.1.23) as was discussed in (2.4.13) in composite field case. The coefficient $\tilde{C}_{i}^{+}$ is defined as in (2.4.13) with the mesonic bound state mode $i$. Then we get from (4.1.23),

$$
i \tilde{S}_{jk}^{(0)-1} \tilde{S}_{im}^{(0)-1} \tilde{S}_{n0}^{(0)-1} \tilde{S}_{pl}^{(0)-1} (A_{kl}C_{mn}D_{op}B_{ij} + A_{kl}C_{mn}B_{op}D_{ij} + A_{kl}B_{mn}C_{op}D_{ij} + A_{kl}B_{mn}D_{op}C_{ij} + A_{kl}D_{mn}B_{op}C_{ij} + A_{kl}D_{mn}C_{op}B_{ij})
$$

(4.1.24)

where $A$, $B$, $C$ or $D$ symbolically represents the wave function of each mesonic mode which is projected out from the whole index space of $\Delta \langle q_i \bar{q}_j \rangle^{(1)}$. The first three terms in the round bracket correspond to $X$, $H$- and $Z$-types of CRD or quark rearrangement diagram (QRD), respectively. Others are given by the same type of diagrams but with the propagator in opposite direction.

Likewise the higher-order corrections can be obtained from (4.1.20) by taking further into account the remaining terms of the effective action (4.1.6). This can be done in a systematic way, see Ref. 1 for more details. Recall that they are represented by the variables defined through Legendre transformations — the full propagators and the dressed three-point vertices in this case. Such changes of the variables are necessary to see the non-perturbative aspects of the corresponding channels. It may be difficult to include the non-perturbative quantities into the scattering diagrams by using only the intuitive graphical approach. The present approach, on the other hand, is suitable to clarify the problem since the non-trivial changes of the variables are completed at the first stage of the formalism, i.e., by the Legendre transformations. The on-shell expansion is convenient especially when we study different many channels in general. Of course, it can also be checked that the result recovers a series of perturbative diagrams if we perturbatively use the stationary condition (4.1.7) of the effective action.
For baryon-meson and baryon-(anti) baryon scattering, similar discussions have been given Ref. 1).

§ 4.2. Two-dimensional QCD

Here we examine the application for two-dimensional QCD (QCD$_2$) with color gauge group $U(N)$ ($N \to \infty$). Since it is a solvable model, to see how our systematic scheme of on-shell expansion works for QCD$_2$ is an interesting subject. For simplicity, here we concentrate only on the meson channel and show that the well-known results are really obtained from on-shell expansion of the effective action.

We start from the Lagrangian density of quarks $q_i$ and gluons $A_\mu$ (in $N \times N$ representation),

$$L_{\text{QCD}_2} = \frac{1}{2} A_{+\mu} D_0^{-1}_{\mu,\nu} A_{+\nu} + \bar{q} i S_0^{-1} \gamma_\mu q + g \bar{q} i \gamma_\mu A_{+\mu} q,$$

$$i D_0^{-1}_{\mu,\nu} \equiv \partial_-^2 \delta_{\mu\nu} \partial_+,$$  

$$i S_0 \equiv (i \partial - m) \delta_+,$$

where $i, j = 1, 2, \ldots, N$ represent the indices of color space. In (4.2.1), we have used the light cone coordinates,

$$x^\pm = x^+ = \frac{1}{\sqrt{2}} (x^0 \pm x^1), \quad (x^0 = x_0, \quad x^1 = - x_1)$$

(similarly for $\gamma_-$) and the light-cone gauge condition,

$$A_- = \frac{1}{\sqrt{2}} (A^0 + A^1) = A^+ = 0,$$

following the original work by 't Hooft. The summation convention is as follows,

$$x^\mu y^\nu = x^+ y^- + x^- y^+ = x^+ y^+ + x^- y^- = x^0 y^1 + x^1 y^0.$$

Let us examine the two-body channels which couple to the meson part; $q_i \bar{q}_j$ and $A_{+\mu} A_{+\nu}$. In this case, assuming that $g^2$ is of the order $1/N$, the corresponding effective action up to the order $N$ takes the following form (see also Appendix C)

$$\Gamma[\bar{S}, \bar{D}] \equiv \frac{1}{2} i D_0^{-1}_{\mu,\nu} \bar{D}_{\mu,\nu} - \frac{1}{2} i \text{Tr} \ln \bar{D}$$

$$- i S_0^{-1} \bar{S}_{ji} + i \text{Tr} \ln \bar{S} + i (ig)^2 \frac{1}{2} \bar{S}_{ji} \gamma_\nu \bar{S}_{ji} \gamma_\nu \bar{D}_{ji,\nu},$$

where the notations $\bar{D}_{\mu,\nu} \equiv \langle A_{+\mu} A_{+\nu} \rangle$ and $\bar{S}_{ji} \equiv \langle q_i \bar{q}_j \rangle$ have been employed. The last term of (4.2.7) represents order $N$ contribution of the two-particle irreducible vacuum diagram. If we explicitly write the color dependence of each variable as $\bar{D}_{\mu,\nu} \equiv D \delta_{\mu\nu} \delta_{ji}$ and $\bar{S}_{ji} \equiv S \delta_{ji}$, the effective action (4.2.7) is written as follows,

$$\Gamma[\bar{S}, \bar{D}] \equiv N^2 \Gamma[\bar{S}, \bar{D}]$$
\[ N^2 \left[ \frac{1}{2} i D^{-1}_\alpha D^{-1} \frac{1}{2} i \text{tr} \ln D + \frac{1}{N^2} i \lambda \sigma^{-1}_{ab} S^{-1}_{ab} + \frac{1}{N} i \text{tr} \ln S - \frac{1}{N^2} \frac{i}{2} \sigma_{a\beta} \gamma_{-\rho\sigma} S_{\rho\sigma} \gamma_{-\beta a} D \right], \quad (4.2.8) \]

where \( \lambda \equiv N g^2 \) and tr denotes the functional trace not including the color degrees of freedom. To clarify the order of the contraction, symbolic indices \( \alpha, \beta, \cdots \) are conveniently used in (4.2.8).

By using \( \Gamma[S, D] \), the on-shell expansion is now straightforward. First, the vacuum solutions are determined by the stationary conditions,

\[ \frac{\delta \Gamma[S, D]}{\delta S_{\rho a}} = -\frac{1}{N} i \sigma^{-1}_{0 a} S^{-1}_{0 a} + \frac{1}{N} i \sigma^{-1}_{a\beta} S^{-1}_{a\beta} - \frac{1}{N^2} i \lambda \sigma_{-\rho a} S_{\rho a} \gamma_{-\beta a} D = 0, \quad (4.2.9) \]

\[ \frac{\delta \Gamma[S, D]}{\delta D} = \frac{i}{2} D_0^{-1} - \frac{i}{2} D^{-1} \left( \frac{1}{N} \frac{i}{2} \lambda \sigma_{-\rho a} S_{\rho a} \gamma_{-} \right) = 0, \quad (4.2.10) \]

which are easily solved in leading order of \( 1/N \),

\[ S^{-1} = S_0^{-1} + \lambda \gamma_{-} S_{-} D_0 + O \left( \frac{1}{N} \right), \quad (4.2.11) \]

\[ D^{-1} = D_0^{-1} + O \left( \frac{1}{N} \right). \quad (4.2.12) \]

The vacuum polarization part of (4.2.12) is suppressed for \( N \to \infty \) since the internal quark loop is involved. Equation (4.2.11) is the 't Hooft equation for quark propagator.

Next, the mode determining equation is obtained in the form,

\[ \begin{bmatrix} \frac{\delta \Gamma}{\delta S} & \frac{\delta \Gamma}{\delta S} \\ \frac{\delta \Gamma}{\delta D} & \frac{\delta \Gamma}{\delta D} \end{bmatrix} \begin{bmatrix} A S^{(1)} \\ A D^{(1)} \end{bmatrix} = 0. \quad (4.2.13) \]

This is given explicitly as

\[ \left( \frac{1}{N} i \sigma_{-}^{-1} S^{-1} + \frac{1}{N} i \lambda \gamma_{-} S_{-} D_0 \right) A S^{(1)} + \left( \frac{1}{N} i \lambda \gamma_{-} S_{-} \right) A D^{(1)} = 0, \quad (4.2.14) \]

\[ \left( \frac{1}{N} i \lambda \gamma_{-} S_{-} \right) A S^{(1)} - \left( \frac{i}{2} D^{-1} D^{-1} \right) A D^{(1)} = 0, \quad (4.2.15) \]

where the subscript 0 denotes the substitution of (4.2.11) and (4.2.12) for \( S \) and \( D \). From (4.2.15), we get

\[ A D^{(1)} = \frac{1}{N} \left( \frac{i}{2} D^{-1} D^{-1} \right) A S^{(1)}. \quad (4.2.16) \]

After eliminating \( A D^{(1)} \) with (4.2.16), one finds that the mode of meson is determined by on-shell condition,
\[ \frac{1}{N} \left[ iS^{(0)-1}S^{(0)-1} + i\gamma - \gamma - D_0 + O(1/N) \right] \Delta S^{(1)} = 0, \]  

(4.2.17)

where \( S^{(0)} \) is the solution of (4.2.11). Equation (4.2.17) is the Bethe-Salpeter equation for mesons obtained by 't Hooft. The scattering among the modes is now determined by the higher-order terms of on-shell expansion. For instance, let us consider the meson-meson scattering amplitude, the general form of which is the same as (4.1.20) with \( S \) in place of \( \tilde{S} \). By (4.2.16), it is easily confirmed that the leading contribution is obtained when we set \( X = Y = \cdots = Y'' = S \) in (4.1.20). The result is given symbolically as follows,

\[
\frac{1}{N} \left[ -\frac{1}{4!} (S^{(0)-1})^4 (\Delta S^{(1)})^4 
+ \frac{12}{4!} i(S^{(0)-1})^2 (\Delta S^{(1)})^2 \left( (iS^{(0)-1}S^{(0)-1} + i\gamma - \gamma - D_0)^{-1} + O\left( \frac{1}{N} \right) \right) i(S^{(0)-1})^2 (\Delta S^{(1)})^2 \right].
\]  

(4.2.18)

Here the quark propagator is the dressed one and the second term includes the bare gluon exchange between non-adjacent quark lines in ladder fashion. The gluon exchanges between adjacent quark lines, which contribute to make up the bound state, have already been included in the second step of our formalism and naturally they are not present here. The result just corresponds to the situation studied in detail by Callan-Coote-Gross. After operating \( (\delta/\delta C^+)^4 (\delta/\delta C^-)^2 \) as in the case of the four dimensional QCD, we get from (4.2.18) the final expression of the connected S-matrix element which we are looking for. \( H^- \), \( X^- \), \( Z \)-types of quark line diagrams are obtained with proper combinations of the external legs.

In this way, the well-known formulas are simply obtained from the effective action step by step. It is also straightforward to include the higher-order terms of \( 1/N \)-expansion, which may require a complicated procedure in the conventional graphical approach. On the basis of the above formalism, direct study of other composite channel is also possible. Especially, combined with the result of § 4.1, the formalism is expected to provide a methodical way of studying \( SU(N) \)-baryon and antibaryon sectors.

The approach of the on-shell expansion presents a systematic way of examining the physical information of a given system and its application is quite wide in the sense that once the Hamiltonian or the Lagrangian is given we can start our program. Aside from QCD there are many examples to which our formalism can be applied straightforwardly. In the usual energy scale, particles are observed in stable localized configurations in the form of the bound states such as atoms and molecules and the interesting phenomena are caused by the interactions or the scattering among them. On-shell expansion scheme is expected to be a useful basis for the analysis of such complicated systems. We can discriminate unambiguously in a diagrammatical language which interaction is responsible for making up the bound state or causing the scattering among bound states. Although some approximation schemes are further required for the actual calculations, our formalism can be used as a frame-
work for the investigation of the atomic scatterings and the chemical reactions. As a preliminary attempt along this line, we will present the study of atomic scattering in § 8.4.

§ 4.3. On-shell variation and different vacua

In this section, the on-shell variation is examined from a different standpoint. Especially we have in mind the on-shell connection of the different vacua in terms of the on-shell variation. All the arguments up to now are essentially based on one selected vacuum solution, while our aim here is to show that the present formalism can also be utilized to clarify the relation between two (or more) possible vacuum solutions.\(^{13}\)

Suppose that the effective action has multiple stationary solutions. Separately for each solution, on-shell variation is defined and determines the physical information above each ground state. We will see, however, that the variation itself can also be chosen to lead to another stationary solution by utilizing the physical quantities only. This will not be the case if we utilize the off-shell interpolation of the vacua, where the condition of \(J=0\) is not satisfied. The problem is thus to see how to connect two different solutions while staying on the physical trajectory \(J=0\). For the case of gauge theories, our approach will provide a gauge invariant way of connecting different two solutions or a gauge invariant variational formalism. More generally, the following studies can be a formal basis for improving variational approach to find out the correct condensed vacuum state, which is expressed by an infinite coherent sum of excited states above the normal vacuum. Below we illustrate our basic ideas through some simple examples.

Our purpose is to suggest (4.3.18) and (4.3.19) below which represent a vacuum state in terms of the excited states defined above different vacuum.

4.3.1. Classical mechanics

First we consider a model of classical particle mechanics. Recall that, in this case, the on-shell variation changes the initial (or final) value of the coordinate: see § 1.1. The use of classical potential is suitable to exemplify the connection of two solutions.

We start from a classical action \(I[q]\) defined in the time interval \(t_i \leq t \leq t_f\),

\[
I[q] = \int_{t_i}^{t_f} dt \left[ \frac{m}{2} \dot{q}(t)^2 + \mu^2 q(t)^2 - \frac{\lambda}{4!} q(t)^4 \right],
\]  

(4.3.1)

where \(q(t)\) signifies the particle coordinate and \(\dot{q}(t)\equiv dq(t)/dt\). Both \(\mu^2\) and \(\lambda\) are assumed to be positive. As one of the solutions of Euler-Lagrange equation of motion, \(\delta I[q]/\delta q(t)=0\) (\(\delta q(t_i)=\delta q(t_f)=0\)), we choose \(q^{(0)}(t)=0\) corresponding to the initial condition \(q^{(0)}(t_i)=\dot{q}^{(0)}(t_i)=0\). This is the unstable vacuum solution. On-shell condition of this case is given by

\[
\int_{t_i}^{t_f} dt \left[ \frac{\delta^2 I[q]}{\delta q(t) \delta q(t')} \right]_{q(t)=q^{(0)}} \Delta q^{(1)}(t') = 0.
\]  

(4.3.2)
It has a blowing up solution,
\[ \Delta q^{(1)}(t) = \bar{C}^+ e^{-i\omega t} + \bar{C}^- e^{i\omega t}, \]
(4.3.3)
where \( \omega^2 = -2\mu^2/m \) and \( \bar{C}^\pm \) indicate arbitrary coefficients. The higher-order terms \( \Delta q^{(n)}(t) \) \( (n \geq 2) \) are similarly introduced just as \( \Delta \phi^{(n)}(x) \) of (2.1.4) and we find that all the terms of on-shell variation can be summed up to obtain
\[ \Delta q(t) = \Delta q^{(1)}(t) + \Delta q^{(2)}(t) + \Delta q^{(3)}(t) + \cdots \]
(4.3.4)
\[ = \Delta q^{(1)}(t) + \frac{\lambda}{3!} \int_{t_1}^{t_2} dt' I^{(2)}(t', t') (\Delta q(t'))^3. \]
(4.3.5)
\( I^{(2)} \) symbolically represents the second derivative of \( I[q] \). Here we have used the fact that the series of (4.3.4) graphically exhausts all kinds of tree diagrams. See the discussion following (2.1.23).

Now we look for the time-independent solution \( \Delta q(t) = \Delta q \) of (4.3.5) besides the trivial one \( \Delta q = 0 \). The solution is expected to represent the stable vacuum solution where the particle is at the bottom of the potential. In order to get this solution, we have to change the initial conditions which are represented by the coefficients \( \bar{C}^\pm \) in \( \Delta q^{(1)}(t) \). We remark that the time-dependence of \( \Delta q^{(1)}(t) \) is essential for the following argument.

For simplicity, we further assume \( t_1 = 0 \) and employ the form of the retarded Green's function \( \Delta_R \) for \( I^{(2)}(t', t') \) in (4.3.5),
\[ \Delta_R(t - t') = -\frac{1}{m\omega} \theta(t - t') \sin \omega(t - t'). \]
By this choice of \( I^{(2)} \), we have fixed the boundary conditions as \( \Delta q(0) = \Delta q^{(1)}(0) \) and \( \Delta \dot{q}(0) = \Delta q^{(1)}(0) \). Then we find, from (4.3.3) and (4.3.5), that the constant \( \Delta q \), if it is a solution, has to satisfy the relation,
\[ \Delta q = \bar{C}^+ e^{-i\omega t} + \bar{C}^- e^{i\omega t} + \frac{\lambda}{2 \cdot 3! \mu^2} (\Delta q)^3 (1 - \cos \omega t). \]
(4.3.6)
As we expect, Eq. (4.3.6) has indeed the non-zero solutions \( \Delta q = \pm (12 \mu^2/\lambda)^{1/2} \) with \( \bar{C}^+ = \bar{C}^- = \Delta q/2 \) in addition to the trivial one \( \Delta q = 0 \) for \( \bar{C}^+ = \bar{C}^- = 0 \). The meaning of these solutions is obvious, since they correspond to the initial condition \( \Delta q(t = 0) = \Delta q \) with \( \Delta \dot{q}(t = 0) = 0 \). The variation \( \Delta q \) now changes the initial position of the particle from the local maximum of the potential to its bottoms. The role of on-shell variation \( \Delta q \) is apparently different from the usual off-shell variation \( \delta q \) whose role is to derive Euler-Lagrange equation of motion itself. Note that \( \delta q \) is usually taken without shifting the initial value.

Of course, the same argument can be made by starting from one of the bottoms of the double-well potential. This is simply done by changing the variable as \( q(t) = q'(t) + q^{(0)} \) \( (q^{(0)} = \pm (12\mu^2/\lambda)^{1/2} \) in this case). Namely we use the action,
\[ I[q'] = \int_{t_1}^{t_2} dt \left( \frac{m}{2} \dot{q}'(t)^2 + \mu^2 (q'(t) + q^{(0)})^2 - \frac{\lambda}{4!} (q'(t) + q^{(0)})^4 \right). \]
(4.3.7)
The condition (4.3.5) is then replaced by
\[ \Delta q'(t) = \Delta q^{(1)}(t) + \int_{t'}^{t} dt' I_{t,t'}^{(2)} \left( \frac{\lambda}{2!} q^{(0)}(\Delta q'(t'))^2 + \frac{\lambda}{3!} (\Delta q'(t'))^3 \right), \]  

(4.3.8)

where \( I_{t,t'}^{(2)} \) is defined as

\[ I_{t,t'}^{(2)} = \left( -m \partial_t^2 + 2\mu^2 - \frac{\lambda}{2} (q^{(0)})^2 \right) \delta(t-t'). \]  

(4.3.9)

The solution \( \Delta q'^{(1)}(t) \) takes the same form as (4.3.3) but with \( \omega^2 = 4\mu^2/m \). Again we take \( t_i = 0 \) and employ the form of the retarded Green’s function for \( I^{(2)-1} \) in (4.3.8), which now leads to the time-independent solutions \( \Delta q' = 0, -q^{(0)}, \) and \(-2q^{(0)}\) with the coefficient \( \tilde{C}^2 = \Delta q'/2 \) for each case. They naturally present the necessary shift of the initial position of the particle in order to stay at the extrema of the potential.

4.3.2. Field theoretical case

Next we examine a model of quantum field theory to see that the change of the boundary states is actually realized. In order to illustrate the essence of our approach, here we assume the following simple form of the effective action as an example,

\[ \Gamma[\phi] = \int d^4x \left\{ \frac{1}{2} \phi(x)(\partial_x^2 + m^2) + m^2 - \frac{1}{4!} \lambda \phi(x)^4 \right\}, \quad m^2 < 0. \]  

(4.3.10)

The quantum corrections are supposed to be effectively included in the coefficients \( m^2 \) and \( \lambda \). We study the constant form of the on-shell variation \( \Delta \phi \), which is now the candidate for space-time translation invariant vacuum solution.

Let us start from a trivial solution \( \phi^{(0)}(x) = 0 \). On-shell condition is written as

\[ (\partial_x^2 + m^2)\Delta \phi^{(1)}(x) = 0, \]  

(4.3.11)

and its solution is simply given by (2.1.17). Like in the previous case, the notation \( p^0 = (p^2 + m^2)^{1/2} \equiv \omega \) will be used in the following. Note here that for small \( p \), the mode becomes unstable: it is tachyonic.

Now we come to the argument of § 2.3 where on-shell variation is effected by the source at the boundary. Recall that the artificially introduced source \( K(x) \) in (2.3.3) is defined first in the finite time interval \( (T_i, T_f) \) and then the limits \( T_{i(f)} \rightarrow (\pm) \infty \) are considered. (Strictly speaking, each reduction process of LSZ defines different \( T_{i,f} \), which satisfy, for example, \( T_{i1} < T_{2f} < \cdots < T_{3f} < T_{4f} \). This fact naturally avoids the appearance of the surface terms like \( \delta(T_{i(f)} - T_{i(f)}) = \delta(0) \) in the actual calculations.) Note here that the similar limiting process should also be considered for the space variables \( x \) to avoid the complete orthogonalization in the case of the infinite volume among the different Hilbert spaces, which are constructed upon different vacua. Namely the non-zero solution \( \Delta \phi(x) \neq 0 \) is assumed to be suitably smoothed out to have its support first in the finite part of its infinite integration region of the space variables and then the limit of the infinite volume is considered. (This is somewhat different from the case for the time variable. Since the reduction is made at arbitrary large but finite time \( T_i \) or \( T_f \), \( \Delta \phi(x) \neq 0 \) is not defined for the region \( x^0 < T_i \) and \( T_f < x^0 \).) The assumption then assures us to omit the surface contribution of the space integration in the original reduction process.
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Now on-shell variation is summed up to satisfy

\[ \Delta \phi(x) = \Delta \phi^{(1)}(x) - \frac{\lambda}{3!} \int_{\mathfrak{A}_I} d^4 x' \Delta \phi(x, x'; m^2)(\Delta \phi(x'))^3. \]  \hspace{1cm} (4.3.12) \]

Here we note that since the effective action is defined starting from \( W[J] \) given in (1.2.1), the kernel corresponding to \( I^{(2)}_{II}^{-1} \) of (4.3.12) is fixed to be represented by the Feynman propagator \( \Delta_F \),

\[ \Delta_F(x, x'; m^2) = i \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2\omega} \left[ \theta(t - t') e^{-i\omega(t - t')} + \theta(t' - t) e^{i\omega(t - t')} \right] e^{i\mathbf{p}\cdot(x - x')}. \]  \hspace{1cm} (4.3.13) \]

After a short calculation, we find from (4.3.12) that the constant solution \( \Delta \phi \) is given by the stationary condition of the effective potential,

\[ \Delta \phi + \frac{\lambda}{3!} \frac{1}{m^2} (\Delta \phi)^3 = 0 \]  \hspace{1cm} (4.3.14) \]

with the coefficients \( \tilde{C}^\pm(p) \) (appearing in \( \Delta \phi^{(1)}(x) \)) having the following form,

\[ \tilde{C}^{\pm(-)}(p) = \frac{1}{2} \Delta \phi \delta^3(p) e^{\pm(-)i\omega_T t_0}. \]  \hspace{1cm} (4.3.15) \]

By inserting these results into (2.2.14), we can see the difference between trivial and non-trivial solutions in terms of the change of the boundary states;

1) \[ \phi^{(0)} = \frac{\langle 0 | \tilde{\phi}(x) | 0 \rangle}{\langle 0 | 0 \rangle} = 0, \]  \hspace{1cm} (4.3.16a) \]

2) \[ \Delta \phi = \frac{\langle \theta^- | \tilde{\phi}(x) | \theta^+ \rangle}{\langle \theta^- | \theta^+ \rangle} = \pm \left( \frac{3|m^2|}{\lambda} \right)^{1/2}, \]  \hspace{1cm} (4.3.16b) \]

where \( |\theta^+\rangle \) and \( |\theta^-\rangle \) are explicitly given by

\[ |\theta^{+(-)}\rangle = \exp \left[ \frac{\Delta \phi}{2} e^{i\omega_{p\cdot x} t_0} a_{\text{in(out)}}(0) \right] |0\rangle. \]  \hspace{1cm} (4.3.17) \]

The phase factors \( \exp(i\omega_{p\cdot x} T_{i(J)}) \) appearing in the exponent of (4.3.17) can be absorbed into the operator if we take the interaction representation and the result (4.3.16b) is reexpressed as follows. Writing \( x = (t, \mathbf{x}) \) we get

\[ \Delta \phi = \frac{\langle \theta^- | U(T, t) \tilde{\phi}(x) U(t, T) | \theta^+ \rangle}{\langle \theta^- | U(T, t) | \theta^+ \rangle} \]  \hspace{1cm} (4.3.18) \]

with the new states \( |\theta^{\pm}\rangle \) defined by the following form,

\[ |\theta^{+(-)}\rangle = \exp \left[ \frac{\Delta \phi}{2} \tilde{a}_I(p=0, t=T_{i(J)}) \right] |0\rangle, \]  \hspace{1cm} (4.3.19) \]

where the subscript \( I \) denotes the interaction representation and \( U \) is the corresponding time evolution operator. All the representations are supposed to coincide with each other at the time \( t=0 \).

The states \( |\theta^{\pm}\rangle \) of (4.3.19) have the same form but only the reference time is
different. They are naturally the candidates for the non-trivial vacuum state which is expressed as a superposition of original modes. So we expect, under the adiabatic hypothesis, that the states should satisfy

$$|\theta^+\rangle = e^{i\eta} U(T_r, T_l)|\theta^+\rangle_l \tag{4.3.20}$$

where $\eta$ is the appropriate phase factor. Then on-shell variation (4.3.18) can be written in both ways,

$$\Delta \phi = i\langle \theta^+| U(T_{i(U)}, t) \tilde{\Phi}_i(x) U(t, T_{i(U)})|\theta^+\rangle_l$$

In the Heisenberg representation, they are now represented by

$$\Delta \phi = \frac{\langle \Theta | \tilde{\Phi}(x) | \Theta \rangle}{\langle \Theta | \Theta \rangle} \tag{4.3.22}$$

with the vacuum state defined as

$$|\Theta\rangle \equiv U(0, T_{i(U)})|\theta^+\rangle_l \tag{4.3.23}$$

where the irrelevant phase factors have been omitted.

We can see explicitly from the above results that $\phi$ is indeed shifted by the amount $\Delta \phi$ in the following way. Take $t = T_r$ (or $T_l$), then it is easily checked that Eq. (4.3.21) straightforwardly becomes

$$\langle 0 | \exp \left( i \Delta \phi \int d^3 x' \tilde{\Phi}_i(x', T_{i(U)})\right) \tilde{\Phi}_i(x, T_{i(U)}) \exp \left( - i \Delta \phi \int d^3 x' \tilde{\Phi}_i(x', T_{i(U)})\right) | 0 \rangle = \phi^{(0)} + \Delta \phi, \quad (\phi^{(0)} = 0) \tag{4.3.24}$$

where $\tilde{\Phi}_i$ denotes the conjugate momentum operator of $\Phi_i$ defined by

$$\tilde{\Phi}_i(x) = - i \int (d^3 p/2(2\pi)^3) [\hat{\alpha}_i(p)e^{-ip\cdot x} - \hat{\alpha}_i(p)e^{ip\cdot x}]$$

For the case of the arbitrary $t$, the relation is proved by unitary transformation of (4.3.24).

Formally, $U(t, T_{i(U)})|\theta^+\rangle_l$ in (4.3.21) can be thought of as a trial state of variational method. Since $|\theta^+\rangle_l$ takes the form of coherent state, it is the commonly used trial state of the conventional approach, while our result suggests that the correct non-trivial vacuum state is obtained by further operating the time evolution operator $U(t, T_{i(U)})$. This fact may answer the question of how we select or improve the trial state of the conventional variational method. In this way, by using on-shell variation, the ground state can be examined in a novel way within the framework of the effective action (and potential) approach in field theory.

It will not be necessary to remark here that Eq. (4.3.23) connects the two vacuums $|0\rangle$ and $|\Theta\rangle$ which are the different ground states of the same system, i.e., the same Hamiltonian. Therefore it is different from the well-known adiabatic formula which relates the vacuum state $|0\rangle$ with that of the free Hamiltonian $|0\rangle_0$,

$$|0\rangle = U(0, t_{i(U)})|0\rangle_0.$$
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References

2) The effective action is used for scattering problem in the case of four body interaction by, M. Lutz and J. Praschifka, Univ. of Regensburg Report No. TPR-90-47, 1990. The method is however an off-shell expansion.
Chapter V. \(N\)-Body Bound State Equation

We apply here on-shell condition (2.1.4a) to derive \(N\)-body bound state equation with arbitrary \(N\) for the relativistic field theory. This \(N\)-body problem has been solved recently\(^1\) and the derivation is given in this chapter. We emphasize the significance of the problem since we have to study, for example, the \(N\)-quark bound state as a hadronic state in the framework of quantum chromodynamics (QCD), the poly-positronium problem in quantum electrodynamics (QED) or the QED correction to the atomic energy levels.

The bound state equation for \(N \geq 4\), as will be discussed in detail in the following, possesses a difficulty inherent in the problem itself: taking the inverse of the \((N-1)\)-particle irreducible Green's function, which is precisely the kernel of the \(N\)-body bound state equation. This is the main part of this chapter and result turns out to be written in an extremely compact form, (5.1.36) with (5.3.16) below.

As we have shown in the previous chapters, it is convenient to utilize the Legendre transformation for the derivation of bound state equation especially for the relativistic problem. The Legendre transformation in the \(N\)-body channel and the resulting effective action has already been discussed by many authors\(^2\)-\(^6\) In particular \(N\)-body equation of Faddeev type has been studied extensively.\(^7\) However the relation between the second derivative of effective action and the BS equation has not been established in these treatments so that the derivation of the \(N\)-body BS equation itself has to be done separately. We have already clarified the direct link between these two in Chapter II in the form of the on-shell expansion of the effective action. By this method, as we have already seen, the BS equation arises as the lowest equation in the expansion. The BS amplitude also naturally emerges in this scheme and a simple proof of \(N\)-particle irreducibility of the kernel can be given.

The external \(N\) sources \(J_1(x_1), J_2(x_1, x_2), \cdots, J_N(x_1, \cdots, x_N)\) are introduced simultaneously and by diagonalizing the \(N\)-channel problem we arrive at the \(N\)-body bound state equation (5.1.36), written in terms of the inverse of the \((N-1)\)-particle irreducible connected \(2N\)-body Green's function \(c_{N, \overline{N}}^{\overline{N}, \overline{N}}\). The appearance of \(c_{N, \overline{N}}^{\overline{N}, \overline{N}}\) here is natural. After giving the interpretation of \(c_{N, \overline{N}}^{\overline{N}, \overline{N}}\) in § 5.2, § 5.3 is devoted to taking the inverse of \(c_{N, \overline{N}}^{\overline{N}, \overline{N}}\), where we encounter the difficulties which come from the combinatorial complexities for \(N \geq 4\). The solution to this problem is given in (5.3.16). It gives us the expression for the correct kernel of the \(N\)-body bound state equation and reproduces the known results for \(N \leq 3\) of course. We discuss in Chapter VIII the non-relativistic case of our equations (5.1.36) and (5.3.16). It will be shown in § 8.1 that our \(N\)-body bound state equation reduces to the \(N\)-body Schrödinger equation after equal time projection.

Here we note that in the past the graphical rule of the Legendre transformation for \(N \geq 5\) was not known which seems to have prevented the derivation for general \(N\) of BS equation from the effective action \(\Gamma[\phi]\). However the crucial point is that to get BS equation only the second derivative of \(\Gamma[\phi]\) is needed. From this fact it is not necessary to have the general rule of calculating \(\Gamma[\phi]\).
§ 5.1. $N$-body bound state equation by Legendre transformation

As in the case of § 1.2, the generating functional $W[J_1, J_2, \cdots, J_N]$ is introduced here by functional integral as

$$
\exp(iW[J_1, \cdots, J_N]) = \frac{\int [d\phi] \exp iI[\phi]}{\int [d\phi] \exp iI[\phi]},
$$

(5.1.1)

where $I[\phi] = J_{i=0}[\phi]$ and $I_i[\phi]$ are defined by the following expression,

$$
I_i[\phi] \equiv \int d^4xL(\phi(x)) + \sum_{j \neq i} \int d^4x_1 \cdots d^4x_{j-1} J_i(x_1, \cdots, x_{j-1}) \times (\phi(x_1)\phi(x_2)\cdots\phi(x_i) - \langle \tilde{\phi}(x_1)\tilde{\phi}(x_2)\cdots\tilde{\phi}(x_i) \rangle_{j=0})
$$

(5.1.2)

$$
\equiv \int d^4xL(\phi(x)) + \sum_{j \neq i} J_i(\phi_i - \langle \tilde{\phi} \rangle_{j=0}).
$$

(5.1.3)

Here the factor $\nu!$ is not inserted in contrast to §3.1 because in the following we do not use explicitly the formula of the Legendre transformation presented in Appendix C. Note also that we have used in (5.1.3) a symbolic notation for the integration over space-time and in (5.1.1) $\exp(iW)$ is defined by dividing through $J$ independent factor. In this section the $c$-number function $J_i(x_1, \cdots, x_i)$ denotes the source coupled to the difference

$$
\phi(x_1)\phi(x_2)\cdots\phi(x_i) - \langle \tilde{\phi}(x_1)\tilde{\phi}(x_2)\cdots\tilde{\phi}(x_i) \rangle_{j=0}.
$$

(5.1.4)

The term $\langle \tilde{\phi}(x_1)\tilde{\phi}(x_2)\cdots\tilde{\phi}(x_i) \rangle_{j=0}$ has been subtracted in contrast to the previous chapters which turns out to be particularly convenient in the discussions in this section. It is defined by

$$
\langle \tilde{\phi}(x_1)\cdots\tilde{\phi}(x_i) \rangle_{j=0} = \frac{\int [d\phi] \phi(x_1)\cdots\phi(x_i) \exp iI[\phi]}{\int [d\phi] \exp iI[\phi]} = \langle 0 | T \phi(x_1)\cdots\phi(x_i) | 0 \rangle.
$$

(5.1.5)

In the discussions that follow, the vacuum state $|0\rangle$ is assumed to be the perturbative one excluding the case where the condensation occurs, otherwise the graphical study is impossible. The discussions in the presence of the condensed vacuum have been given in Chapter III for $N \leq 3$ and will be given in Chapter VI for $N \leq 4$, using slightly different method. The case of condensed vacuum definitely requires the rule of the Legendre transformation. The reason why the sources $J_1 \sim J_N$ are introduced is that we want to decompose $N$-channels into the diagonal $i$-body channel with $1 \leq i \leq N$ as will become clear.

Here we introduce the effective action $I'[\phi_1, \phi_2, \cdots, \phi_N]$ as

$$
\phi_i \equiv \phi_i(x_1, \cdots, x_i) = \frac{\delta W[J_1, \cdots, J_N]}{\delta f_i(x_1, \cdots, x_i)},
$$

(5.1.6)
\[ \Gamma[\phi_1, \ldots, \phi_N] = W[J_1, \ldots, J_N] - \sum_{i=1}^{N} J_i \phi_i. \]  

(5.1.7)

The symbol \( \phi_i \) introduced above is used only in this chapter and the notation \( J_i \phi_i \) includes the space-time integration. There is an identity (A-5),

\[ \frac{\delta \Gamma[\phi_1, \ldots, \phi_N]}{\delta \phi_i(x_1, \ldots, x_i)} = -J_i(x_1, \ldots, x_i) \equiv -J_i. \]  

(5.1.8)

For the stationary solution of \( \Gamma \), i.e., for \( J_i = 0 \) \((i = 1, \ldots, N)\), the variables \( \phi_j \) \((j = 1, \ldots, N)\) vanish owing to the above choice of \( J_i \), which makes the problem clear. We need the quadratic part of \( \Gamma \) evaluated at \( \phi_i = 0 \):

\[ \frac{\delta^2 \Gamma[\phi_1, \ldots, \phi_N]}{\delta \phi_i(x_1, \ldots, x_i) \delta \phi_j(x_1, \ldots, x_i)} = \frac{\delta^2 \Gamma}{\delta \phi_i \delta \phi_j}, \]

which is related to the quadratic part of \( W \) in \( J_i \) through the following identity, see (A-8):

\[ \sum_{i=1}^{N} \frac{\delta^2 \Gamma}{\delta \phi_i \delta \phi_j} \frac{\delta^2 W}{\delta J_i \delta J_j} = \sum_{i=1}^{N} \frac{\delta^2 W}{\delta J_i \delta J_j} \frac{\delta^2 \Gamma}{\delta \phi_i \delta \phi_j} = -\delta_{ik}. \]  

(5.1.9)

Only the quadratic part of \( W \) is therefore required since we set \( J_i \) to zero in the end of calculation. Thus \( W \) is expanded as

\[ W[J_1, \ldots, J_N] = \frac{i}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} \int d^4x_1 \cdots d^4x_k d^4x_i \cdots d^4x_l J_k(x_1, \ldots, x_k) J_l(x_i, \ldots, x_l) \]

\[ \times \langle \phi(x_1) \cdots \phi(x_k) \phi(x_i) \cdots \phi(x_l) \rangle_c + O(J^3) \]

\[ = \frac{i}{2} \sum_{k=1}^{N} \sum_{l=1}^{N} J_k J_l \langle \phi \phi \rangle_c + O(J^3). \]  

(5.1.10)

Here the subscript \( c \) means the connected part which is defined by the graphs whose external points \( x_1, \ldots, x_k \) and \( x_i, \ldots, x_l \) are connected by at least one propagator.

Now we perform the Legendre transformation step by step as follows. For \( i \geq 0 \), we define

\[ \Gamma_0[J_1, \ldots, J_N] = W[J_1, \ldots, J_N], \]  

(5.1.11)

\[ \phi_{i+1}(x_1, \ldots, x_{i+1}) = \frac{\delta \Gamma_i[\phi_1, \ldots, \phi_i, J_{i+1}, \ldots, J_N]}{\delta J_{i+1}(x_1, \ldots, x_{i+1})}, \]  

(5.1.12)

\[ \Gamma_{i+1}[\phi_1, \ldots, \phi_{i+1}, J_{i+2}, \ldots, J_N] = \Gamma_i[\phi_1, \ldots, \phi_{i+1}, J_{i+2}, \ldots, J_N] - J_{i+1} \phi_{i+1}. \]  

(5.1.13)

Equations (5.1.11) \~ (5.1.13) lead to \( \Gamma_N \) which is equivalent to \( \Gamma \) defined in (5.1.6) and (5.1.7), see Appendix A for the successive Legendre transformation. Let us derive \( \Gamma_N \) up to the second order of \( \phi \). The term \( O(J^3) \) in (5.1.10) is discarded and we write \( W \) as

\[ \Gamma_0 = W[J_1, \ldots, J_N] = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_i \phi_i J_j, \]  

(5.1.14)

where from (5.1.10)
\[ c_{i,j} = i\langle \hat{\phi}(x_1) \cdots \hat{\phi}(x_i) \hat{\phi}(x_{i+1}) \cdots \hat{\phi}(x_f) \rangle_c . \]  

(5.1.15)

For general \( i, \Gamma_i \) has the following quadratic form,

\[
\Gamma_i[\phi_1, \ldots, \phi_i, J_{i+1}, \ldots, J_N] = \frac{1}{2} \left( \sum_{j=1}^{i} \sum_{k=1}^{j} \phi_j a_{j,k} \phi_k + \sum_{j=1}^{i} \sum_{k=1}^{N} \phi_j b_{j,k} J_k + \frac{1}{2} \sum_{j=1}^{i} \sum_{k=1}^{N} J_k c_{j,k} J_k \right)
\]

\[
= \frac{1}{2} \begin{pmatrix} a_{i,1} & \cdots & a_{i,i} & b_{i,1} & \vdots & \vdots & \vdots & \cdots & b_{i,N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ a_{i,1} & \cdots & a_{i,i} & b_{i,1} & \vdots & \vdots & \vdots & \cdots & b_{i,N} \\ b_{i,1} & \cdots & b_{i,1} & c_{i,1,i} & \vdots & \vdots & \vdots & \cdots & c_{i,1,N} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ b_{i,1} & \cdots & b_{i,1} & c_{k,1,i} & \cdots & c_{k,1,N} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_i \\ J_{i+1} \\ \vdots \\ J_N \end{pmatrix}
\]

(5.1.16)

\[
= \frac{1}{2} (\phi_1, \ldots, \phi_i, J_{i+1}, \ldots, J_N)
\]

(5.1.17)

where \( a_{j,k} = a_{k,j} \), \( b_{j,k} = b_{k,j} \) and \( c_{j,k} = c_{k,j} \). It is not unique to write down the above \( N \times N \) matrix, but the above form is a convenient one. The superscript \( i \) appearing in \( a_{j,k} \), \( b_{j,k} \) or \( c_{j,k} \) stands for the number of steps of the Legendre transformation which has been carried out. The coefficients \( a_{j,k} \), \( b_{j,k} \), \( c_{j,k} \) are calculable perturbatively using propagators and vertices determined by the form of the starting Lagrangian.

Now using (5.1.12), (5.1.13) and (5.1.16) \( \Gamma_{i+1} \) can be written by \( a_{j,k} \), \( b_{j,k} \), \( c_{j,k} \) which are the coefficients of \( \Gamma_i \),

\[
\Gamma_{i+1} = \frac{1}{2} \left( \sum_{j=1}^{i} \sum_{k=1}^{j} \phi_j (a_{j,k} - b_{j,1} (c_{i,1,i+1})^{-1} b_{i,1} \phi_k \right)
\]

\[
+ \sum_{j=1}^{i} \sum_{k=1}^{N} \phi_j b_{j,1} (c_{i,1,i+1})^{-1} \phi_{i+1} - \frac{1}{2} \phi_{i+1} (c_{i,1,i+1})^{-1} \phi_{i+1}
\]

\[
+ \sum_{j=1}^{i} \sum_{k=1}^{N} \phi_j (b_{j,k} - b_{j,1} (c_{i,1,i+1})^{-1} c_{i,1,k} J_k + \sum_{j=i+2}^{N} \phi_j (c_{i,1,i+1})^{-1} c_{i,1,j} J_j
\]

\[
+ \frac{1}{2} \sum_{j=i+2}^{N} \sum_{k=1}^{N} J_k (c_{j,k} - c_{i,j+1} (c_{i,1,i+1})^{-1} c_{i,1,k} J_k ,
\]

(5.1.18)

where \( (c_{i,1,i+1})^{-1} \) is defined through the symmetrized identity operator \( I_i \) as follows,

\[
(c_{i,1,i+1})^{-1} c_{i,1,i+1} = c_{i,1,i+1} (c_{i,1,i+1})^{-1} \equiv I_{i+1} ,
\]

(5.1.19)

\[
(I_i)(x_1, \ldots, x_i, y_1, \ldots, y_i) = \frac{1}{i!} \sum_{\pi} \delta^i(x_j - y_{a_i}) .
\]

(5.1.20)

In (5.1.20) \( \Sigma_F \) means the summation over all possible \( \{ a_1, \ldots, a_i \} \)'s, which are permutations of \( 1, 2, \ldots, i \). If we rearrange (5.1.18) in the form of (5.1.16), the recursion formulas for the coefficients of \( \Gamma_i \) and \( \Gamma_{i+1} \) are obtained as follows,

\[
a_{j,k}^{i+1} = a_{j,k} - b_{j,1} (c_{i,1,i+1}^{-1}) b_{i,1} , \quad (1 \leq j, k \leq i)
\]

(5.1.21)

\[
a_{j,i}^{i+1} = a_{j+1,i}^{i+1} = b_{j,1} (c_{i,1,i+1}^{-1}) , \quad (1 \leq j \leq i)
\]

(5.1.22)
\[ a^t_{i+1,i+1} = -(c_{i+1,i+1})^{-1}, \quad (5.1.23) \]
\[ b^t_{j,k} = b^t_{j,k} - b^t_{i,i+1}(c_{i+1,i+1})^{-1}c_{i+1,k}, \quad (1 \leq j \leq i, \quad i + 2 \leq k \leq N) \quad (5.1.24) \]
\[ b^t_{i+1,i} = (c_{i+1,i+1})^{-1}c_{i+1,i}, \quad (i + 2 \leq j \leq N) \quad (5.1.25) \]
\[ c^t_{j,k} = c^t_{j,k} - c^t_{i,i+1}(c_{i+1,i+1})^{-1}c_{i+1,k}. \quad (i + 2 \leq j, \ k \leq N) \quad (5.1.26) \]

The coefficients \( c^t_{i,k} \) \((1 \leq j, k \leq N)\) are given by \((5.1.15)\). Now \( a^t_{j,k}, b^t_{j,k}, c^t_{j,k} \) are determined step by step through the use of \((5.1.21)\) \(\sim\) \((5.1.26)\) and \((5.1.15)\). In spite of its appearance, these are easily solved by noting the fact that \( a^t_{j,k} \), for instance, is an \( i \times i \) matrix in the index space of \( j, k \).

We need the quadratic form of \( \Gamma_N \),

\[ \Gamma_N = \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} \phi_j a^t_{j,k} \phi_k. \quad (5.1.27) \]

Let us apply the on-shell condition to our problem. Consider first our bound state equation which is a generalization of \((2.1.4a)\). Suppose a solution to

\[ \frac{\delta \Gamma_N[\phi_1, \ldots, \phi_N]}{\delta \phi_j} = 0, \quad (j=1, 2, \ldots, N) \quad (5.1.28) \]

be given by \( \phi^{(0)} = 0 \) in our case and write \( \phi_j = \phi^{(0)}_j + \Delta \phi_j \). This is inserted into the above equation and we get the mode determining on-shell equation,

\[ \sum_{k=1}^{N} \left( \frac{\delta^2 \Gamma_N}{\delta \phi_j \delta \phi_k} \right)_0 \Delta \phi_k = 0. \quad (5.1.29) \]

By \((5.1.27)\), it takes the form

\[ \sum_{k=1}^{N} a^t_{j,k} \Delta \phi_k = 0. \quad (j=1, \ldots, N) \quad (5.1.30) \]

As is seen in \((5.1.31)\) below \( a^t_{j,k} \) is not a diagonal matrix and we have to decompose these \( N \)-channels into \( k \)-body channel separately by diagonalizing the matrix \( a^t_{j,k} \).

From \((5.1.21) \sim (5.1.23)\) and \((5.1.27)\), we get

\[ \Gamma_N[\phi_1, \ldots, \phi_N] = \frac{1}{2} \sum_{j,k=1}^{N} \phi_j \left\{ -(c_{j,j-1})^{-1} \delta_{j,k} + (c_{j,j})^{-1} b^t_{j,k} \right\} + b^t_{j,k} \right\} \phi_k, \quad (5.1.31) \]

The right-hand side can be written in matrix form as

\[ \Gamma_N[\phi_1, \ldots, \phi_N] = -\frac{1}{2} \phi B^t C B \phi, \quad (5.1.32) \]

where we have defined the vector \( \phi \) and the matrices \( C, B \) as \( \phi_i \equiv \phi_i, \ (C)_{i,j} \equiv (c_{i,i})^{-1} \delta_{i,j}, \)


\[
(B)_{i,j} = \begin{cases} 
-b_i^{-1}, & (i > j) \\
I_i^0, & (i = j) \\
0, & (i < j)
\end{cases}
\]  

(5.1.33)

The fact that \( B \) is a lower triangular matrix makes things easy and in (5.1.33) \( I_i^0 \) is defined as \( I_i^0 = \prod_{k=1}^{i} \delta^4(x_k - y_k) \). We then introduce a new variable and rewrite (5.1.32):

\[
\phi'_i = \sum_{j=1}^{N} (B)_{i,j} \phi_j, \quad (5.1.34)
\]

\[
\Gamma_N[\phi'_1, \cdots, \phi'_N] = -\frac{1}{2} \sum_{i=1}^{N} \phi'_i (c_i^{(i-1)})^{-1} \phi'_i. \quad (5.1.35)
\]

With this diagonalized form, \( N \)-body bound state equation and the BS amplitude becomes

\[
(c_{N,N}^{N-1})^{-1} \Delta \phi_N = 0, \quad (5.1.36)
\]

\[
\Delta \phi_N = \sum_{i=1}^{N} (B)_{N,i} \langle 0 | T \bar{\phi}_1 \cdots \bar{\phi}_j | B \rangle + \text{c.c.} \quad (5.1.37)
\]

Actually Eq. (5.1.36) holds for any \( N \). Note that \( c_{N,N}^{N-1} \) is evaluated at \( J_i=0 \) \( (i=1, 2, \cdots, N) \) and that the transformation from \( \phi \) to \( \phi' \) is not singular since the inverse of \( B \) exists. Before taking the inverse of \( c_{N,N}^{N-1} \) explicitly in § 5.3, the interpretation of \( c_{N,N}^{N-1} \) is given in the next section.

§ 5.2. Interpretation of \( c_{N,N}^{N-1} \)

The coefficient matrix \( c_{j,k} \) is the sum of all graphs with \( j \)-external lines on the left-hand side of the diagram and \( k \)-external lines on the right-hand side, see Fig. 5.1.

From the relation (5.1.26), we will show an important property of \( c_{j,k} \) that there are at least \( i+1 \) propagators in the channel starting from left to right in Fig. 5.1. Remember that \( j, k \geq i+1 \) from (5.1.16). \( c_{j,k} \) becomes \( i \)-particle irreducible in the conventional terminology whose precise definition will be given in § 5.3. This is shown below by mathematical induction although this property is a direct conse-

![Fig. 5.1. Diagrammatical expression of \( c_{j,k} \).](image-url)
quence of the Legendre transformation. In what follows, $i$ is taken as the variable of mathematical induction with indices $j$ and $k$ fixed.

Now $c_{j,k}^i$ defined by (5.1.15) is equal to $i_i \phi(x_i) \phi(x_j) \phi(y_i) \phi(y_j) \phi(y_k)$ which is the sum of connected graphs satisfying the following condition: At least one propagator is connected with at least one of the $j$-external lines and with at least one of the $k$-external lines. Therefore the statement holds for $i=0$. Next we assume that the assumption is satisfied for $i=l$. Substituting the identity (5.1.19), we can write (5.1.26) as

$$c_{j,k}^{l+1} = c_{j,k}^l - c_{j,l+1}(c_{l+1,l+1}^{-1}c_{l+1,l+1}^{-1}c_{l+1,l+1}^{-1}c_{l+1,l+1}^{-1}c_{l+1,k}^{-1}) (l+2 \leq j, k \leq N) \quad (5.2.1)$$

The graphical structure of $c_{l+1,l+1}^{-1}$ is now investigated. By the assumption of the induction each of the $l+1$ external lines on the left-hand side of the graph (or the right-hand side) is connected with at least one external line on the right-hand side (or the left-hand side). In (5.2.1), $c_{j,l+1}(c_{l+1,l+1}^{-1}$ is the sum of all graphs which have $j$ external lines on the left-hand side and $l+1$ amputated external lines on the right-hand side. It also satisfies the condition that there are at least $l+2$ propagators along the channel. This is because we have got rid of the part with $l+1$ propagators along the channel by the operation $(c_{l+1,l+1}^{-1})^{-1}$. The factor $(c_{l+1,l+1}^{-1})^{-1}c_{l+1,k}$ in (5.2.1) has the same meaning. It is easy to understand that all the diagrams which have $l+1$ propagators along the horizontal channel from left to right are subtracted from $c_{j,k}$ in (5.2.1). Thus the right-hand side of (5.2.1) represents the graphs which have $j(k)$-external lines on the left (right)-hand side having at least $l+2$ propagators along the channel. The assumption is thus proved for $i=l+1$. In particular $c_{N,N}^{N,N}$ is the sum of all graphs with $N$ external lines on both sides and in these graphs there are at least $N$ propagators along the channel.

We can similarly obtain the graphical interpretation of $b_{j,k}^{i}$. The meaning of $a_{j,k}^{i}$ becomes clear in the following section where we study $(c_{N,N}^{N,N})^{-1}$.

§ 5.3. Inverse of $c_{N,N}^{N,N}$

We are in a position to take the inverse of $c_{N,N}^{N,N}$ to derive the $N$-body bound state equations (5.1.36) and (5.3.16) below. Before discussing general $N$, the cases with $N=1, 2, 3, 4$ are illustrated first and then proceed to the general proof.

It is easy to check that for the case $N=1$ our result (5.1.36) reproduces the well-known Klein-Gordon equation with full order quantum correction included. For $N=2, 3$, the following is another derivation of 2, 3-body BS equation shown in § 3.1.

(i) The case $N=2$

We know for $N=2$ that $c_{2,2}$ satisfies the integral equation,

$$(c_{2,2})_{x_1,x_2;y_1,y_2} = i \Delta F(x_1-y_1) \Delta F(x_2-y_2) 2!(I_2)_{y_1,y_2;y_1,y_2}$$

$$+ \frac{1}{2!} \overline{\Delta F}(x_1, x_2; y_1, y_2) \Delta F^{-1}(y_1-y_2) \Delta F^{-1}(y_2-y_1)(c_{2,2})_{y_1,y_2;y_1,y_2} \quad (5.3.1)$$
where $\tilde{V}_2$ is the sum of the two particle irreducible graphs along the channel from $(x_1, x_2)$ to $(y_1', y_2')$ and $\Delta_F(x-y)$ is the connected part of the full propagator. Both $\Delta_F$ and $\tilde{V}_2$ are evaluated for $J_i=0$ and each propagator contained in $\tilde{V}_2$ is the full propagator. The inverse is easily taken as

$$
((c^{L3}_{\pm})^{-1})_{x_1,x_2:y_1,y_2} = \frac{1}{2!} \{ \Delta_F^{-1}(x_1-y_1')\Delta_F^{-1}(x_2-y_2') - \frac{1}{2!} V_2(x_1, x_2; y_1', y_2') \}(I_2)_{y_1',y_2':y_1,y_2} \\
= \frac{1}{(2!)^2} \{ \Delta_F^{-1}(x_1-y_1')\Delta_F^{-1}(x_2-y_2') + \Delta_F^{-1}(x_1-y_2')\Delta_F^{-1}(x_2-y_1') \\
- V_2(x_1, x_2; y_1', y_2') \},
$$

(5.3.2)

where $V_2$ is used for $\tilde{V}_2$ with all external lines amputated.

From (5.1.36) we get BS equation as the on-shell condition for $\Delta\phi_2$,

$$
\int d^4y_1 d^4y_2 \{ \Delta_F^{-1}(x_1-y_1')\Delta_F^{-1}(x_2-y_2') - \frac{1}{2!} V_2(x_1, x_2; y_1, y_2) \} \Delta\phi_2(y_1, y_2) = 0.
$$

(5.3.3)

Here we have introduced a new definition of $\Delta\phi_2$ as

$$
\Delta\phi_2(x_1, x_2) = \int d^4y_1 d^4y_2 (I_2)_{x_1,x_2:y_1,y_2} \Delta\phi_2(y_1, y_2) \\
= \langle 0 | T\tilde{\phi}(x_1)\tilde{\phi}(x_2)|B_2\rangle - \int d^4x_1 b_{x_1}(x_1, x_2; x_1')\langle 0 | \tilde{\phi}(x_1') | B_2 \rangle + c.c.,
$$

(5.3.4)

where $|B_2\rangle$ represents two particle bound state and c.c. implies complex conjugation.

(ii) The case $N=3$

We introduce here the concept of the 'pure $i$-particle irreducible graph'. For this purpose we first define 'i-particle irreducible graph along the channel' from $(x_i, \cdots, x_1)$ to $(y_1, \cdots, y_i)$. Let the external points $(x_i, \cdots, x_1)$ of a chosen graph contract temporarily to a single point $x$ and $(y_1, \cdots, y_i)$ to $y$. Cut the resulting vacuum-like graph into two graphs in such a way that $x$ and $y$ are separated from each other. If there is no way to perform such an operation except that one of the graphs, after division, consists only of the bare vertex specified by $x$ or $y$, we call the original graph as $i$-particle irreducible graph along the channel. Now 'pure $i$-particle irreducible graph' is the $i$-particle irreducible graph along the channel from $(x_i, \cdots, x_1)$ to $(y_1, \cdots, y_i)$ satisfying further the condition that every external point is not connected to other external points directly. We then define $\tilde{V}_i$ as the sum of all the topologically different pure $i$-particle irreducible graphs. Recall that the definition of $\tilde{V}_i$ is the same as $\tilde{V}_2$. Also we use $V_i$ for $\tilde{V}_i$ with all the external lines amputated.

Recall that $c^{L3}_{\pm}$ represents the graphs which have three external lines on both sides and have at least three propagators along the channel we are interested in. It satisfies the following integral equation,
\[(c_{3,3})_{123,1'2'3'} = i \Delta_F(1, 1'', 2'') \Delta_F(3, 3'') \Delta_F(I_3)_{1''2''3''1'2'3'} + \frac{1}{3!} \left[ P[\Delta_F V_2] + P[\bar{V}_3] \right]_{123,1''2''3''} \times \Delta_F^{-1}(1'', 1'') \Delta_F^{-1}(2'', 2'') \Delta_F^{-1}(3'', 3'')(c_{3,3})_{1''2''3''1'2'3'} \times \Delta_F^{-1}(1'', 1'') \Delta_F^{-1}(2'', 2'') \Delta_F^{-1}(3'', 3'')(c_{3,3})_{1''2''3''1'2'3'} \quad (5.3.5)\]

Here we have defined $P$ as follows, which is written explicitly in order to make the notations clear,

\[(P[\Delta_F V_2])_{123,1'2'3'} = \Delta_F(1, 1') \bar{V}_2(2, 3; 2', 3') + \Delta_F(1, 2') \bar{V}_2(2, 3; 1', 3') + \Delta_F(1, 3') \bar{V}_2(2, 3; 1', 2') + \Delta_F(2, 1') \bar{V}_2(1, 3; 2', 3') + \Delta_F(2, 2') \bar{V}_2(1, 3; 1', 3') + \Delta_F(2, 3') \bar{V}_2(1, 3; 1', 2') + \Delta_F(3, 1') \bar{V}_2(1, 2; 2', 3') + \Delta_F(3, 2') \bar{V}_2(1, 2; 1', 3') + \Delta_F(3, 3') \bar{V}_2(1, 2; 1', 2'), \quad (5.3.6)\]

\[(P[\bar{V}_3])_{123,1'2'3'} = \bar{V}_3(1, 2; 1', 2'), \quad (5.3.7)\]

\[(P[\bar{V}_3])_{123,1'2'3'} = \bar{V}_3(1, 2, 3; 1', 2', 3'), \quad (5.3.8)\]

where $\Delta_F(1, 1')$ and $\bar{V}_2(1, 2; 1', 2')$ imply $\Delta_F(x_1 - y_1)$ and $\bar{V}_2(x_1, x_2; y_1, y_2)$, etc. (Generalization of $P$ to the case $N \geq 4$ is straightforward.) The integrations over the repeated numbers are implied of course. From (5.3.5) the inverse of $c_{3,3}$ is readily obtained as

\[
((c_{3,3}^{-1})_{123,1'2'3'} = -\frac{1}{3!} \left[ \Delta_F^{-1}(1, 1'') \Delta_F^{-1}(2, 2'') \Delta_F^{-1}(3, 3'') - \frac{1}{4!} \left[ P[\Delta_F^{-1} V_2] + P[\bar{V}_3] \right]_{123,1''2''3''} \right] (I_3)_{1''2''3''1'2'3'} \quad (5.3.9)\]

After we insert (5.3.9) into (5.1.36), the correct three-body bound state equation is obtained.

(iii) The case $N=4$

A new and troublesome situation arises for $N \geq 4$, due to the combinatorics of the diagrams. This is illustrated for $N=4$ as an example. The point is that a simple extension of (5.3.9) does not work for $N \geq 4$. To show this, consider $T_{4,4}$ which is defined simple mindedly as

\[
(T_{4,4})_{1234,1'2'3'4'} = i \Delta_F(1, 1'') \Delta_F(2, 2'') \Delta_F(3, 3'') \Delta_F(4, 4'') \Delta_F(4'') (I_4)_{1''2''3''4''1'2'3'4'} + \frac{1}{4!} \left[ P[\Delta_F \Delta_F V_2] + P[\Delta_F \bar{V}_3] + P[\bar{V}_4] \right]_{1234,1''2''3''4''} \times \Delta_F^{-1}(1'', 1'') \Delta_F^{-1}(2'', 2'') \Delta_F^{-1}(3'', 3'') \Delta_F^{-1}(4'', 4'') (T_{4,4})_{1''2''3''4''1'2'3'4'} \quad (5.3.10)\]

Simbolically this is represented as
\begin{equation}
A = \left( A_0 N! + K + K \frac{1}{N!} A_0^{-1} K + K \frac{1}{N!} A_0^{-1} K \frac{1}{N!} A_0^{-1} K + \cdots \right) I_N
\end{equation}

\begin{equation}
= A_0 N! I_N + \frac{1}{N!} KA_0^{-1} A
\end{equation}

with the obvious notation; \( A = T_{4,4} \), \( A_0 = \Delta_F \Delta_P \Delta_F \Delta_P \) and \( K = P[\Delta_F \bar{V}_2] + P[\Delta_F \bar{V}_3] + P[\bar{V}_4] \). In (5.3.11), each \( A_0^{-1} \) appears in combination with the factor \( 1/N! \). This is due to the combinatorial number appearing when we connect \( N \) lines of two groups of graphs each of which is symmetric under the exchange of the \( N \) external lines. The weight factors of several diagrams appearing in \( KA_0^{-1} K \) are as follows. The terms like

\begin{equation}
\bar{V}_4(1, 2, 3, 4; 1'', 2'', 3'', 4'') \Delta_F^{-1}(1'', 1''') \Delta_F^{-1}(2'', 2''')
\end{equation}

appear with the same weight. This weight is easily seen to be a correct one, i.e., unity. But we notice that

\begin{equation}
\bar{V}_3(1, 2; 1', 2') \bar{V}_3(3, 4; 3', 4')
\end{equation}

have twice as much weight. This is because there are two ways to get \( \bar{V}_3(1, 2; 1', 2') \bar{V}_3(3, 4; 3', 4') \) from \( K^2 \) term in the expansion (5.3.11). The first type Fig. 5.2(d1) is obtained by combining the term \( \Delta_F(3, 3') \Delta_F(4, 4') \bar{V}_3(1, 2; 1', 2') \) in the first \( K \) and \( \Delta_F(1, 1') \Delta_F(2, 2') \bar{V}_3(3, 4; 3', 4') \) in the second \( K \). The second type Fig. 5.2(d2) is just the reverse of it. All the terms in \( T_{4,4} \) which show the similar structure as in

Fig. 5.2. Diagrams appearing in \( KA_0^{-1} K \).
(5·3·13) have incorrect weights. We conclude that

\[ c_{44}^3 \neq T_{44}. \]

Thus we have seen that the graph of the type shown in Fig. 5.2(d) is the source of the trouble which prevents us from writing down in a straightforward way the correct bound state equation for \( N \geq 4 \).

The correct equation for \( c_{44}^3 \) is obtained by modifying \( K \) as \( K \rightarrow K = K - P[\tilde{V}_2 \tilde{V}_2] \) in (5·3·11). Therefore \( c_{44}^3 \) satisfies

\[
(c_{44}^3)_{1234,1'2'3'4'}
= i\Delta_f(1, 1')\Delta_f(2, 2')\Delta_f(3, 3')\Delta_f(4, 4')4!(I_4)_{1'2'3'4',1'2'3'4'}
+ \frac{1}{4!}[P[\Delta_f \Delta_f \tilde{V}_2] - P[\tilde{V}_2 \tilde{V}_2] + P[\Delta_f \tilde{V}_3] + P[\tilde{V}_3]]_{1234,1'2'3'4'}
\times \Delta_f^{-1}(1', 1'')\Delta_f^{-1}(2', 2'')\Delta_f^{-1}(3', 3'')\Delta_f^{-1}(4', 4'')(c_{44}^3)_{1'2'3'4',1'2'3'4'}. \tag{5·3·14}
\]

We can prove (5·3·14) as follows. For this purpose consider the iterative expansion of (5·3·14) in the form of (5·3·11). What we have to prove is that the right-hand side of (5·3·11) with \( \tilde{K} \) substituted for \( K \) indeed produces \( c_{44}^3 \); all the topologically different graphs of \( c_{44}^3 \) appear and the weight for each different graph is a correct one, i.e., unity.

This can be shown by mathematical induction. Assume that any topologically different graphs which are \( k \)-th-order in \( \tilde{V}_i \) (\( i = 2, 3, 4 \)) have the correct weight on the right-hand side of (5·3·11). Let us consider then the graphs of the \( (k+1) \)-th-order in \( \tilde{V}_i \). In the present case \( A \) in (5·3·11) stands for \( c_{44}^3 \) and \( \tilde{K} \) consists now of the graphs of the first and second order in \( \tilde{V}_i \), see (5·3·14). The way how an arbitrary graph of the \( (k+1) \)-th-order in \( \tilde{V}_i \) appears from up to the order \( \tilde{K}^{k+1} \) diagrams in (5·3·11) is as follows. Consider the case where the \( (k+1) \)-th-order diagram is made up by \( k \)-th-order diagram together with \( P[\tilde{V}_4] \) or \( P[\Delta_f \tilde{V}_3] \) at the right end of a given graph. Since all the \( k \)-th-order graphs have the proper weight by the assumption of the induction and since the multiplication of \( A_{0}^{-1}\tilde{K} \) (\( P[\tilde{V}_4] \) or \( P[\Delta_f \tilde{V}_3] \) in this case) at the right end apparently does not change its weight, the correct weight factor is obtained.

We can use, however, this type of argument only for the case in which the right end of the graph is uniquely determined. We call this type of graph the determinative graph. An example of diagram which is not determinative is precisely the one corresponding to (5·3·13), since it comes from \( KA_0^{-1}\tilde{K} and from \( \tilde{K} \). Let us discuss such an exceptional case. The right end of the \( (k+1) \)-th-order graphs in this case is represented by \( \tilde{V}_2(1, 2; 1', 2') \tilde{V}_3(3, 4; 3', 4') \) or \( \tilde{V}_2(1, 3; 1', 3') \tilde{V}_3(2, 4; 2', 4') \) or \( \tilde{V}_2(1, 4; 1', 4') \tilde{V}_3(2, 3; 2', 3') \). We consider the case \( \tilde{V}_2(1, 2; 1', 2') \tilde{V}_3(3, 4; 3', 4') \) (other terms can be discussed in a similar way). This type of graph is constructed in three different ways as shown in Figs. 5.3(a), (b), (c).

Now we observe the following: Fig. 5.3(a) contains the factor \( \Delta_f(3, 3')\Delta_f(4, 4') \tilde{V}_2(1, 2; 1', 2') \) at the right end while Fig. 5.3(b) \( \Delta_f(1, 1')\Delta_f(2, 2') \tilde{V}_3(3, 4; 3', 4') \). The last graph Fig. 5.3(c) contains the factor \( \tilde{V}_2(1, 2; 1', 2') \tilde{V}_3(3, 4; 3', 4') \) on the right end.
Fig. 5.3. Diagrams for the illustration of the weight factor of \((k+1)\)th order in \(V\).

Figures 5.3(a) and (b) have the unit weight. Figure 5.3(c) has also the unit weight but with the negative sign, since \(P[\tilde{V}_2 \tilde{V}_3] \) has the relative minus sign in \(\tilde{K}\) (see (5·3·14)). So the sum of these three types yields the correct weight factor, i.e., the same weight as the determinative graph has. In this way, all the topologically different \((k+1)\)th-order graphs appear in \(c_{k,l}^t\) with the desirable weight. Since it is straightforward to show that the assumption is correct for the lower orders in \(\tilde{V}_t\), the proof is completed. From (5·3·14) we finally get a very compact expression of \((c_{k,t}^l)^{-1}\),

\[
((c_{k,t}^l)^{-1})_{1234,1'2'3'4'} = \frac{1}{4!} \left\{ \Delta^{-1}_F(1, 1')\Delta^{-1}_F(2, 2')\Delta^{-1}_F(3, 3')\Delta^{-1}_F(4, 4') \\
+ \frac{1}{4!} \left( -P[\Delta^{-1} F^{-1} V_2] + P[V_2 V_2] - P[\Delta^{-1} F^{-1} V_3] - P[V_3] \right)_{1234,1'2'3'4'} \right\} \\
\times (I_4)_{1'2'3'4',1234'}, \tag{5·3·15}
\]

which can easily be checked to satisfy (5·3·11).

(iv) The \(N\)-body case

The general \(N\)-body channels can be discussed once we have understood the case \(N=4\). The result of \((c_{N,t}^N)^{-1}\) is expressed as:

**THEOREM**

\[
((c_{N,t}^N)^{-1})_{12…N,1'2'…N'} = \frac{1}{N!} \left\{ \Delta^{-1}_F(1, 1')\Delta^{-1}_F(2, 2')…\Delta^{-1}_F(N, N') \\
+ \sum_{(k,a_k)} \frac{1}{N!} \left( P[(-1)^k V_{a_1} V_{a_2}…V_{a_k}(\Delta^{-1}_F)^{(N-\sum_{i=1}^k a_i)}]_{12…N,1'2'…N'} \right) \right\} \\
\times (I_N)_{1'2'…N',12…N'}, \tag{5·3·16}
\]

where the summation is taken over all the combinations of \(V_{a_i}\) which satisfy \(\sum_{i=1}^k a_i \leq N\) and \(2 \leq a_i \leq N\) for each \(i\). If we use bare propagator \(\Delta_{bare}\) instead of \(\Delta_F\), the
theorem holds with the summation modified as $1 \leq a_i \leq N$ with the definition $V_i \equiv \Sigma$, the full self-energy function.

**Proof**

If we use
\[
\bar{K} = - \sum_{(k,a)} P[(-1)^k \tilde{V}_{a_1} \tilde{V}_{a_2} \cdots \tilde{V}_{a_k}(\mathcal{A}_F)^{N-\sum a_i a_i}]
\]  

instead of $K$ in (5.3.11), then it has to be shown that $A$ is equal to $c_{\vec{n}, \vec{n}}^{\vec{k}}$; all the topologically different graphs of $c_{\vec{n}, \vec{n}}^{\vec{k}}$ appear on the right-hand side of (5.3.11) and the weight for each different graph is correct. We first assume that any topologically different graphs of $k$th-order in $V_i \sim V_n$ have the proper weight on the right-hand side of (5.3.11). Take then the graphs of the $(k+1)$th-order in $V_i \sim V_n$. Here we notice that any graphs can be written as shown in Fig. 5.4, where $k+1 \geq i$ and all the $V_{a_i}$'s ($1 \leq j \leq i$) are pushed to the right as far as possible. We have written explicitly in Fig. 5.4 the vertices appearing on the right end.

As is easily understood all the contributions to any graphs up to the $(k+1)$th-order in $V_i$ come from some graphs up to the $k$th-order in $V_i$ together with $A^{-1}_{a_i} \bar{K}$ on the right end. The first contribution comes from the graphs which are constructed by taking away one of the $V_{a_i}$'s ($1 \leq j \leq i$) from Fig. 5.4. There are $iC_1$ ways to do this and each graph has the unit weight because of the assumption. So they contribute $iC_1$ to the weight. The second contribution comes from the graphs which are obtained by taking away $V_{a_i}$ and $V_{a_i}$ ($1 \leq j, l \leq i, j \neq l$) from Fig. 5.4. There are $iC_2$ ways and each graph has the unit weight by assumption. Here we notice that in $\bar{K}$ the graphs of the second-order in $V$ have negative sign. So the contribution is $-iC_2$. We continue the discussions and the total contribution for the graph turns out to be
\[
iC_1 - iC_2 + iC_3 - \cdots + (-1)^{i+1}iC_i = 1.
\]  

Of course any graphs of the first-order in $V_i$ can be shown explicitly to have the proper weight. So the proof is completed except for the last statement of the theo-
rem, the proof of which is quite straightforward.

Equation (5·3·16) is a natural generalization of the formula for $N=2$ and agrees with the expression presented in Ref. 2). The $N$-body bound state equation is then given by (5·1·36) using (5·3·16) for $(e^N, \gamma)^{-1}$.

In Chapter VIII, our method is applied to non-relativistic atomic system (in §§ 8.1.4 and 8.1.5) where we will see that the simple structure of non-relativistic ground state makes formulas simpler than the relativistic case.

References

Chapter VI. Legendre Transformation through Diagrams

The main aim of the Legendre transformation is, as has been stressed already, to rewrite the theory in terms of the expectation value of small number of operators that have been chosen depending on the nature of the problems we are going to discuss. For this purpose we first introduce the c-number source \( J \) as a probe of the corresponding operator \( \hat{O} \) and calculate the expectation value \( \phi = \langle \hat{O} \rangle \) of this operator in the presence of the probe. The essential part of the Legendre transformation is to invert the functional relation; \( \phi = \phi[J] \) in order to express the source in terms of the expectation value; \( J = J[\phi] \).

The graphical rule of the Legendre transformation is given in Appendix C, where the combinatorial relation of vacuum diagrams plays an essential role. The method is due to De Dominicis and Martin.\(^1\) However the graphs with external lines are easier than the vacuum diagrams in the sense that the former allow a simple minded insertion of sub-diagrams. On the basis of this fact and following the method of Ref. 2) we explain in this chapter a sum-up rule for the diagrams having external lines and derive a direct inversion formulas in which external source is represented as a functional of the expectation value of product of non-local operators, i.e., the Green's functions. It leads us to the BS equation of up to 4-body channel. Compared with the results of Chapter V, the present BS equation applies also to the case where the vacuum state is a non-perturbatively condensed state.

\[ \text{§ 6.1. Sum-up rule for general } i \text{-point connected Green's functions} \]

Let us take a single component scalar field \( \varphi(x) \) for brevity and define as before \( W[J] \), the generating functional for the Green's functions, using path integral formula,

\[
\exp\left(\frac{i}{\hbar} W[J]\right) = \int [d\varphi] \exp \left(\frac{i}{\hbar} I_1 \right),
\]

\[ I_1 = \frac{1}{2} \int d^4x \left( \partial_\mu \varphi(x) \partial^\mu \varphi(x) - m^2 \varphi(x)^2 \right) \]

\[ + \sum_{j=1}^N \int d^4x_1 \cdots \int d^4x_N \frac{1}{j!} J_1(x_1, \ldots, x_j) \varphi(x_1) \cdots \varphi(x_j) \]

\[ = \frac{1}{2} \frac{\hbar}{i} \varphi [G_2^0]^{-1} \varphi + \sum_{j \neq k} \frac{1}{j!} J_j \varphi^j. \]

Here the bare propagator \( G_2^0 \) includes the source \( J_2 \) for convenience,

\[ [G_2^0]^{-1} = \frac{i}{\hbar} (\Box + m^2 - J_2). \]

We have employed the symbolic notation by suppressing the space-time integration. This is used throughout this chapter. Note that (6·1·2) is different from (5·1·2) — here we have the factor \( (1/j!) \) in front of \( J_j \) and have no subtraction term
\( \langle \varphi(x_1) \cdots \varphi(x_j) \rangle_{\beta=0} \) appeared in (5.1.2). This is connected with our aim that the subsequent formulae are applicable to the case of condensed vacuum. Another reason for this notational change is to see the correspondence between our formulae and those of Appendix C where we have followed the definition of Ref. 1). The interaction will be introduced by adjusting the values of \( J_i \). For example if we consider \( \lambda \phi^4 \) theory we set \( J_i = \lambda \delta \phi_i \) at the end of calculation.

The \( i \)-th effective action, \( \Gamma_i[\phi] \), is the \( i \)-fold Legendre transform of \( W[J] \). Let us define the \( i \)-body Green's function \( \phi_i \) and \( \Gamma_i \),

\[
\phi_i(x_1, x_2, \cdots, x_i) = i! \frac{\delta W[J]}{\delta J_i(x_1, x_2, \cdots, x_i)} = i! \frac{\delta W[J]}{\delta J_i}, \quad (6.1.3)
\]

\[
\Gamma_i = W - \sum_{j=1}^{i} \frac{1}{j!} J_j \phi_j. \quad (6.1.4)
\]

Then the following equations are easily verified by (A.5) and (A.11),

\[
J_i = -i! \frac{\delta \Gamma_i}{\delta \phi_i}, \quad (i \leq j) \quad (6.1.5)
\]

\[
\phi_i = i! \frac{\delta \Gamma_i}{\delta J_i} = i! \frac{\delta W}{\delta J_i}. \quad (i > j) \quad (6.1.6)
\]

Note in the above formulae that the space-time variables are included in the indices \((i \text{ and } j)\). Note also that the \( \Gamma_i \)'s are functionals of \( \phi_j \) and \( J_k \) where \( j \leq i \) and \( k > i \), that is, \( \Gamma_i = \Gamma_i[\phi_1, \cdots, \phi_i, J_{i+1}, \cdots, J_N] \). The connected part of the \( i \)-point Green's function \( \phi_i \) is denoted as \( G_i[J_1 J_2 \cdots] \) hereafter emphasizing the dependence on the \( i \)-point vertices \( J_i \).

6.1.1. Transformation from \( J_1 \) to \( G_1 \)

Let us take \( G_i[J_1 J_2 \cdots] \) \((i \geq 2)\). The essential step of the Legendre transformation is to invert the relation (6.1.3) and to express \( J_i \) as a functional of \( \phi_j \) \((j \leq i)\). This is done graphically as follows. We are going to rewrite \( G_i[J_1 J_2 \cdots] \) as a functional of \( G_1, J_2, J_3, \cdots \); thus \( G_i = G_i[G_1 J_2 J_3 \cdots] \). Now in any diagram the part connected to the remainder by one line, i.e., by one bare propagator \( G_2^0 \) (see the left-hand side of (6.1.7) below), seems to be summed up to a single \( \tilde{G}_1 \) \((G_1 = (G_2^0)^{-1} G_i)\). Stated in other words, \( \tilde{G}_1 \) on the right-hand side of (6.1.7) generates all the graphs on the left-hand side. Here \( \tilde{G}_1 \) is \( G_1 \) with an external leg amputated.

\[
\text{(6.1.7)}
\]

We start from this well-known fact, since it is a prototype of the following discussions.

However Eq. (6.1.7) does not necessarily hold for all diagrams. Consider the vacuum graph shown in Fig. 6.1, corresponding to \((i/\hbar) W[J_1 \cdots J_N] \) which has no external legs. In this case each term on the right-hand side which is contained in
appears with different (i.e., incorrect) weight. So we cannot sum up all possible vacuum graphs having correct weight, i.e., unit weight, into \( \mathcal{G}_1 \). We have to exploit topological relation (C·6), for example, as in Appendix C.

But if we consider the graphs of \( G_i[J_1 \cdots] \), having external legs, such is not the case. To prove this, let us define a 1-legged part that is a connected subgraph which itself is connected to the rest through only one line (an example is the part A of Fig. 6.2). We distinguish this part by using a closed (solid or broken) line which encircles the subgraph and intersects only one line. In what follows we draw such a closed line in a way that it cuts as small number of lines as possible. Then the following theorem can be proved.

**Theorem 1** If, in a connected graph with at least one external line, two different 1-legged parts have a common part, one completely contains the other.

The theorem is easily proved if we consider the case shown in Fig. 6.2. In Fig. 6.2 the part A is one of the 1-legged part. Let us consider candidates for another 1-legged part which have some part in common with A. There seem to be three ways ((a), (b), (c)) described as a dotted line in Fig. 6.2. But we readily realize that only the case (b) is possible because a closed dotted line intersects only one propagator line. In the cases (a) and (c), a closed line intersects lines at least two times owing to the connectivity of the graph and the existence of (at least one) external line. The case (b) leads to Theorem 1.

It follows from Theorem 1 that we can unambiguously proceed to a larger 1-legged part to reach the largest 1-legged part (see Fig. 6.3). This procedure can be repeated to reach the largest 1-legged part starting from another 1-legged part which is not contained in the former largest 1-legged parts. We continue this until there are no 1-legged parts other than the largest ones. This is done for all the graphs of \( G_i[J_1 \cdots] \). Two graphs are said to belong to the same element of \( G_i[J_1 \cdots] \) if the two graphs have the same largest 1-legged structure (see Fig. 6.4). Then we put together

![Fig. 6.1. An example of troublesome graph: the left (right) part enclosed by a dotted circle in each term on the right-hand side comes from the left (right) \( \mathcal{G}_1 \) on the left-hand side.](image1)

![Fig. 6.2. Explanation of Theorem 1.](image2)
all the graphs belonging to the same element of \( G_i \). It is easy to see that this class of graphs corresponds with correct weight to just one graph which is obtained by replacing each of the largest 1-legged part by \( \bar{G}_1 \) vertex. Through the above sum-up process we have eliminated \( J_1 \) and accomplished the transformation from \( J_1 \) to \( \bar{G}_1 \) and hence to \( G_1 \).

To summarize the result let us define \( i \)-particle irreducible vacuum graph or \( i \)PI graph \((i=1, 2, \ldots)\). A given connected vacuum graph is called \( i \)PI if it is separated into two parts only when at least \((i+1)\) lines are cut except for the case that one of the separated parts is a trivial vertex. Here the trivial vertex implies \( \bar{G}_1, \bar{G}_2, \ldots, \bar{G}_i \) where \( \bar{G}_i \) \((i \geq 2)\) is defined as follows: external \( i \) legs of \( G_i \) are all amputated by the propagator \( G_2; \bar{G}_i=(G_2^{-1})iG_i \). Using this terminology the above result is written as

\[
G_i[J_1J_2\ldots]=i \text{ lines} \begin{array}{c}
\text{1PI}
\end{array}, \quad (i \geq 2) \tag{6.1.8}
\]

where 1PI implies that if the external lines are connected by a \( J_i \) vertex then the subsequent vacuum graph is 1PI.

6.1.2. Transformation from \( J_2 \) to \( G_2 \)

We assume here that \( G_i \) is already a functional of \( G_1 \). Our aim is then to show that \( G_i \) can be written as a functional of \( G_1 \) and \( G_2 \) instead of \( J_1 \) and \( J_2 \) if \( i \geq 3 \).

As in the previous subsection, we define a 2-legged part as a connected subgraph which is connected to the rest by two lines. Let us show the following statement:

**Theorem 2** In a connected graph with at least one external line (which is already written in terms of \( \bar{G}_1 \) vertex instead of \( J_1 \) vertex), if two different 2-legged parts have a common part, only two cases 1. and 2. are possible;

1. one completely contains the other,
2. there is another larger 2-legged part that completely contains these two 2-legged parts.
To prove this, see Fig. 6.5. The part B being one of the 2-legged part, candidates for another 2-legged part having some part in common with A are described by dotted circles in Fig. 6.5. Noting that if a closed dotted circle is truly another 2-legged part it must intersect just two lines and noting that graphs are connected ones, the graphs of Figs. 6.5 (b), (c) cannot be examples of another 2-legged part and Figs. 6.5 (a), (d) have the structure illustrated in Fig. 6.6. We notice that the case Fig. 6.6 (d) does not exist from the beginning because we are dealing with 1PI graphs which are already functionals of $G_1$. In the case Fig. 6.6 (a) there are three ways to encompass 2-legged part as shown in Fig. 6.6 (a') but there is the largest 2-legged part which completely includes the others. It is an example of the case 2. of Theorem 2. The cases (e) and (f) of Fig. 6.5 are examples of the case 1. of Theorem 2. In this way we have established Theorem 2. Note that if A part does not have any external lines Theorem 2 no longer holds (see Fig. 6.7). Theorem 2 ensures us to proceed unambiguously to the largest 2-legged part to find the 2-legged structure of the graph. Thus we can sum up all the graphs having the same largest 2-legged structure to a single graph obtained by replacing each largest 2-legged part with $G_2$. Thus we have eliminated $J_2$ and finished the transformation from $J_2$ to $G_2$. From now on the lines in the graph are assumed to represent $G_2$. Then the results are summarized as

$$G_{i}[G_1 G_2J_3 \ldots] = i \text{ lines} \quad 2\text{PI}. \quad (i \geq 3) \quad (6.1.9)$$

Here 2PI implies that if $i$-external lines are connected by a $J_i$ vertex then the resulting vacuum graph is 2PI.
6.1.3. **Transformation from \( J_i \) to \( G_i \)**

Now \( G_i \) is assumed to be already a functional of \( G_1 \) and \( G_2 \) (lines in the graph imply \( G_3 \)). We are going to show that \( G_i \) can be written as a functional of \( G_1 \), \( G_2 \) and \( G_3 \) instead of \( J_1 \), \( J_2 \) and \( J_3 \) if \( i \geq 4 \).

As in the previous subsection we define a 3-legged part in the same way and derive the following theorem.

**Theorem 3** In a connected graph with at least one external line (which is already written in terms of \( G_1 \) vertex and \( G_2 \) line), if two different 3-legged parts have a common part, only two cases 1. and 2. are possible,

1. one completely contains the other,
2. there is another larger 3-legged part that completely contains these two 3-legged parts.

As in the case of Theorem 2, this statement is in fact proved by considering all possible ways of drawing another 3-legged part having a common part with B part which is itself 3-legged part (see Fig. 6.8). Then we can sum up the graphs having the same largest 3-legged structure to give the following result,

\[
G_i[G_1 G_2 G_3 J_4 \cdots] = i \text{ lines} \left( \begin{array}{c}
\begin{array}{c}
\vdots \\
\text{3PI}
\end{array}
\end{array} \right). \quad (i \geq 4)
\]

(6.1.10)

Here the meaning of 3PI may be clear.

6.1.4. **Transformation from \( J_i \) to \( G_4 \)**

\( G_i \) is now a functional of \( G_1 \), \( G_2 \) and \( G_3 \) and we prove that \( G_i \) can be regarded as a functional of \( G_1 \), \( G_2 \), \( G_3 \) and \( G_4^p \) instead of \( J_1 \), \( \cdots \), \( J_4 \) if \( i \geq 5 \). \( G_4^p \) is slightly different from \( G_4 \) as discussed below.

Suppose that we define a 4-legged part as in Fig. 6.9 in the same way as in the previous subsections and assume similar theorem as Theorem 2 or 3 given above. But this turns out to be a wrong statement because of the appearance of the structure shown in Fig. 6.10. The two 4-legged parts (B, C in Fig. 6.10 (a), (b), (c)) have a common part but there does not exist a third 4-legged part which completely contains B- and C-parts. These three cases are only ones which violate the desired theorem.*

Thus we cannot proceed to a larger 4-legged part without ambiguity. But this difficulty is avoided by introducing another variable \( G_4^p \) and by trying to make a transformation from \( J_4 \) not to \( G_4 \) but to \( G_4^p \). \( G_4^p \) is defined as follows,

\[
G_4^p(1, 2, 3, 4) \equiv G_4(1, 2, 3, 4) - \begin{pmatrix}
3 & 4 \\
1 & 2
\end{pmatrix} + \begin{pmatrix}
2 & 4 \\
1 & 3
\end{pmatrix} + \begin{pmatrix}
2 & 3 \\
1 & 4
\end{pmatrix},
\]

(6.1.11)

where black dots stand for \( \bar{G}_3 \) vertices. We call these three graphs contained in the parenthesis of (6.1.11) pseudo 4-vertices after 4 external lines (\( G_2 \)) are amputated.

* We can see this fact after considering all possible cases of drawing another 4-legged part having a common part with B of Fig. 6.9 (for details, see Ref. 2).
Fig. 6.8. 3-legged part B in the graph.

Fig. 6.9. 4-legged part B in the graph.

Fig. 6.10. Examples of troublesome structure: the a- or b-(b')-part corresponds to subparts of A- or B-part respectively.

The pseudo 4-vertices are excluded from the definition of 4-legged parts but they appear as independent elements. Then in Figs. 6.10 (a), (b) there is only one way to draw a closed dotted line as a 4-legged part, i.e., the line B for Fig. 6.10 (a) and C for Fig. 6.10 (b), and no way in Fig. 6.10 (c). Figures 6.10 (a) and (b) correspond to \( \overline{G_3} \circ G_4 \otimes \overline{G_3} \) and \( \overline{G_3} \circ G_4 \otimes G_3 \) respectively. The structure like Fig. 6.10 (c) should be kept as it is, or interpreted as a product of three \( \overline{G_3} \) vertices; \( \overline{G_3} \circ \overline{G_3} \circ \overline{G_3} \). Now we can proceed to the largest 4-legged part to transform \( J_i \) to \( G_4^i \). The result is

\[
G_i[G_1 G_2 G_3 G_4^i \cdots] = i \text{ lines } (\overline{4PI}) \quad (i \geq 5) \tag{6.1.12}
\]

Here the definition of 4PI is slightly different from the original one defined just above (6.1.8) in that trivial \( \overline{G_i} \), \( \cdots \), \( \overline{G_4} \) vertices are turned into \( \overline{G_i} \), \( \overline{G_2} \), \( \overline{G_3} \), \( \overline{G_4} \) and pseudo 4-vertex (\( \overline{G_4}^i \) is the amputated \( G_4^i \); \( \overline{G_4}^i = (G_2^{-1})^i G_4^i \)).

6.1.5. Difficulty of transformation from \( J_i \) to \( G_i \) (i \geq 5)

If we consider all possible ways to draw another 5-legged part having a common part with a 5-legged part we encounter several troublesome cases two of which are shown in Fig. 6.11. Unlike the case for 4-legged part it seems to be difficult to give
new definition of 5-legged part, like $G_4^p$ of (6.1.11), to remove ambiguity in proceeding to a larger 5-legged part. We do not have the answer to this problem yet.

§ 6.2. Derivation of generalized bound state equation

As an application of sum-up rules discussed in § 6.1 we derive in this section 1, 2, 3 and 4-body bound-state equation (BS eq.). As have been stated, the results are more general than those of Chapter V since they can be used for the case of non-perturbatively condensed vacuum.

Let us recall some results of on-shell expansion. Hereafter we consider $\lambda \phi^4$ theory. The stationary solution $\phi_i^{(0)}$ to

$$\begin{align*}
\frac{\delta \Gamma_N}{\delta \phi_4} &= \lambda, \\
\frac{\delta \Gamma_N}{\delta \phi_i} &= 0, \quad (i \neq 4)
\end{align*}$$

determines the vacuum and zero eigenvalue equation

$$\sum_j \left( \frac{\delta^2 \Gamma_N}{\delta \phi_i \delta \phi_j} \right)_0 \Delta \phi_j = 0 \quad (6.2.1)$$

or equivalently, as is proved in Appendix A of Ref. 2), we can use a simplified equation

$$\left( \frac{\delta^2 \Gamma_N}{\delta \phi_N \delta \phi_N} \right)_0 \Delta \phi_N = 0, \quad (6.2.2)$$

which is nothing but the mode-determining equation in the $N$-body channel, i.e., $N$-body BS equation in our case. Here $\Sigma_j$ implies the integral $\prod_{i=1}^N d^4 x_i$ and $(\cdots)_0$ signifies that it is evaluated at the solution $\phi_i^{(0)}$ which can be either the perturbative or the non-perturbative condensed vacuum. This applicability to the non-perturbatively condensed vacuum case is an advantage of sum-up rule compared with Chapter V. Recall here that, in case the ground state is a perturbative one, $\phi_i^{(0)}$ can be expanded in the coupling constant so that the diagrammatic expansion of the kernel $(\delta^2 \Gamma_N/\delta \phi_N \delta \phi_N)_0$ is available. If, on the other hand, the theory realizes the non-perturbative vacuum, $\phi_i^{(0)}$ has no perturbative expansion in the coupling constant but the rule for $(\delta^2 \Gamma_N/\delta \phi_N \delta \phi_N)_0$ can be obtained in our case since the full vertices $\phi_i$ are our independent variables.

Noting that the Green's function $\phi_i$ defined by $\phi_i \equiv \langle 0 | T \phi(x_1) \phi(x_2) \cdots \phi(x_i) | 0 \rangle$ is expressed as a sum of terms each of which is written by connected Green's function $G_i$, 

\begin{center}
Fig. 6.11. Troublesome graphs.
\end{center}
\( \phi_i = G_i + \text{polynomial of } G_j, \) \( \text{where } j < i, \) \( \text{(especially } \phi_i = G_i) \) \hfill (6.2.3)

\( \Gamma_i \) can be regarded as a functional of \( G_i \) and \( J_k \) where \( j \leq i \) and \( k > i, \) that is, \( \Gamma_i = \Gamma_i^i[G_i, \ldots, G_i, J_{i+1}, \ldots, J_N]. \) We have then the relation, using (6.2.3),

\[
\frac{\delta \Gamma_i^c}{\delta G_N} = \frac{\delta \Gamma_i^c}{\delta \phi_N} = \frac{1}{N!} J_N, \quad \frac{\delta^2 \Gamma_i^c}{\delta G_N \delta G_N} = \frac{\delta^2 \Gamma_i^c}{\delta \phi_N \delta \phi_N}.
\] (6.2.4)

In each equation of (6.2.4) the first (second) expression implies that the derivative is taken by regarding \( G_i (\phi_i) (j = 1, 2, \ldots, N-1) \) as constant. Thus we get

\[
\frac{\delta G_N}{\delta J_N} \bigg|_{G_1, \ldots, G_{N-1}} = \left( \frac{\delta J_N}{\delta G_N} \right)^{-1} = \left[ N! - \frac{\delta^2 \Gamma_i^c}{\delta G_N \delta G_N} \right]^{-1},
\] (6.2.5)

where both on the left- and right-hand side the derivative is taken for fixed \( G_i (j = 1, 2, \ldots, N-1) \). Equation (6.2.5) enables us to study the second derivative of the effective action or BS equation (see (6.2.2)) through the graphical rule of the first derivative of \( G_i \) with respect to \( J_N \).

**6.2.1. 1, 2 and 3-body BS equations**

We notice that \( J_1 \) vertex in \( \delta G_1/\delta J_1 \) can be replaced by \( \bar{G}_1 \) vertex as in § 6.1.1 and we get

\[
\frac{\delta G_1}{\delta J_1} \bigg|_{J_2, J_3, J_4} = \frac{\text{a.l.1}}{\text{a.l.2}}.
\] (6.2.6)

The definition of the set of a.l. 1 (at least one) and a.l. 2 (at least two) is the special case of the following definition: the set of a.l. \( i \) and a.l. \( i+1 \) means that the graphs satisfy the constraints given below. Suppose that there are \( i \) external lines on both sides (we call (a) side and (b) side) of graph and suppose that they are connected by two extra \( \bar{G}_i(a) \) and \( \bar{G}_i(b) \) vertices to make a vacuum graph. The constraints we impose are the following: The resultant vacuum graph can be separated into two parts (which are not trivial vertices) only when at least \( i \) lines are cut if the cutting process leads to the separation of the two attached vertices \( \bar{G}_i(a) \) and \( \bar{G}_i(b). \) On the other hand, if the cutting process keeps the two attached \( \bar{G}_i(a) \) and \( \bar{G}_i(b) \) vertices connected, the resultant vacuum graph becomes two disconnected parts (which are not trivial vertices) only when at least \( i+1 \) lines are cut.

We now classify the graphs of the right-hand side of (6.2.6) by the number of lines which lead to the separation of the graph if each one of them is cut

\[
\frac{\delta G_1}{\delta J_1} = -a(1\text{PI}) + + + + + + + + + + + + (1\text{PI})^{(-1)} \cdots = \left( \frac{(-1)^{i-1} (1\text{PI})^{-1}}{(-1)^{i-1} (1\text{PI})^{-1}} \right.
\] (6.2.7)

Here \( a(1\text{PI})b \) is usually called the self-energy part and 1PI implies that if each external point \( a, b \) is closed by a \( \bar{G}_1 \) vertex with bare propagator \( \cdots \bar{G}_1 \) then the subsequent vacuum graph is 1PI. Then from (6.2.5) and (6.2.2) we get the second
derivative of the first effective action $I_1^c$ and BS equation for 1-body case,

\[ -\frac{\delta^2 I_1^c}{\delta G_1 \delta G_1} = (-)^{-1} - \begin{array}{c} \text{1PI} \end{array}, \quad (6.2.8) \]

\[ \left((-)^{-1} - \begin{array}{c} \text{1PI} \end{array}\right)_0 \delta G_1 = 0. \quad (6.2.9) \]

In order to study the 2-body case we notice that $J_1$ vertex in $G_2$ can be relaced by $\tilde{G}_1$ as in § 6.1.1 and get

\[ G_2 = \begin{array}{c} \text{1PI} \end{array}, \quad (6.2.10) \]

where 1PI means that the vacuum graph obtained by supplying a $J_2$ vertex is 1PI. $G_2$ is a functional of $G_1, J_2, J_3, \ldots$. Then replacing $J_2$ with $\tilde{G}_2$ in $\delta G_2/\delta J_2$ we get

\[ 2! \frac{\delta G_2}{\delta J_2} = \begin{array}{c} \text{al. 2} \end{array} \begin{array}{c} \text{al. 3} \end{array}. \quad (6.2.11) \]

The meaning of the set of al. 2 and 3 has already been defined. Note that lines here are the $G_2$'s. Then as in (6.2.7) we notice that

\[ 2! \frac{\delta G_2}{\delta J_2} = \left[\frac{1}{2!}\right]^2 \begin{array}{c} \text{2PI} \end{array}, \quad (6.2.12) \]

where $[\text{sym}]$ is the symmetrized product of two propagators $G_2$,

\[ \begin{bmatrix} 1 & 2 \n 3 & 4 \end{bmatrix}^{-1} = \frac{1}{3!} \begin{bmatrix} 1 & 2 \n 3 & 4 \end{bmatrix} + \frac{1}{3!} \begin{bmatrix} 1 & 2 \n 3 & 4 \end{bmatrix}. \]

Thus the second derivatives of the effective action and the generalized 2-body BS equation are given by

\[ -\frac{\delta^2 I_2^c}{\delta G_2 \delta G_2} = \left[\frac{1}{2!}\right]^2 \begin{array}{c} \text{2PI} \end{array}, \quad (6.2.13) \]

\[ \left[\frac{1}{2!}\right]^2 \begin{array}{c} \text{2PI} \end{array}_0 \delta G_2 = 0. \quad (6.2.14) \]

In a similar way we get

\[ -\frac{\delta^2 I_3^c}{\delta G_3 \delta G_3} = \left[\frac{1}{3!}\right]^2 \begin{array}{c} \text{3PI} \end{array}, \quad (6.2.15) \]

\[ \left[\frac{1}{3!}\right]^2 \begin{array}{c} \text{3PI} \end{array}_0 \delta G_3 = 0, \quad (6.2.16) \]

where $[\text{sym}]$ contains 3! graphs such as
Equations (6.2.8), (6.2.13) and (6.2.15) agree with the results given in Ref. 1. In case the vacuum is not a condensed one, Eqs. (6.2.9) and (6.2.14) coincide with the well-known BS equation (for instance see Refs. 3 and 4). Equation (6.2.16) for three-body BS equation has been derived with a different method in Ref. 4) which, for the un-condensed case, reduces to the result of Ref. 5).

6.2.2. 4-body BS equation

Owing to the special definition of 4-legged part made in § 6.1.4 we get

\[ 4! \frac{\delta G_4(a)}{\delta f_4(b)} = a \xrightarrow{\text{a.l. 4}} \circ \xrightarrow{\text{a.l. 5}} b. \]  

(6.2.17)

The definition of the set of a.l. 4 and a.l. 5 is the same as before if we replace \( \bar{G}_4 \) by \( \bar{G}_4^p \) in the previous definition and consider \( \bar{G}_4^p \) and pseudo 4-vertex as the trivial 4-point vertex.

In order to take the inverse of the above expression let us study the graph shown in Fig. 6.12. In what follows, the square bracket [⋯] implies the sum of the permutation of the external lines on the left- and right-hand side of the graph. In this definition the permutation of one external line on the right-hand side with the one on the left-hand side is not allowed. Now a particular class of graphs called simple net is introduced. It is a class of graphs generated by taking products of the graphs shown in Fig. 6.12 that satisfy a.l. 4 and 5 conditions of (6.2.17) (see Fig. 6.13). This set does not contain such parts as Fig. 6.14 (a) because it is inconsistent with the fact that we have already taken the largest 4-legged parts in (6.2.17) by using \( G_4^p \). The pseudo 4-vertex can appear in \( \circ \) only in a way of Fig. 6.14 (b) because if it is contained in the graph like Fig. 6.14 (c) this part contradicts with a.l. 4 condition of (6.2.17).

It is easily understood that simple net which is composed of the combination of the \( G_4^p \)'s and pseudo 4-vertices can be written by a simple net built only with \( D_4 \) defined as

\[ \quad \text{Fig. 6.12. Generator of the simple net: the circle stands for } G_4^p \text{ (or pseudo 4-vertex).} \]

\[ \quad \text{Fig. 6.13. Graphs representing simple net: the first term is included for convenience.} \]

\[ \quad \text{Fig. 6.14. Explanation of simple net: the circle and black dots stand for } G_4^p \text{ (or pseudo 4-vertex) and } \bar{G}_4 \text{ respectively.} \]
\[ D_4(1, 2; 3, 4) = G_4^p(1, 2, 3, 4) + \frac{1}{2} \frac{3}{4} + \frac{1}{2} \frac{4}{3} \]

\[ = G_4(1, 2, 3, 4) - \frac{1}{2} \frac{3}{4} \]

\[ = \frac{3}{4} + \frac{1}{2} \]

(6.2.18)

Note that \( D_4 \) should be used in such way that it is consistent with a.l. 4 condition of (6.2.17). We call this simple net \( D_4 \) simple net. The graphs appearing in (6.2.17) are able to be classified by the number of \( D_4 \) simple net. Note that the entire graph is separated into two parts by cutting 4 lines of each \( D_4 \) simple net. The following relation is readily written down.

\[ \frac{\delta G_4}{\delta I_4} = 4! \left( \left( \begin{array}{c} D_4 \text{ simple net} \\ \end{array} \right) \right)^{-1} - \frac{1}{4!} \left( \begin{array}{c} 4\text{PI} \\ \end{array} \right)^{-1} \]

(6.2.19)

Here \( \{4\text{PI}\} \) means the class of graphs which satisfies the following condition.

Suppose that 4 external lines on both sides of the graph be connected by two extra \( G_4^p(a) \), \( G_4^p(b) \) to get a vacuum graph. If this vacuum graph is separated into two parts, at least 5 lines must be cut except for the case that one of the separated parts is a trivial \( \bar{G}_1 \), \( \bar{G}_2 \), \( \bar{G}_3 \), \( \bar{G}_4 \), or pseudo 4-vertex.

Let us use here the following very interesting theorem (see Ref. 2) for the proof which is a statement about the property of Feynman graph.

**THEOREM 4** \( D_4 \) simple net = [\( D_4 \) chain]^{-1}

Here \( D_4 \) chain means the class of graphs illustrated in Fig. 6.15. It is a class of graphs created through taking the second derivative by \( D_4 \) of the sum of the cyclic vacuum graphs shown in Fig. 6.16. Thus we arrive at

\[ -\frac{\delta^2 I_4^e}{\delta G_4 \delta G_4} = \left( \begin{array}{c} D_4 \text{ chain} \\ \end{array} \right) - \left( \frac{1}{4!} \right)^2 \left( \begin{array}{c} 4\text{PI} \\ \end{array} \right) \]

(6.2.20)

This result coincides with the second derivative of \( I_4^e \) obtained in Ref. 1). Notice here that exceptional graphs appearing in Ref. 1) are all eliminated if one takes the second derivative in terms of \( G_4 \). Thus our result does not contain such exceptional graphs indicating that the vacuum graph is more complex than graphs with external

Fig. 6.15. Definition of \( D_4 \) chain.

Fig. 6.16. Cyclic vacuum graph.
Therefore, the following equation,
\[
\left( D_4 \text{ chain} \right) - \left( \frac{1}{4!} \right)^2 \left( 4\Pi \right)_0^3 \Delta G_4 = 0 \tag{6.2.21}
\]
is our generalized 4-body BS equation.

§ 6.3. Graphical rule for \( J_i \): inversion formula

As another application of sum-up rule, the graphical rule for \( J_i \) in terms of \( \bar{G}_i \), \( \cdots \), \( \bar{G}_i \), \( J_{i+1} \), \( \cdots \), \( J_N \) vertices is derived in this section. This is the inversion formula in terms of diagrams: \( G_i = G_i[G_1, \cdots, G_{i-1}, J_i, \cdots] \) is solved for \( J_i \), which is an essential step of the Legendre transformation.

So far the transformations from \( J_j \) to \( G_j \) \( (j \leq i) \) are considered for the Green's function \( G_{i+1} \). But in order to get the inversion formula, we need the transformation from \( J_i \) to \( G_i \) \( (j \leq i) \) for the Green's function \( G_i \) (not \( G_{i+1} \)) itself. Such a transformation can be achieved if we exploit the concept of the second largest structure as follows.

What we want to do is to invert \( \bar{G}_1, \bar{G}_2, \cdots, \bar{G}_i \), which are written in terms of \( J_1, J_2, \cdots, J_N \) and express \( J_1, J_2, \cdots, J_N \) by \( \bar{G}_1, \bar{G}_2, \cdots, \bar{G}_i, J_{i+1}, \cdots, J_N \). In this way one gets graphical rule for \( J_i \) which is constructed using \( \bar{G}_1, \cdots, \bar{G}_i, J_{i+1}, \cdots, J_N \). Recalling (6.2.5) or
\[
\frac{\delta J_N}{\delta G_N} = -N! \frac{\delta^2 \Gamma_N^c}{\delta G_N \delta G_N},
\]
one can again obtain BS equations through this graphical rules of \( J_N \) by removing one \( G_N \) vertex and by evaluating the quantity at the stationary point determined by
\[
N! \frac{\delta \Gamma_N^c}{\delta G_N} = -J_N = 0.
\]

First, consider the graphical rule for \( J_i \). If we try to use sum-up rule for \( G_i \), we notice that all graphs have the same largest 1-legged structure and are trivially summed-up to be a single \( \bar{G}_1 \) vertex. But if we sum up the graphs having the same second largest (1-legged part) structure (see Fig. 6.17) we get
\[
-\bar{G}_1 = J_1 + \text{1PI} \tag{6.3.1}
\]
We have used the following notation for the case of single component scalar field,
\[
\bar{G}_2^0 = \frac{\hat{\lambda}}{i} (\Box + m^2 - J_2)^{-1}.
\]
In (6.3.1) 1PI implies that, after attaching \( \bar{G}_1 \) vertex, resultant vacuum graph is 1PI. Here \(-\text{1PI}\) is written of course not by \( J_1 \) vertex but by \( \bar{G}_1 \) vertex. This relation can
be easily solved for $J_1$ which is the desired inversion formula,

$$\frac{i}{\hbar} J_1 = - \bar{G}_1 + \left[ \Pi \right].$$

(6.3.2)

Second, we go to the case $i=2$. Consider the graphs of $G_2$ which is already built with $G_1$ vertex. We can classify these by the number of the lines which, if one of them is cut, lead to the disconnected graphs, namely,

$$G_2 = + \left[ \frac{\text{a.l. 2}}{\text{a.l. 2}} \right] + \left[ \frac{\text{a.l. 2}}{\text{a.l. 2}} \right] + \cdots = \left( (-)^{-1} \left[ \frac{\text{a.l. 2}}{\text{a.l. 2}} \right] \right)^{-1},$$

(6.3.3)

where $\left[ \frac{\text{a.l. 2}}{\text{a.l. 2}} \right]$ is the usual self-energy part which is still described by $J_2$ or by $G_2^0$ (bare propagator) lines. If we sum up the graphs contained in $\left[ \frac{\text{a.l. 2}}{\text{a.l. 2}} \right]$ having the same second largest (2-legged part) structure (see Fig. 6.18) to transform from $J_2$ to $G_2$ we get which is now expressed by $G_2$ lines. This should be denoted as $\left[ \Pi \right]$. 

Fig. 6.17. Examples of the second largest structure for 1-legged part.

Fig. 6.18. Examples of the second largest structure for 2-legged part.
instead of \( \square \). The former means that if we make a vacuum graph \( \square 2\Pi \) by attaching \( G_2 \) lines to the two external points of \( 2\Pi \) the resulting vacuum graph is \( 2\Pi \). On the other hand the latter implies that the vacuum graph \( \overline{G}_1 2\Pi \overline{G}_1 \) made by attaching two \( G_1 \) to the external points of the \( 2\Pi \) is \( 2\Pi \). Thus we have

\[
G_2 = \left( (-)^{-1} \right) \left( \square 2\Pi \right)^{-1} \tag{6.3.4}
\]

or

\[
(G_2)^{-1} = [G_2^0]^{-1} - \square 2\Pi. \tag{6.3.5}
\]

Using \( G_2^0 = (\hbar/i)(\square + m^2 - J_2)^{-1} \) again we get the inversion formula for \( J_2 \),

\[
\frac{i}{\hbar} J_2 = \frac{i}{\hbar} (\square + m^2) - G_2^{-1} - \square 2\Pi. \tag{6.3.6}
\]

Next we consider the case \( i = 3 \). The graphs of \( G_3 \) which are already written by \( \overline{G}_1 \) vertex and \( G_2 \) line are summed-up after being classified by the second largest (3-legged part) structures (see Fig. 6.19),

\[
\square \overline{G}_3 \equiv \triangleleft J_3 + \square 3\Pi. \tag{6.3.7}
\]

Then we get

\[
\frac{i}{\hbar} J_3 = - \overline{G}_3 + \square 3\Pi. \tag{6.3.8}
\]

The case \( i = 4 \) can be treated in a similar (although somewhat tedious) manner to
give the graphical rules for $J_4$ in terms of $\bar{G}_1$, $\bar{G}_3$, $\bar{G}_4^p$, pseudo 4-vertices and $G_2$ line. The result is basically the same as (72) of Ref. 1).

As mentioned before BS equations obtained in § 6.2 are also derived using the above inversion formulae. Namely the on-shell condition

$$J_N[G^{(0)} + \Delta G] = 0$$

leads to

$$\left( \frac{\delta J_N}{\delta G_N} \right)_{G=G^{(0)}} \Delta G = 0,$$

which is the BS equation. Graphically speaking we remove one $G_N$ vertex from the graphs of $J_N$ to get BS kernel. BS equations thus obtained of course agree with the results in § 6.2 or with

$$\left( \frac{\delta^2 J_N}{\delta \phi_N \delta \phi_N} \right)_{G} \Delta \phi_N = 0.$$  \hspace{1cm} (6.3.9)

References

   For recent developments, see the following review articles: Modern Three-Particle Physics, ed. A. W. Thomas (Topics in Current Physics, vol. 2) (Springer, Berlin, 1977).
Chapter VII. Inversion Method

Up to now we have been mainly concerned with the problem of how to extract physical information from the effective action by using the formalism of on-shell expansion. How to calculate the effective action is our next subject.

In this chapter we are interested in the cases where the symmetry of the Hamiltonian does not coincide with that of the state in some region of the temperature, pressure, density or some other parameters such as the coupling strength contained in the Hamiltonian. The study on the transition between phases of different symmetry is one of the main interests of many body problem. The use of the free energy or the effective potential in zero temperature case which is defined through the Legendre transformation is known to be of particular help to discuss the characteristics of the symmetry breaking.

However, as has been stated in the Introduction, we know at present the diagrammatical rule of the Legendre transformation only for several special types of operators: non-local product of up to four field operators (see Appendix C for up to three). For the case where the auxiliary field can be introduced by Hubbard-Stratonovich transformation, the rules are applicable but we may encounter many other situations where the closed formula of the Legendre transformation does not exist.

Inversion method is one of the formalisms to circumvent these difficulties and the purpose of this chapter is to explain and apply the method of inversion, recently introduced by one of the authors,\(^1\)~\(^3\) to some typical systems which are known to possess the symmetry breaking solution. As will be explained, the process is nothing but the one used in obtaining the equation of state in equilibrium system in statistical physics and has long been applied to Ising model, for example. We refer to earlier works of Ref. 4) which are related to ours in some sense. One of the purposes of this article is to point out that it has a wide applicability covering the whole subjects of field theory, equilibrium or non-equilibrium, relativistic or non-relativistic and also microscopic or macroscopic.

After stating the principle and formulas, some examples of lowest order inversion method are first given which coincide with the mean-field results. Inclusion of fluctuations is done by considering higher-order terms which are quite straightforward in the present method. Combined with the scale invariance or with the renormalization group equation, the process of taking higher terms into account is then illustrated.

The detailed discussions of higher orders of inversion series will be given in Chapter XI, where we take a local composite operator and study the diagrammatical structure in full order.

§ 7.1. Basic principle

For the explanation of inversion method, let us take a spin system and discuss the ferromagnetic-paramagnetic phase transition in order to exemplify the role of the
Legendre transformation. This helps us to get a physical picture of our inversion method. The model Hamiltonian of this system without external magnetic field is written as

$$H_{ss} = -g \sum_i S_i \cdot S_j,$$  \hspace{1cm} (7.1.1)

where $S_i$ is the spin operator of site $i$ and $g$ is assumed to be positive. Although this Hamiltonian has rotational symmetry, the state realizes the spontaneous magnetization, i.e., the state does not have rotational symmetry, below some critical temperature known as the Curie point. In order to introduce the Legendre transformation, we shall define Gibbs free energy $G[H, g]$ by

$$G[H, g] = -\beta^{-1} \ln \{T \exp[-\beta(H_{ss} + H_{sh})]\},$$  \hspace{1cm} (7.1.2)

where $T = \beta^{-1}$ is the temperature of the system (Boltzmann constant is set to unity) and $H_{sh} = H \cdot \sum_i S_i$ stands for artificially introduced interaction Hamiltonian with external magnetic field $H$, which is set to zero in the end of the calculation. This term breaks the rotational symmetry and we shall call it the source term from now on. The spontaneous magnetization is characterized by the fact that even for $H=0$, non-vanishing magnetization remains. In this sense, $H$ serves as an infinitesimal probe. From (7.1.2), it follows that the magnetization is given by

$$M = \frac{\partial G[H, g]}{\partial H}.$$  \hspace{1cm} (7.1.3)

However, if we calculate $G[H, g]$ perturbatively in power series of $g$, for example, (7.1.3) gives vanishing $M$ for all orders of perturbation.

Now Helmholtz free energy $F[M, g]$ is defined as the Legendre transform of $G[H, g]$,

$$F[M, g] = G[H[M, g], g] - M \cdot H[M, g],$$ \hspace{1cm} (7.1.4)

where $H[M, g]$ is obtained by inverting (7.1.3). Once Helmholtz free energy is obtained, the spontaneous magnetization, which we choose as an order parameter, is given by a non-trivial solution of the reciprocal relation of (7.1.3)

$$H = -\frac{\partial F[M, g]}{\partial M}.$$ \hspace{1cm} (7.1.5)

with $H=0$. Removal of $H$ is nothing but a self-consistent condition to determine $M$.

The situation here is quite different from (7.1.3). Suppose we are given a perturbative calculation of $F[M, g]$ in powers of $g$ regarding $M$ as order unity in $g$. Then for $H=0$, non-vanishing $M$ can be found, if it exists at all, for any finite order expression of $F[M, g]$. The essential point here is the change of variable from $(H, g)$ to $(M, g)$ by inverting (7.1.3). By this process, infinitely many terms of the expansion series of $G[H, g]$ have been included in each term of the expansion coefficients of $F[M, g]$. Usually the lowest non-trivial solution to (7.1.5) with $H=0$ coincides with the mean-field result.

Now inversion method is a generalization of the Legendre transformation in the
sense that it takes into account only the essential step of the latter: add the source term (magnetic field $H$ in the preceding example) to break the symmetry of the Hamiltonian and calculate perturbatively in some parameter ($g$) the order parameter (magnetization) as a function of the external symmetry breaking field (or the source), invert then this relation to represent the symmetry breaking field as a function of this order parameter. Find finally the zero of this last relation. We point out here that the source term and order parameter can be chosen quite freely. It is not necessary that they are conjugate each other, like $H$ and $M$. The only requirement is that the source term breaks the symmetry and order parameter represents the required property of the system which vanishes when the source term is removed. In this sense, inversion method is a generalization of the Legendre transformation. However we are mainly concerned with the case where the probe and order parameter are conjugate each other. The method has been applied to various models, some of which are illustrated below.

§ 7.2. Inversion formula

The general procedure of inversion method is now explained. The method of determining expectation value is first presented and then we proceed to the problem of excited levels.

7.2.1. Static case

Let us consider the Hamiltonian $\hat{H}$ ( $\hat{\ }$ denotes the operator) of the system with some parameter $g$ contained in it. For convenience of the following discussions, we assume that it can be divided into two parts, the free part and the interaction part:

$$\hat{H} = \hat{H}_0 + g\hat{H}_1,$$  \hspace{1cm} (7.2.1)

where $g$ is the coupling constant. In order to investigate the characteristics of the symmetry breaking phase, order parameter is defined. It does not matter whether the system is in zero temperature or not. If the expectation value of some operator, say $\hat{\phi}$, is chosen to be an order parameter, it vanishes for all orders of the perturbation series in $g$. We add the source term $\hat{H}_f$ to $\hat{H}$ so as to break the symmetry of $\hat{H}$. Here $J$ is some parameter corresponding to the external field (source). The restriction on the source term is to give a non-zero perturbation series of $\phi = \langle \hat{\phi} \rangle$ and to vanish when $J=0$. Hence, it is not necessary to be of the form $\hat{H}_f = \hat{H} + J\hat{\phi}$. In order to get back to the starting theory, the source is made to vanish in the end of the calculation.

Then the order parameter $\phi$ can be calculated perturbatively and expressed as the following series,

$$\phi = f[J] = \sum_{n=0}^{\infty} g^n f_n[J].$$  \hspace{1cm} (7.2.2)

This is called the original series in what follows. While (7.2.2) is the relation defining $\phi = \phi[J, g]$, we take another view that $J$ is given by the relation $J = J[\phi, g]$. This can be done by looking upon $\phi$ as a quantity independent of $g$ (i.e., as the order
of unity) and by inverting the function \( \phi = f(J) \) to get
\[
J = h[\phi] = \sum_{n=0}^{\infty} g^n h_n[\phi]. \tag{7.2.3}
\]
We call (7.2.3) the inverted series. Whereas only finite number of coefficient functions \( f_m[J] \) of the original series, \( m \leq N \) for example, can actually be calculated, it is possible to obtain \( h_m[\phi] \) of the inverted series for \( m \leq N \). Indeed substituting (7.2.3) into (7.2.2) and expanding the right-hand side in a power series of \( g \), the following identity is to be obtained
\[
\phi = f[h[\phi]] = \sum_{n=0}^{\infty} g^n f_n \left[ \sum_{m=0}^{\infty} g^m h_m[\phi] \right]
= f_0[h_0[\phi]] + g[f_0[h_0[\phi]] h_1[\phi] + f_1[h_0[\phi]]] + g^2 \left[ f_0[h_0[\phi]] h_2[\phi] + \frac{1}{2} f_0^2[h_0[\phi]] h_1^2[\phi] + f_1[h_0[\phi]] h_1[\phi] + f_2[h_0[\phi]] \right] + \cdots,
\]
where the prime stands for the differentiation with respect to \( J \). If we consider \( \phi \) as order unity, \( h_n[\phi] \) can be expressed in terms of the function \( f_n \):
\[
h_0[\phi] = f_0^{-1}[\phi], \tag{7.2.4}
\]
\[
h_1[\phi] = -\left[ \frac{f_1[J]}{f_0[J]} \right]_{J=h_0[\phi]}, \tag{7.2.5}
\]
\[
h_2[\phi] = \left[ \frac{1}{2} f_0[h_0[\phi]] h_1[\phi] + f_1[h_0[\phi]] h_1[\phi] + f_2[J]}{f_0[J]} \right]_{J=h_0[\phi]}, \tag{7.2.6}
\]
and so forth. Here \( f_0^{-1} \) is the inverse function of \( f_0 \). The set of equations presented in (7.2.4)~(7.2.6), etc., is all that is required in inversion method.

Since we can only perform a calculation for finite order in \( g \), setting \( J = 0 \) in (7.2.2) gives trivial solution \( \phi = 0 \) only. But once we invert (7.2.2) with respect to \( J \) and set \( J = 0 \), the non-trivial solution \( \phi \neq 0 \) is obtainable with finite order calculation. This is the most essential point of this formalism. Although Eqs. (7.2.2) and (7.2.3) are equivalent to each other, the finite order version of them are not, of course.

The above technique is common to the formalism of free energy in statistical mechanics and also to that of the effective action or potential in quantum field theory. Several comments are in order here.

(1) Truncation of the original series (7.2.2) implies that we have kept finite number of diagrams. However if we truncate the series of (7.2.3) at some finite order, an infinite number of specific diagrams are included. These diagrams consist of those that can be written as a repetition of simple sub-diagram. This happens because we have regarded \( \phi \) as order unity and makes it possible to get a non-perturbative solution. The situation is clearly seen by the discussion of Chapter VI where an infinite number of sub-diagrams are represented by single variable \( \phi \).
(2) In case the source term is chosen as
\[ \hat{H} = \hat{H} + J\hat{\phi}, \tag{7.2.7} \]
then our inversion method coincides with the usual method of the Legendre transformation. Let us explain this fact by taking an equilibrium system. First, introduce Gibbs-type free energy \( W[J] \) in the presence of \( J\hat{\phi} \) by
\[ e^{-\beta W[J]} = \text{Tr} e^{-\beta (\hat{H} + J\hat{\phi})}. \tag{7.2.8} \]

Then
\[ \phi = \langle \hat{\phi} \rangle = \frac{\partial W[J]}{\partial J}, \tag{7.2.9} \]
can be calculated using diagrams and get the original series (7.2.2). Then the inverted series (7.2.3) is just the series for
\[ J = -\frac{\partial \Gamma[\phi]}{\partial \phi}, \tag{7.2.10} \]
where Helmholtz-type free energy is defined by the Legendre transformation as
\[ \Gamma[\phi] = W[J] - J \frac{\partial W[J]}{\partial J}. \tag{7.2.11} \]
In the case of single variable \( \phi \), \( \Gamma[\phi] \) is obtained by simply integrating the series (7.2.3),
\[ \Gamma[\phi] = -\int^\phi d\phi J = -\sum_{n=0}^\infty g^n \int^\phi d\phi h_n[\phi], \tag{7.2.12} \]
where the integration constant is an irrelevant quantity. For the case of several variables \( \phi_i \), \( \Gamma[\phi_i] \) can be obtained as a solution of partial differential equation \( J_i[\phi] = -\partial \Gamma/\partial \phi_i \). Examples will be given in §7.3 and in Chapters IX and X.

More generally, if \( \phi \) is expressed as the derivative of some function \( W[J] \), \( \Gamma[\phi] \) can be written using the perturbative series of \( W[J] \). Let us expand \( W \) in powers of \( g \)
\[ W[J] = W^{(0)}[J] + g W^{(1)}[J] + g^2 W^{(2)}[J] + g^3 W^{(3)}[J] + \cdots. \]
(Do not mix with the notation \( W^{(2)} \) or \( \Gamma^{(2)} \) of Chapter II, which denotes the second derivative.) Then each term produces \( \phi \) of corresponding order by differentiation,
\[ \phi^{(i)} = \frac{dW^{(i)}}{dJ}. \tag{7.2.13} \]

Now construct the inverted series (7.2.3) and calculate \( \Gamma[\phi] = W[J] - J\phi \) perturbatively. Here both \( W \) and \( J \) have to be expanded regarding \( \phi \) to be order unity. Using the inversion formulas (7.2.4), (7.2.5), etc., it is straightforward to get \( \Gamma \) up to order \( g^2 \),
\[ \Gamma[\phi] = W^{(0)} - h_0 \phi \tag{7.2.14} \]
+ \frac{g}{2} \left[ W^{(2)} - \frac{1}{2} \left( \frac{W^{(1)}}{W^{(0)}} \right)^{12} \right] 
\tag{7.2.16}
+ g^3 \left[ W^{(3)} - \frac{1}{3!} \left( \frac{W^{(1)}}{W^{(0)}} \right)^{13} + \frac{1}{2!} \left( \frac{W^{(1)}}{W^{(0)}} \right)^{12} \left( \frac{W^{(1)}}{W^{(0)}} \right)^{(1)} - \left( \frac{W^{(1)}}{W^{(0)}} \right)^{(2)} \right] 
\tag{7.2.17}
+ \cdots

where \( W^{(1)} \) for example implies the differentiation of \( W \) by its argument and all the \( W^{(i)} \)'s in the above formulas are evaluated at the value \( J = h_0(\phi) \). We have arranged in the above formulas the terms according to the order of \( g \). The graphical meaning of the above expressions can be studied in arbitrary order of \( g \) by taking a specific model Hamiltonian and the operator \( \hat{O} \). Roughly speaking, the terms that follow the first term \( W^{(1)} \) in the \( i \)-th formula play the role of subtracting the reducible part contained in \( W^{(i)} \). These terms are the consequence of changing the variable from \( J \) to \( \phi \) by the Legendre transformation. See Chapters X and XI.

The formulas (7.2.14)\( \sim \) (7.2.17) can also be obtained by simple integrations. Let us expand

\[
\Gamma[\phi] = \Gamma^{(0)}[\phi] + g\Gamma^{(1)}[\phi] + g^2\Gamma^{(2)}[\phi] + \cdots,
\]

then order by order we have the relation

\[
\frac{\partial \Gamma^{(i)}}{\partial \phi} = - h_1[\phi].
\]

Then by using (7.2.13) and (7.2.4)\( \sim \) (7.2.6), we get

\[
\Gamma^{(0)}[\phi] = - \int h_0[\phi] d\phi = - \int h_0 \frac{d\phi}{dh_0} dh_0 = - \int h_0(W^{(0)}) dh_0 = - h_0(W^{(0)}) + W^{(0)},
\]

\[
\Gamma^{(1)}[\phi] = - \int h_1[\phi] d\phi = - \int h_1 \frac{d\phi}{dh_0} dh_0 = \int (W^{(0)})^{-1} (W^{(1)}) (W^{(0)}) dh_0 = W^{(1)}
\]

and so forth.

(3) When the chosen operator \( \hat{\phi} \) is one of the non-local product of field operators up to four, then the result of the Legendre transformation is known as a diagrammatic rule, i.e., for \( \hat{\phi} = \hat{\phi}(x), \hat{\phi}(x) \hat{\phi}(y), \hat{\phi}(x) \hat{\phi}(y) \hat{\phi}(z), \hat{\phi}(x) \hat{\phi}(y) \hat{\phi}(z) \hat{\phi}(w) \). See Appendix C for the rule up to three body operators. However there are many cases where we are interested in operators other than these four. Because of this, the use of the Legendre transformation has actually been limited to rather special kinds of problems which allow the direct use of the graphical rule. However the inversion method is applicable for any cases.

(4) From the applications of the present method to several typical models of quantum field theory or statistical mechanics, some of which are shown below, it is known empirically that in the lowest non-trivial approximation inversion method
gives the equation which is the same as the one obtained by mean-field theory or variational calculation in its simplest form of the trial state. Our inversion method provides a systematic improvement of mean-field results, as is obvious from the arguments already presented.

(5) Inversion method can also be utilized for the time-dependent dynamical phenomena. We have only to introduce time-dependent probe \( J(t) \) and calculate the time evolution of the expectation value \( \phi(t) \) of order parameter in the presence of \( J(t) \). Inverting this relation by expressing \( J(t) \) as a function(al) of \( \phi(t) \) and setting \( J(t) \) to be zero, we get the equation of motion for \( \phi(t) \). The method will be applied to non-equilibrium case in Chapters IX, XII, XIII and XIV. In the next subsection the time-dependent inversion method is applied to get the excitation modes which are excited above the stationary solution \( \phi(t) \).

(6) The quantity \( \phi \) which we called the order parameter does not necessarily have to be an expectation value of some operator. We can take any physical quantity and calculate it as a function(al) of \( J \). (Evenmore it can be a symmetry preserving quantity.) After this is done, the steps we take are the same as above. Examples of such \( \phi \)'s are; the gap parameter in superconductor, the energy of the excited level of the condensed phase, or even the scattering matrix element among excited levels. These are not expressible as an expectation value of any operator. Investigation along this line may be an interesting subject.

(7) The source term or the probe \( J \) can be anything as long as it has a correct quantum number corresponding to the channel we are going to probe. Since \( J \) is set to zero in the end, difference in the way how \( J \) is introduced disappears as is usually believed. This is a full order argument. The problem is, however, what happens if we use approximate series by truncating (7-2-3) at some finite order. The numerical value of \( \phi \) obtained by solving \( J=0 \) will be different in this case depending on the choice of \( J \). Although the difference is small for small \( g \), we have somehow to investigate for each specific problem the form of the probe \( J \) which reproduces the best value of \( \phi \).

(8) It looks that in the above inversion formulas, we need an explicit form of the inverse function \( f_{0}^{-1}(\phi) \). But this is circumvented by changing the order parameter from \( \phi \) to \( h_{0}(\phi) \). Indeed the inverted series has the structure

\[
J = h_{0}(\phi) + h_{1}[h_{0}(\phi)] + h_{2}[h_{0}(\phi)] + h_{3}[h_{0}(\phi)] + \cdots,
\]

so that the solution to \( J=0 \) determines \( h_{0}(\phi) \). The parameter \( h_{0}(\phi) \) thus obtained has a physical meaning: It is the (lowest order value of) internally produced field when the original order parameter \( \phi \) takes a non-zero value. For example in the case of ferromagnetic order, we add the term \( H \cdot M \) to the Hamiltonian, where \( H \) is the external magnetic field introduced as a probe, which is set to zero in the end, and \( M \) is the magnetization operator. In this case \( h_{0}(\phi) \) is the internal magnetic field due to the spontaneous magnetization \( M \). Another example is the chiral symmetry breaking in massless fermion theory. Here the source term \( \int d^{4}x \bar{\psi}(x)\psi(x) \) is added to the action and \( h_{0}(\phi) \) is the dynamical mass generated by non-zero \( \phi = \langle 0 | \bar{\psi}(x)\psi(x) | 0 \rangle \).
We summarize below the relation between the order parameter and $h_0(\phi)$:

| magnetic system | order parameter $\bar{\phi}(x)\phi(x)$ | $h_0(\phi)$ dynamical mass |
| massless fermion | magnetization | internal magnetic field |
| superconductor | pairing field | gap parameter |
| fluid system | current operator | velocity field |

In all examples, the original parameter $\phi$ is obtained by inverting $h_0(\phi)$ but this is done graphically in $\phi - h_0(\phi)$ plane. Note that if the source term breaks the symmetry of the Hamiltonian then $h_0(\phi)$ vanishes when we set $\phi = 0$. Therefore we can use $h_0(\phi)$ as a symmetry breaking order parameter.

(9) In case we are interested in multiple channels, many sources have to be introduced and the inversion formulas become of the matrix form connecting the probes $\mathcal{J}^a$ and the order parameters $\phi^a (a=1\sim N)$. Such a case will be discussed in appropriate places (see Appendix I for necessary formulas).

(10) One comment about the numerical value. For our perturbative treatment to be reliable numerically, the expansion parameter $g$ has to be small in the first place. Since we are interested only in the stationary point corresponding to $\mathcal{J}=0$, the true requirement for the reliability is, however, that the neglected terms are indeed small at the stationary solution $\phi^{(0)}$. Consider (7·2·3) keeping up to the term with $n=1$. Then $\phi^{(0)}$ will be a complicated function of $g$ depending on the functional form of $h_0[\phi]$ and $h_1[\phi]$. A possible way to judge whether the effect of the term with $n \geq 2$ is really small if $g$ is small is to evaluate the term $n=2$ at $\phi^{(0)}$. If it is small then there is a possibility that the approximation is good. In §7.4, we discuss an example where $g=0$ is the ultraviolet fixed point of the theory and all the higher terms are shown to be small indeed.

(11) In statistical physics, the relation between the two types of free energy $\Omega(\mu, T, V)$ and $F(N, T, V)$ has long been studied. Here $\mu$, $N$, $T$ and $V$ are the chemical potential, number, temperature and the volume respectively. Concerning the perturbative inversion from $\mu$ to $N$, especially the limit $T \to 0$, there is a well-known continuity theorem for the fermionic system.\(^5\)

We want to stress here that in contrast to the inversion between $\mu \leftrightarrow N$, which has nothing to do with the symmetry, the main interest in this article lies in the search for the symmetry breaking solution.

7.2.2. Excited state by inversion method —generalization of on-shell equation—

The procedure of on-shell expansion explained in Chapter II can be applied to inversion method and we get the generalized on-shell equation to determine the excited state. Let us assume that the Hamiltonian contains time-dependent parameters $\mathcal{J}_i(t)$ with $i=1\sim n$; $H(t) = H(\mathcal{J}(t))$. It is convenient to discuss separately the two cases:

(i) **Zero temperature case** Consider the expectation value of a set of operators $\bar{\mathcal{O}}_i$
(i=1~n) at time t:
\[
\phi_i(t) = \langle | \tilde{O}_i(t) \rangle \\
= \frac{\int [d\phi] O_i(\phi(t), \dot{\phi}(t)) \exp \frac{i}{\hbar} \{ \int_{-\infty}^{\infty} dt \ L(\phi(t), \dot{\phi}(t), J(t)) \}}{\int [d\phi] \exp \frac{i}{\hbar} \{ \int_{-\infty}^{\infty} dt \ L(\phi(t), \dot{\phi}(t), J(t)) \}}.
\] (7.2.18)

Here \( \tilde{O}_i(t) \) is the Heisenberg operator and \( | \rangle \) is the ground state in the presence of the source \( J(t) \). We need not bother about the notion of the ground state of the time-dependent Hamiltonian. The probe \( J(t) \) is a temporarily introduced parameter and is set to zero in the end after taking necessary functional derivatives with respect to \( J_i(t) \). Therefore only the ground state for \( J(t)=0 \) comes into the formulas. In (7.2.18) the Lagrangian is assumed to be written by \( \phi \) and \( \dot{\phi} \) and \( \int [d\phi] \) implies the path integrals. Further the operators are expressed as a function of \( \phi \) and \( \dot{\phi} \).

Now \( \phi_i(t) \) is a functional of \( J_i(t) \) and a function of \( t \): \( \phi_i(t) = \phi_i[J, t] \). We invert this relation functionally to get \( J_i(t) = J_i[\phi, t] \). Setting \( J_i(t)=0 \) in this inverted relation, which is the equation of motion of \( \phi \), determines \( \phi_i(t) \). Let us take a static solution \( \phi_i(t) = \phi_i^{(0)} \) and look for a solution of small oscillation around \( \phi_i^{(0)} \) by writing \( \phi_i(t) = \phi_i^{(0)} + \Delta \phi_i(t) \),
\[
0 = J_i[\phi^{(0)} + \Delta \phi_i, t] \\
= -\sum_j \int_{-\infty}^{\infty} dt' \Gamma_i^{(2)}(t - t') \Delta \phi_i(t') ,
\] (7.2.19)
where we have defined
\[
\Gamma_i^{(2)}(t - t') = -\left( \frac{\delta J_i(t)}{\delta \phi_i(t')} \right)_0.
\] (7.2.20)

Here the notation \( (\cdots)_0 \) implies that \( (\cdots) \) is evaluated at \( \phi_i^{(0)} \). Equation (7.2.19) is the on-shell equation for arbitrary source and operator.

In order to see the relation of (7.2.19) to the pole of the Green's function and also to the wave function of the excited state, we use the following identity of the inverse function:
\[
\delta \phi(t - t') = \frac{\delta J_i(t)}{\delta J_i(t')} = \sum \int_{-\infty}^{\infty} dt'' \frac{\delta J_i(t)}{\delta \phi_i(t'')} \frac{\delta \phi_i(t'')}{\delta J_i(t')} \\
= -\sum \int_{-\infty}^{\infty} dt'' \Gamma_i^{(2)}(t - t'') W_i^{(2)}(t'' - t') ,
\] (7.2.21)
where \( W^{(2)} \) is defined as
\[
W_i^{(2)}(t - t') = \left( \frac{\delta \phi_i(t)}{\delta J_i(t')} \right)_0 = \left( \frac{\delta}{\delta J_i(t')} \langle 0 | O_i(t) | 0 \rangle \right)_0 \\
= \langle 0 | T \tilde{O}_i(t) \tilde{X}_i(t') | 0 \rangle.
\] (7.2.22)

Here the time ordered Green's function appears as is seen by the path integral form of (7.2.18) and the operators are in the Heisenberg representation and \( \tilde{X}_i \) is an
operator defined by

\[ \tilde{X}_j(t) = -\frac{i}{\hbar} \frac{\partial \tilde{H}(J(t))}{\partial J_j(t)} . \] (7.2.23)

In Fourier space (7.2.21) is written as

\[ \sum_I \Gamma^{(2)}_I(\omega) W^{(2)}_I(\omega) = -\delta_0 \] (7.2.24)

and \( W^{(2)} \) has the following expression using the complete set of the eigenstates of the Hamiltonian \( H(J=0) \) with eigenvalue \( E_n \),

\[ W^{(2)}_I(\omega) = i \sum_n \frac{\langle 0 | \tilde{O}_I(0) | n \rangle \langle n | \tilde{X}_j(0) | 0 \rangle}{\omega - (E_n - E_0) + i\epsilon} - i \sum_n \frac{\langle 0 | \tilde{X}_j(0) | n \rangle \langle n | \tilde{O}_I(0) | 0 \rangle}{\omega + (E_n - E_0) - i\epsilon} . \] (7.2.25)

Now taking the residue at \( \omega = (E_n - E_0) \), for example, we get from (7.2.24)

\[ \sum_I \Gamma^{(2)}_I(\omega = E_n - E_0) \langle 0 | \tilde{O}_I(0) | n \rangle = 0 . \] (7.2.26)

Remembering (7.2.19) written in Fourier space, we conclude that

\[ \Delta \phi_I(\omega) = \langle 0 | \tilde{O}_I(0) | n \rangle . \] (7.2.27)

**ii) Finite temperature case** For non-zero temperature, we proceed as follows. Let us write the initial density matrix by \( \rho_I \) and for simplicity we take the initial time \( t_I = -\infty \). The general case is discussed in Chapter XII, see also Chapters IX, XIII and XIV. The time evolution kernel \( \tilde{K}_I \) is defined by using time ordering operation as

\[ \tilde{K}_I = \text{Tr} \left\{ \frac{i}{\hbar} \int_{-\infty}^t dt' \tilde{H}(J(t')) \right\} \] (7.2.28)

and we have the expression for \( \phi_I(t) \) and its inverted relation as

\[ \phi_I(t) = \text{Tr} \left\{ \rho_I \tilde{K}_I \tilde{O}_I \tilde{K}_I \right\} \equiv \phi_I[J_I(t), t_I] \rightarrow J_I(t) = J_I[\phi, t] . \] (7.2.29)

The formulas (7.2.19)~(7.2.24) hold except for (7.2.22). \( W^{(2)} \) in this case is the retarded Green's function instead of T-product function,

\[ W^{(2)}_I(t - t') = \theta(t - t') \text{Tr} \left\{ \rho_I[\tilde{O}_I(t), \tilde{X}_j(t')] \right\} . \] (7.2.30)

In Fourier representation \( W^{(2)}_I(\omega) \) is given by (7.2.25) where in the last term of the right-hand side \( -i\epsilon \) is replaced by \( +i\epsilon \). We have of course to replace the ground state expectation value by the trace over \( \rho_I \).

Taking the residue of (7.2.25) at \( \omega = E_n - E_0 \) and comparing the result with (7.2.19), the following identification is obtained (apart from a constant factor)

\[ \Delta \phi_I(\omega) = \text{Tr} \left\{ \rho_I \tilde{O}_I(0) | n \rangle \langle n | \tilde{X}_j \right\} . \] (7.2.31)

The above formula suggests that for each fixed \( j \), the expression given on the right-hand side of (7.2.31) is the eigenvector of the matrix \( \Gamma_I^{(2)}(\omega) \) (where \( \omega = E_n - E_0 \) with zero eigenvalue.
§ 7.3. Some examples

Inversion method is illustrated below using four examples. Three of them are relativistic ones and first two terms of inversion series are studied. The last example is the Ising model where first three terms are included. We discuss specific subjects separately in Chapters IX and X. The general structure of higher-order terms of inverted series will be investigated in detail in Chapter XI.

7.3.1. Contact 2-body interaction

As a first example, let us take $d$-dimensional relativistic fermion system with zero mass. The interaction is assumed to be of contact four-Fermi type and we discuss a solution which breaks the chiral symmetry. We will see in this case that application of the lowest order inversion method reproduces the well-known mean-field results. Below, $d$-dimensional Dirac field $\phi$ is assumed to have $N$-components and the Lagrangian density $L$ takes the form,

$$L = i\bar{\phi}(x) \slashed{D} \phi(x) + \frac{1}{2} g^2 (\bar{\phi}(x) \phi(x))^2 + J \bar{\phi}(x) \phi(x), \quad (7.3.1)$$

where $\gamma$ is the $d$-dimensional $\gamma$ matrix and $g^2$ the coupling strength. For $d=2$ the model is called Gross-Neveu model $^9$ and for $d=4$ Nambu-Jona-Lasinio model.$^7$ We have added the source term with constant $J$ in order to probe the chiral symmetry of the ground state. Order parameter we take as $\phi$ is the expectation value of $\bar{\phi}(x) \phi(x)$.

The first task is to calculate the original series (7.2.2) in the presence of $J$ which is given by two diagrams shown in Fig. 7.1 in the lowest non-trivial approximation. The result of straightforward computation is

$$\phi = \langle \bar{\phi}(x) \phi(x) \rangle_J$$

$$= - DNF(J) - g^2 DNF(DN - 1) F(J) F'(J), \quad (7.3.2)$$

$$F(J) = \int \frac{d^d k}{(2\pi)^d} \frac{J}{k^2 + J^2}, \quad F'(J) = \frac{dF(J)}{dJ}. \quad (7.3.3)$$

We have defined $D=2^{\frac{d}{2}}$ which is the dimension of the $\gamma$ matrix and Wick-rotation has been assumed. The structure of (7.3.2) makes inversion process very simple. The first inversion formula (7.2.4) gives

$$h_0[\phi] = F^{-1}(-\phi/DN). \quad (7.3.4)$$

In the second relation (7.2.5), the factor $F'(J)$ cancels out and we get

\[ \begin{array}{c}
\text{Fig. 7.1. Diagrams leading to (7.3.2).}
\end{array} \]
\[ h_1[\phi] = -g^2(DN-1)F(J = h_0[\phi]), \]  
(7.3.5)

which becomes, after using (7.3.4),

\[ h_1[\phi] = \frac{DN-1}{DN} g^2 \phi. \]  
(7.3.6)

Thus we arrive at

\[ J = F^{-1}(\phi/DN) + \frac{DN-1}{DN} g^2 \phi. \]  
(7.3.7)

For \( J = 0 \), the explicit form of \( F^{-1} \) is not required and the following mean-field type equation is obtained,

\[ -\phi = DNF\left( -\frac{DN-1}{DN} g^2 \phi \right). \]  
(7.3.8)

The function \( F(J) \) is calculated as

\[ F(J) = \begin{cases} \frac{J}{4\pi} \ln\left( \frac{A^2 + J^2}{J^2} \right), & (d=2) \\ \frac{J}{16\pi^2} \left( A^2 - J^2 \ln\left( \frac{A^2 + J^2}{J^2} \right) \right), & (d=4) \end{cases} \]

Here we have introduced the cut off \( A \). The above equations say that the critical coupling \( g_c^2 \) of chiral symmetry breaking is zero for \( d=2 \) and non-zero for \( d=4 \), which is a well-known fact.

### 7.3.2. Schwinger-Dyson equation in the ladder approximation

As a second example, we will show for QED that the Schwinger-Dyson (SD) equation of electron propagator in the ladder approximation is recovered by using the above formalism. The action of QED including the gauge term \((1/2\lambda)(\partial^\mu A_\mu)^2\) is written as

\[ I = \int d^4x d^4y \left[ \bar{\phi}(x)iG_0^{-1}(x,y)\phi(y) + \frac{1}{2} A_\mu(x)iD_0^{-1\mu\nu}(x,y)A_\nu(y) \right] \]  
\[ -e \int d^4x \bar{\phi}(x)A(x)\phi(x), \]  
(7.3.9)

where

\[ iG_0^{-1}(x,y) = (i\partial - m)\delta^4(x-y), \]
\[ iD_0^{-1\mu\nu}(x,y) = -[\Box g^\mu\nu - (1-1/\lambda)\partial^\mu \partial^\nu] \delta^4(x-y). \]

We take electron propagator itself as an order parameter \( \phi \), that is

\[ \phi(x,y) = \langle T\bar{\phi}(x)\phi(y) \rangle = -G(y,x), \]  
(7.3.10)

and \( J(x,y)\bar{\phi}(x)\phi(y) \) as the source term, which is of the form \( J\tilde{\phi} \) in this case. Note that both \( \phi(x,y) \) and \( J(x,y) \) are matrixes in Dirac space. Then the action is changed into the following \( I_\phi \),
\[ I_i = \int d^4x d^4y \left[ \bar{\phi}(x) iG_0^{-1}(x, y) \phi(y) + \frac{1}{2} A_\mu(x) iD_0^{-1} A^\mu(y) \right] \]
\[ - e \int d^4x \bar{\phi}(x) A(x) \phi(x), \quad (7.3.11) \]

where \( G_0^{-1}(x, y) = G_0^{-1}(x, y) - iJ(x, y) \). If we assume translationally invariant case, \( G \) is expressed in momentum space as \( G(p) \). Then, in the approximation up to second order in \( e \), \( G(p) \) is written as follows,
\[ G(p) = G_0'(p) - e^2 G_0'(p) \int \frac{d^4q}{(2\pi)^4} [ \gamma_\mu G_0'(p+q) \gamma_\nu D_0^{\mu\nu}(q) ] G_0'(p), \quad (7.3.12) \]

where \( G \) is a functional of \( J \) as well as a function of momentum \( p \). Regarding \( G \) as order unity, we invert functional \( G \) by the formulas \((7.2.4)\) and \((7.2.5)\). After some calculations, we get
\[ J(p) = iG^{-1}(p) - iG^{-1}(p) - ie^2 \int \frac{d^4q}{(2\pi)^4} \gamma_\mu G(p+q) \gamma_\nu D_0^{\mu\nu}(q). \quad (7.3.13) \]

If we set \( J = 0 \), Eq. (7.3.13) coincides with SD equation in the ladder approximation.

As is well known, the results from the ladder SD equation depend on the gauge parameter \( \lambda \). In the next section, we present a gauge invariant calculation of the order parameter of the chiral symmetry breaking using the inversion technique.

### 7.3.3. Gauge invariant study of strong coupling phase of massless QED

Recently much attention has been paid to the possibility of the phase in massless (i.e., zero electron mass) QED especially in relation to the technicolor theory\(^8\) and to GSI anomalous \( e^+e^- \) event in heavy ion collision.\(^9\) In this phase, the chiral symmetry of the original massless QED Lagrangian is spontaneously broken and the mass of the electron is dynamically generated. These conclusions are obtained by approaches which are mainly based on the ladder SD equation\(^{10,11}\) and on the numerical studies of the lattice QED.\(^{12}\)

If one wants to study continuum QED, there arise several difficult problems: the results depend on the gauge we choose since the approximation scheme depends on the gauge. For covariant gauge expressed by \( (1/2\lambda)(\partial_\mu A^\mu)^2 \), the outcome of the ladder SD equation is dependent on the gauge parameter \( \lambda \). However, inversion method makes it possible to study the problem in a gauge invariant way.

Now we take as an operator for investigating the strong coupling phase the local operator \( \bar{\phi}(x) = \bar{\phi}(x) \phi(x) \).\(^2\) This is of course gauge invariant and we adopt the source term as \( J \bar{\phi}(x) = J \bar{\phi}(x) \phi(x) \). We want now to calculate \( \phi(J) = \langle \phi \rangle \) with the action \( S + i \int d^4x J \bar{\phi}(x) \phi(x) \). This choice makes things simpler than the conventional SD approach since we have only to handle single (i.e., local) gauge invariant constant order parameter instead of the non-local gauge non-invariant function (i.e., propagator).

Fig. 7.2. Diagrams leading to (7.3.14).
Note that the diagrammatical rule of the effective action or the potential has not been known for the local bilinear operator as $\hat{\phi}$. (See, however, Chapter XI for general rule.) The advantage of inversion method is that the perturbation calculation is straightforward even in such a case, which proceeds as follows. The diagrams to be calculated are shown in Fig. 7.2.

Using Pauli-Villars auxiliary field method, we get, up to order $a$ (fine structure constant),

$$\phi(J) = J\Lambda^2 \frac{1}{4\pi^2} + J\Lambda^2 \frac{3a}{8\pi^4} \left[ 1 - \frac{J^2}{\Lambda^2} \left( \ln \left( \frac{J^2}{\Lambda^2} \right) \right)^2 \right] + O(a^3 \ln(J^2)),$$

(7.3.14)

where $\Lambda$ is the momentum cut-off which is taken to be equal for electron and photon for simplicity. We have also assumed $J$ to be a small quantity since $J$ is set to zero in the end. The result (7.3.14) is indeed gauge invariant.

Now, by using inversion formulas (7.2.4) and (7.2.5), we get up to order $a$ again,

$$J(\phi) = \frac{(2\pi)^2}{\Lambda^2} \phi \left( 1 + \frac{a}{\alpha_c} \frac{(2\pi)^4}{\Lambda^8} \phi^4 \left[ \ln \left( \frac{(2\pi)^4}{\Lambda^4} \phi^2 \right) \right]^2 + O(\phi^3 \ln(\phi^2)) \right).$$

(7.3.15)

In this equation, the notation $\alpha_c = 2\pi/3$ is used. Putting $J=0$ in (7.3.15), we find that the sign of the first term determines the phase in the same way as in the Landau theory of phase transition: the temperature dependent term proportional to $-(1 - T/T_c)\phi^2$ appearing in the Landau free energy is replaced here by $(1 - a/\alpha_c)\phi^2$. Note here that, since we have chosen the form $J\hat{\phi}$ as a source term, the relation $J(\phi) = dV(\phi)/d\phi$ holds, where $V(\phi)$ is the usual effective potential of $\phi$. See (7.2.12) or (A.5) of Appendix A. By integrating (7.3.15) over $\phi$ we get

$$V(\phi) = \frac{(2\pi^2}{\Lambda^2} (1 - a/\alpha_c)\phi^2 + \frac{a}{\alpha_c} \frac{16\pi^6}{\Lambda^8} \phi^4 \left[ \ln \left( \frac{(2\pi)^4}{\Lambda^4} \phi^2 \right) \right]^2 + O(\phi^3 \ln(\phi^2)) \right).$$

(7.3.16)

It is seen that for $a > \alpha_c$ the chiral symmetry breaking solution is realized. In this phase, if $|1 - a/\alpha_c|$ is small enough, a nontrivial solution of $J=0$ is consistently obtained from (7.3.15) by neglecting the terms of $O(\phi^3 \ln(\phi^2))$. So we conclude that the symmetry breakdown occurs and the value of the critical coupling constant is $\alpha_c$. The solution $\phi$ behaves near $a=\alpha_c$ as

$$|\phi| \approx -\frac{\Lambda^8}{(2\pi)^2} \frac{(1 - \alpha_c/a)^{1/2}/2}{\ln((1 - \alpha_c/a)^{1/2}/2)}.$$  

(7.3.17)

Apart from logarithm, this is the mean-field type behavior. For more details of the calculation, see Ref. 2).

Similar result has been obtained in Refs. 14) and 15) by solving non-local SD equation which takes into account higher-order corrections to vacuum polarization. Here we notice that $\alpha_c = 2\pi/3$ and this is twice as large as the well known result ($\alpha_c = \pi/3$) given by the Landau gauge ladder SD equation.

Recently Kondo has extended above gauge invariant inversion formalism to more general models such as gauged Nambu-Jona-Lasinio type.

The higher orders of inversion series of this problem will be discussed in Chapter XI in a diagrammatical language.
7.3.4. Ising model by inversion method

As a last example of this section, we take Ising model and illustrate the calculation of first three terms of the inversion series. See § 11.7 for higher orders. It is clear from the discussions presented up to now, especially from Chapter VI, that our method is equivalent to summing up infinite number of sub-diagrams which can be written as an order parameter itself. Sometimes this process is called the renormalization of vertices because the process amounts to replacing the bare vertex by its full order expression. Indeed in Ref. 17) the results of De Dominicis-Martin were extended to Ising system following the idea of renormalization. The aim of the discussions below is the same as Ref. 17) but the procedure is simpler and more straightforward since we can perform calculations without knowing the complicated graphical results of renormalization. The inversion process applied to equilibrium system leads us to, as has been stated in § 7.1, Helmholtz free energy or the equation of state, which has been studied for the Ising system by Ref. 19), in combination with the scale invariance.

We start from the following Hamiltonian $\mathcal{H}$,

$$-\beta \mathcal{H} = K \sum_{\langle ij \rangle} S_i S_j + H \sum_i S_i. \quad (7.3.18)$$

Here, $\beta = 1/T$, $K \equiv \beta J$ is the strength of the exchange interaction between the nearest-neighbor sites. $H$ denotes (non-dimensional) magnetic field, which plays the role of external probe in our inversion method formalism. $S_i$ takes two values, $S_i = \pm 1$, and its mean value $\phi = \langle S_i \rangle = m$ is taken as the order parameter. Here the artificial probe $J$, which is transformed away by the Legendre transformation, is not necessary. Such a probe appears in combination $H + J$, therefore $H$ plays the necessary role. By a straightforward application of linked-cluster expansion, we get a perturbative series of $m$ with respect to coupling $K$:

$$m = M_1 + K q M_1 M_2 + K^2 \left[ \frac{q}{2} M_2 M_3 + \frac{q^2}{2} (2M_1 M_2^2 + M_1 M_3 M_2) \right]$$

$$+ K^3 \left[ 3P(\Delta) M_2 M_3 M_4 + \frac{q}{6} M_3 M_4 + \frac{q^2}{2} (M_2^2 M_4 + M_1 M_3 M_4 + M_1 M_2 M_4) \right.$$  

$$+ \frac{q^3}{6} (9M_1^2 M_2 M_3 + M_3^2 M_4 + 6M_1 M_3^2) \right] + O(K^4). \quad (7.3.19)$$

Here $q$ is the number of nearest-neighbor of each site and $P(\Delta)$ is a constant, which depends on the shape of the lattice. For the close-packed lattice, it has nonzero value: $P(\Delta) = 2$ for two-dimensional triangular lattice and $P(\Delta) = 8$ for face-centered cubic, otherwise it vanished. $M_n$ is a function of $H$, defined as

$$M_0 = \ln(2 \cosh H), \quad M_n = \frac{d^n M_0}{dH^n}. (n \geq 1) \quad (7.3.20)$$

Each term on the right-hand side of (7.3.19) has an obvious origin. A way to see how it comes about is to take magnetic field which has an independent value at each lattice point and change $H \sum_i S_i$ into $\sum_i H_i S_i$. All the terms of perturbation in $K$ are
obtained by appropriate differentiation with respect \( H_i \) of the function \( \ln(2\cosh H_i) \).

Inversion process is very simple because \( M_2 = (dM_1/dH) \) so that the original series has the same structure as (7·3·2) up to first order. After some straightforward calculations by using inversion formula we get

\[
H = M_1^{-1}(m) - K q M_1 - \frac{1}{2} K^2 q M_3 - \frac{1}{6} K^3 \left[ 18 P(\Delta) M_2 M_3 + q \frac{M_4 M_4}{M_2} \right] + O(K^4),
\]

(7·3·21)

where \( M_1^{-1}(m) \) denotes the inverse function of \( M_1(H) = \tanh H \) and \( M_n \)'s are evaluated at \( H = M_1^{-1}(m) \). Here, in addition to the formulas (7·2·4)~(7·2·6), the third-order formula of the inversion

\[
h_3(\phi) = - \left[ f_3(h_0(\phi)) + f_2(h_0(\phi)) h_1(\phi) + \frac{1}{2} f_1''(h_0(\phi)) h_1^2(\phi) 
+ f_1'(h_0(\phi)) h_2(\phi) + \frac{1}{3!} f_1''(h_0(\phi)) h_1^3(\phi) 
+ f_0''(h_0(\phi)) h_1(\phi) h_2(\phi) \right] / f_0'(h_0(\phi))
\]

(7·3·22)

has been used. By using the definition (7·3·20), it is easily found that every \( M_{n \geq 2} \) is written as a polynomial of \( m \). Equation (7·3·21) is thus calculated as

\[
H = \arctanh m - K q m + K^2 q m (1 - m^2) + \frac{2}{3} K^3 [9 P(\Delta) m (1 - m^2)^2 - q m (1 - m^2) (1 - 3m^2)] + O(K^4).
\]

(7·3·23)

Here we note that the terms including \( q^2 \) or \( q^3 \) vanish in (7·3·21) or (7·3·23). These terms describe the effect from the next-nearest-neighbor \( (q^2) \) or the third-nearest-neighbor sites \( (q^3) \) in (7·3·19). Equation (7·3·21) or (7·3·23) tells us that these effects are included, or renormalized, into a local interaction between the nearest neighbors in the process of inversion. The exceptional term including \( P(\Delta) \) in the third order term does not vanish; it remains unrenormalized. This is because it corresponds to a triangle graph in the linked-cluster expansion, so that it cannot be absorbed into the nearest-neighbor interaction. As is known from the conventional high temperature expansion scheme, this term brings us a crucial difference between the close-packed lattice and the loose-packed one. Apart from the first term \( \arctanh m \), all the higher terms can be shown to be polynomials in \( m \). Now we obtain a series of approximation for \( m \) by taking into account higher-order terms successively:

(i) \( m = \tanh(H + K q m) \),

(ii) \( m = \tanh(H + K q m - K^2 q m (1 - m^2)) \),

(iii) \( m = \tanh \left( H + K q m - K^2 q m (1 - m^2) - \frac{2}{3} K^3 [9 P(\Delta) m (1 - m^2)^2 - q m (1 - m^2) (1 - 3m^2)] \right) \).
The first approximation (i) is nothing but an expression given by the mean-field theory. The cases (ii) and (iii) include the corrections to the mean-field approximation (i). We expect that inversion method will improve the mean-field approximation as we proceed to higher order. It is clear that our series is a canonical one defined in Ref. 21).

The numerical study based on the above results combined with the coherent anomaly method (CAM)\textsuperscript{21} has been performed by Ukita.\textsuperscript{20}

§ 7.4. Improvement by renormalization group: case of QCD

7.4.1. Callan-Symanzik equation

In Ref. 20), the inverted series of Ising model was combined with scaling form to get an approximate expression which is better than the original one near the critical point. Another way of improving our series is discussed here taking a scale invariant relativistic field theory. It utilizes Callan-Symanzik type differential equation. The use of renormalization group for the improvement of perturbative series has long been known, especially for the case of vacuum polarization in QED.\textsuperscript{22} The application of renormalization group to effective action or potential was studied by many authors and especially its perturbative structure was studied in Refs. 23)\textemdash 25). Here we discuss the problem in connection with inversion method\textsuperscript{23} and the special attention is paid to the stationary solution corresponding to vanishing source.

An attempt at improving inversion series is illustrated by taking a relativistic field theory which does not contain any dimensional parameter. To be more specific, we discuss massless Quantum Chromodynamics (QCD) where all the quarks are assumed to be massless. Thereby we will see an important connection between the sign of anomalous dimension and the condensation. The order parameter we take is the chiral symmetry breaking operator \( \bar{\phi}(x)\psi(x) \) where \( \phi(x) \) denotes the quark field operator, and for that purpose the source term \( J\bar{\phi}(x)\phi(x) \) is added to the Lagrangian density of QCD. In the following all the renormalization programs are assumed to have been finished including that of \( J \). Note that \( J \) can be renormalized by \( Z_m \) corresponding to mass renormalization factor through replacing the mass parameter \( m \) by \( J \). Therefore any quantities that appear below are the renormalized ones. We denote by \( \mu \) the renormalization point assuming that we have fixed the renormalization scheme.

Let us introduce

\[
\phi = \langle \bar{\phi}(x)\phi(x) \rangle, \tag{7.4.1}
\]

and look at the inverted series (7.2.3). Since QCD is (believed to be) one-phase theory, \( \phi \) is non-zero for arbitrarily small coupling constant \( g \) and its behavior near \( g=0 \) is given as

\[
\phi^{1/3} \sim \mu \exp\left(\frac{1}{2\beta_0 g^2}\right), \tag{7.4.2}
\]

where we have used the fact that \( \phi \) has mass dimension 3 and \( \beta_0<0 \) is related to \( \beta \)
function as
\[ \mu \frac{dg}{d\mu} = \beta(g) = b_0 g^0 + b_1 g^0 + \cdots. \]  
\[ (7.4.3) \]

Instead of \( \phi \) we use the variable
\[ t = g^2 \ln \left( \frac{\phi^{1/3}}{\mu} \right), \]
\[ (7.4.4) \]

which is order unity near the expected solution (7.4.2). Our new inverted series is now,
\[ J = \phi^{1/3} f(t, g) = \phi^{1/3} \sum_{n=0}^{\infty} (g^2)^n f_n(t). \]  
\[ (7.4.5) \]

We have employed the fact that for QCD the perturbation series is that of \( g^2 \). Our task is thus to find the solution to \( J = 0 \) other than \( \phi = 0 \), that is, to look for the solution to \( f(t, g) = 0 \).

The function \( f_n \) for finite \( n \) is calculable from finite terms of original series. Now we know that the correct non-perturbative solution has the expansion,
\[ t = \frac{1}{2b_0} - \frac{1}{2b_0} \left( \frac{\gamma_1}{3} + \frac{b_1}{b_0} \right) g^2 \ln g^2 + d_0 g^2 + d_1 (g^2)^2 + \cdots. \]
\[ (7.4.6) \]

Here the anomalous dimension of \( \bar{\psi}(x) \psi(x) \) has been denoted by \( \gamma(g) \) which is defined as
\[ \mu \frac{d\phi}{d\mu} = \gamma(g) \phi, \]  
\[ (7.4.7) \]

\[ \mu \frac{dJ}{d\mu} = -\gamma(g) J, \]  
\[ (7.4.8) \]

\[ \gamma(g) = \gamma_0 g^2 + \gamma_2 g^4 + \cdots. \]  
\[ (7.4.9) \]

In (7.4.6), the coefficients \( d_0 \) and \( d_1 \) are some numerical constants. In actual calculation we truncate (7.4.5) so that we have to see how good or bad our approximation is compared with the exact form (7.4.6).

The function \( f_n(t) \) is largely determined by the renormalization group equation. In order to simplify the arguments, we take Landau gauge and write down (7.4.8) in terms of \( f_n(t) \). For this purpose let us apply \( \mu d/d\mu \) on both sides of (7.4.5). Since we are finally interested in the case \( J = 0 \), we get
\[ \mu \frac{d}{d\mu} \left[ \phi^{1/3} \sum_{n=0}^{\infty} (g^2)^n f_n(t) \right] = 0. \]
\[ (7.4.10) \]

The above equation can be cast into a differential equation by noting that
\[ \mu \frac{dt}{d\mu} = \left( \frac{1}{3} \gamma(g) - 1 \right) g^2 + 2 \frac{\beta(g)}{g} t. \]  
\[ (7.4.11) \]

Equation (7.4.10) is arranged according to the power of \( g^2 \) and the lowest equation arises from \( g^2 \) term,
\[(2b_{0}t-1)f_{0}(t)+\frac{\gamma_{1}}{3}f_{0}(t)=0 . \quad (f_{0}(t)=\frac{df_{0}(t)}{dt}) \quad (7.4.12)\]

The solution is
\[f_{0}(t)=C\left(t-\frac{1}{2b_{0}}\right)^{\eta}, \quad \eta=-\frac{\gamma_{1}}{6b_{0}}. \quad (7.4.13)\]

where \(C\) is an integration constant. The solution to \(J=0\) of (7.4.5) other than trivial one, \(\phi=0\), is given by \(f_{0}(t)=0\). We conclude that non-trivial solution \(\phi=1/2b_{0}\) exists provided \(\eta>0\), i.e., \(\gamma_{1}>0\), which is assumed to be the case in the following.

There is a theorem about the physical meaning of \(\gamma_{1}>0:\)²³

**Theorem** Following correspondence exists:
\[\gamma_{1}>0(<0) \leftrightarrow \text{attractive (repulsive) force in corresponding channel}. \quad (7.4.14)\]

The above theorem shows that the positiveness of \(\gamma_{1}\) for the operator \(\bar{\phi}(x)\phi(x)\) is a consequence of the attractive force between quark-antiquark pair in color singlet channel. See Ref. 23 for details.

Higher terms \(f_{n}\) with \(n>0\) are most conveniently discussed by defining
\[\bar{f}(t, g)=K(g)^{-1}f(t, g)^{1/3}, \quad (7.4.15)\]

\[K(g)^{-1}\equiv\lim_{g_{0}\to0}g_{0}^{-2}\exp\left\{\frac{g}{3}\int_{g_{0}}^{g}dx'\gamma(x')\right\}\]
\[=g^{2}\left\{1+\left(\frac{\gamma_{2}}{\gamma_{1}}\frac{b_{1}}{b_{0}}\right)g^{2}+\cdots\right\}. \quad (7.4.16)\]

Then, at \(J=0\), \(\bar{f}(t)\) satisfies
\[\left\{\mu\frac{\partial}{\partial \mu}+\bar{\beta}(g)\frac{\partial}{\partial g}\right\}\bar{f}(\mu, g, \phi)=0 , \quad (7.4.17)\]

\[\bar{\beta}(g)=\frac{\beta(g)}{1-\gamma(g)}b_{0}g^{3}+\bar{b}_{1}g^{6}+\cdots, \quad (7.4.17)\]

\[\bar{b}_{1}=b_{1}+\frac{\gamma_{1}b_{0}}{3}. \quad (7.4.17)\]

In (7.4.17), \(\bar{f}\) is regarded as a function of \(\mu, g\) and \(\phi\) and the derivative \(\partial/\partial \mu\) or \(\partial/\partial g\) is taken with fixed \(\phi\). Now \(\bar{f}(t, g)\) is expanded as
\[\bar{f}(t, g)=g^{-2}W_{1}(t)+W_{0}(t)+g^{2}W_{1}(t)+\cdots. \quad (7.4.18)\]

In the definition of \(K(g)\), \(g_{0}^{-2}\) can be a finite quantity but the limit \(g_{0}\to0\) has been taken for convenience. For finite \(g_{0}^{-2}\) the arguments below should be modified slightly. A hierarchy of equations for \(W_{n}(t)\) is obtained as
\[(1-2b_{0}t)W_{1}(t)+2b_{0}W_{0}(t)=0, \quad (7.4.19)\]
\[(1-2b_{0}t)W_{0}(t)+2\bar{b}_{1}(1-2b_{0}t)W_{-1}(t)=0, \quad (7.4.19)\]
and so forth. Therefore the solution up to $W_0$ is given by

$$\bar{f}(t, g) = C^{-1}_{-1} \left( t - \frac{1}{2b_0} \right) - \frac{C^{-1}_{-1} \tilde{b}_1}{2b_0^2} \ln(1 - 2b_0t) + C_0, \quad (7.4.20)$$

where $C_{-1}$ and $C_0$ are integration constants. These are calculable in the sense that they are determined by the original series which is obtained through digrams.

The solution to $\bar{f}(t, g) = 0$ is illustrated in Fig. 7.3 where we have assumed $C_{-1} > 0$ without loss of generality. In Fig. 7.3, the line (a) represents the first term on the right-hand side of (7.4.20) and line (b) is the sum of the first and second terms. We see that the lowest order solution $t = 1/2b_0$ at $A$ in the figure is shifted slightly to $B$ and it behaves for small coupling as

$$t = \frac{1}{2b_0} - \frac{\tilde{b}_1}{2b_0^2} g^2 \ln g^{-2} + O(g^2 \ln g^{-2}). \quad (7.4.21)$$

It corresponds to

$$g^{2\pi \phi^{1/3}} \sim \mu \exp \left\{ \frac{1}{2b_0g^2} - \frac{b_1}{2b_0^2} \ln g^{-2} \right\}. \quad (7.4.22)$$

Equation (7.4.21) agrees with (7.4.6) up to second order and we expect that if higher-order terms are included the solution approaches the exact expression (7.4.6).

**Higher orders:** Let us assume that

$$\frac{\beta}{1 - \gamma^3} = b_0 g^3 + \tilde{b}_1 g^5. \quad (7.4.23)$$

This is always possible by the redefinition of renormalized coupling constant, $g \to g'$ $= g + a_1 g^3 + a_2 g^5 + \cdots$. In this case we get for $l \geq -1$,

$$(1 - 2b_0t) W_l - 2b_0 t W_{l-2} \tilde{b}_1 [t W_{l-1} + (l-1) W_{l-1}] = 0 \quad (7.4.24)$$

with $W_{-2} = 0$. In order to see that $g^2 \ln g^{-2}$ term in (7.4.21) is cancelled by higher-
order terms, the leading singularity of $W_i$ (with $l > 0$) near $s \equiv 1 - 2b_0t \approx 0$ is summed up. From (7.4.24) we get near $s = 0$,

$$\frac{dW_i}{ds} + 2W_i \approx \frac{\bar{b}_1}{b_0} \frac{dW_{i-1}}{ds}. \quad (7.4.25)$$

The solution behaves like

$$W_i \approx C \left( -\frac{\bar{b}_1}{b_0} \ln s \right)^i, \quad (7.4.26)$$

where the constant $C$ can be calculated explicitly to be $C = -(\bar{b}_1/b_0)$. Then we get

$$\sum_{l=0}^{\infty} g^{2l} W_l = \frac{\bar{b}_1}{b_0} \ln \left( s + g^2 \frac{\bar{b}_1}{b_0} \ln s \right). \quad (7.4.27)$$

The zero of the sum of this expression and $W_{-1}/g^2$ behaves as (7.4.21) but the term $g^2 \ln \ln g^{-2}$ is now replaced by $g^2 \ln \ln \ln g^{-2}$. The process can be continued until we get the exact expression (7.4.6) and it shows how our result approaches the exact formula. However there is a way\(^{24}\) to achieve full invariance under the renormalization group transformation, as will be seen in the next subsection.

### 7.4.2. Scale invariant formula

Let us define $M(s, e^2)$ by\(^{24}\)

$$M(s, e^2) = -\frac{2b_0^2}{\bar{b}_1} \sum_{l=0}^{\infty} (g^2)^l W_l, \quad (7.4.28)$$

where $e^2 = (\bar{b}_1/b_0)g^2$. By multiplying $(g^2)^l$ to (7.4.24) and summing over $l(l \geq -1)$, $M$ is seen to satisfy

$$\left\{ (1 + e^2)s - e^2 \frac{\partial}{\partial s} + (1 + e^2)e^2 \frac{\partial}{\partial e^2} \right\} M(s, e^2) = 1. \quad (7.4.29)$$

We collect the terms of the form $(\ln s)^m/s^l$, $1 \leq m \leq l$ appearing in $W_i$. By explicitly writing down the perturbative solution, it is easily seen that this can be accomplished by looking for the solution of (7.4.29) with the factor $(1 + e^2)$ replaced by unity. The neglected terms contribute $(\ln s)^m/s^{l-n}(1 \leq n \leq l, 1 \leq m \leq l - n)$ for $W_i$. These terms make no contribution to the solution to $\bar{f} = 0$ in the limit $g \to 0$. Now we solve

$$\left[ (s - e^2) \frac{\partial}{\partial s} + e^2 \frac{\partial}{\partial e^2} \right] M(s, e^2) = 1 \quad (7.4.30)$$

with the solution given by an implicit form

$$M = \ln(s + e^2 M). \quad (7.4.31)$$

The lowest solution $M = \ln s$ and the second iterative solution $M = \ln(s + e^2 \ln s)$ reproduce the previous results of $(g^2)^n \varphi^{1/3}$, given in (7.4.22). There is a freedom of adding the solution of the homogeneous equation. These involve integration constants which are fixed by explicit calculation of diagrams, $C_{-1}/C_0$ appearing in (7.4.20) for example. For small $g$, the solution $M + (C_0/C_{-1})$ is sufficient for our purpose where $M$
satisfies \((7.4 \cdot 31)\).

Now our non-perturbative solution is given by solving simultaneously \((7.4 \cdot 31)\) and

\[
\frac{s}{g} + \left( \frac{\beta_1}{b_0} \right) M + C = 0 ,
\]

\[(7.4 \cdot 32)\]

where \(C = -2 b_0 C_0 / C_1\). Equations \((7.4 \cdot 31)\) and \((7.4 \cdot 32)\) can be solved algebraically and we get \(M = \ln(-g^2 C)\), which leads to the following solution for \(\phi^{1/3}\):

\[
\phi^{1/3} = \mu \exp\left[ \frac{1}{2 b_0 g^2} + \frac{C}{2 b_0} + \frac{\beta_1}{2 b_0} \ln(-g^2 C) \right].
\]

\[(7.4 \cdot 33)\]

Now the parameter \(\mu\) is eliminated using the usual \(\Lambda_{\text{QCD}}\) defined by

\[
\Lambda_{\text{QCD}} = \mu \exp\left[ \frac{1}{2 b_0 g^2} + \frac{b_1}{2 b_0} \ln\left( \frac{b_0 g^2}{1 + \frac{b_1 g^2}{b_0}} \right) \right].
\]

\[(7.4 \cdot 34)\]

This is the expression obtained by assuming \(\beta(g) = b_0 g^2 + b_1 g^5\) which is sufficient since we are working in the region of small \(g\). In this way the final scale invariant formula is obtained by taking the limit \(g \to 0\),

\[
\left( \frac{g^2}{4 \pi} \right)^\gamma \phi^{1/3} = D \Lambda_{\text{QCD}},
\]

\[
D = \exp\left[ \frac{C}{2 b_0} + \frac{b_1}{2 b_0} \ln\left( \frac{C}{b_0} \right) + \frac{\gamma_1}{6 b_0} \ln(-4 \pi C) \right]
\]

\[
= \exp\left[ \frac{C}{2 b_0} + \frac{\beta_1}{2 b_0} \ln\left( \frac{C}{b_0} \right) + \frac{\gamma_1}{6 b_0} \ln(-4 \pi b_0) \right] .
\]

\[(7.4 \cdot 35)\]

The above two expressions for \(D\) are equivalent. Since the relation we have obtained is the one among scale invariant quantities, we are justified to take the limit \(g \to 0\) or \(\mu \to \infty\) because they can be evaluated for any \(g\) or \(\mu\). Thus, for example, assumed form of \(\beta(g)\) can be used without the redefinition of the coupling constant. Besides the requirement \(\gamma_1 > 0\), the above formulas imply that the real valued non-perturbative solution exists as long as \(C < 0\), which can be shown to be the case (for several physically interesting order parameters \(\phi\)) in the theory of QCD. For details see Ref. 24).

Although we have discussed a specific theory, QCD, the above consideration may cast some hint for other theories.

References

12) J. B. Komut, Rev. Mod. Phys. 51 (1979), 659.
13) See, for example, the textbook by, C. Itzykson and J. B. Zuber, Quantum Field Theory (McGraw-Hill, New York, 1980).
Chapter VIII. Atomic System

The purpose of this chapter is to apply the formalism developed so far to atomic system. Because of the simple structure of the ground state of non-relativistic system, formulas are simpler than those of relativistic case. We can write down various types of wave equations as our on-shell equations all of which are equivalent to the Schrödinger equation. These are obtained by different choices of source term added as a probe to Hamiltonian of the system.

After deriving the multi-time Schrödinger equation for $N$-electron atom, the reduction to the ordinary Schrödinger equation is studied. Then the method of the Legendre transformation is applied to the density functional theory. In fact we will see that rewriting the theory in terms of density is quite transparently done by the use of the Legendre transformation. As another application of the Legendre transformation, an atomic wave equation that determines ionization (affinity) energy as an eigenvalue is also derived.

A novel picture of scattering process among bound states is finally discussed as higher-order terms of on-shell expansion.

§ 8.1. Multi-time Schrödinger equation

We examine below various types of equations to determine the atomic energy levels. Here our on-shell condition itself is the desired equation and we apply it within a purely non-relativistic framework. In this section a generalized form of Schrödinger equation for $N$ electrons which contains multiple time variables is derived by the technique developed so far. In order to handle with the electron system, we need the Legendre transformation by Grassmann numbers. This has been discussed in § 2.5. In the following, the expectation value of electron field operator $\hat{\phi}$ or $\hat{\phi}^\dagger$ is denoted as $\langle \phi \rangle \equiv \langle \hat{\phi} \rangle$, or $\langle \phi^\dagger \rangle \equiv \langle \hat{\phi}^\dagger \rangle$ respectively.

We start from the Hamiltonian $\hat{H}$ in Heisenberg representation for interacting electrons,

$$\hat{H} = \int d^3x \hat{\phi}^\dagger(t, x) \left(-\frac{\nabla^2}{2m} - v(x)\right) \hat{\phi}(t, x)$$

$$+ \frac{1}{2} \int d^3x d^3y \hat{\phi}^\dagger(t, x) \hat{\phi}^\dagger(t, y) V(x-y) \hat{\phi}(t, y) \hat{\phi}(t, x), \quad (8\cdot1\cdot1)$$

$$[\hat{\phi}^\dagger(t, x), \hat{\phi}(t, y)]_+ = \delta^3(x-y), \quad \text{(others are zero)} \quad (8\cdot1\cdot2)$$

where $[ , ]_+$ denotes anti-commutator, $v(x) = Ze^2/|x|$ is the nuclear potential energy, and $V(x-y) = e^2/|x-y|$ represents the interaction between two electrons. In this section the spin index is neglected for simplicity which is easily recovered.

The conjugate momentum $\Pi$ is defined by the relation,

$$[\hat{H}(t, x), \hat{\phi}(t, y)]_+ = -i\delta^3(x-y). \quad (8\cdot1\cdot3)$$
From (8.1.2), $\bar{H}$ is seen to be given by

$$\bar{H}(t, x) = -i\hat{\phi}^\dagger(t, x).$$  \hfill (8.1.4)

Then the Hamiltonian (8.1.1) is written by $\hat{\phi}$ and $\bar{H}$ and the Lagrangian $\bar{L}$ is defined as

$$\bar{L} = \int d^3x \partial_t \hat{\phi}(t, x) \cdot \bar{H}(t, x) - \bar{H}. \quad \left( \partial_t \phi(t, x) = \frac{\partial \phi(t, x)}{\partial t} \right)$$  \hfill (8.1.5)

We see that $\bar{H}$ introduced in (8.1.4) satisfies the well-known relation,

$$\bar{H}(t, x) \equiv \frac{\delta \bar{L}}{\delta \partial_t \hat{\phi}(t, x)}.$$  \hfill (8.1.6)

The action $\bar{I} = \int dt \bar{L}$ of the model is thus written as follows,

$$\bar{I} = \int d^4x d^4y \left\{ \hat{\phi}^\dagger(x) iS_0^{-1}(x, y) \hat{\phi}(y) - \frac{1}{2} \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(y) V(x-y) \delta(t_x - t_y) \hat{\phi}(y) \hat{\phi}(x) \right\},$$  \hfill (8.1.7)

$$iS_0^{-1}(x, y) = \left( i\partial_0 + \frac{p_x^2}{2m} + v(x) \right) \delta^4(x-y).$$  \hfill (8.1.8)

8.1.1. **Hydrogen atom**

Let us study one-electron channel of (8.1.7). For this purpose, external sources are required for $\hat{\phi}$- and $\hat{\phi}^\dagger$-channel. We add the term

$$\int d^4x \left( J_\phi(x) \hat{\phi}(x) + J_{\phi^\dagger}(x) \hat{\phi}^\dagger(x) \right) \equiv J_a \Psi_a$$

to $I$. Once the action $I$ is fixed it is straightforward to introduce $W[J]$ of (2.5.1). After the Legendre transformation, effective action (2.5.3) in this case is obtained,

$$\Gamma[\phi, \phi^\dagger] = \int d^4x d^4y \phi^\dagger(x) iS_0^{-1}(x, y) \phi(y) - i\kappa^{(1)}. \hfill (8.1.9)$$

Here $\kappa^{(1)}$ represents the sum of all 1-particle irreducible vacuum graphs\(^\text{6}\) (see Appendix C). By using the vacuum solutions corresponding to $J_a = 0$ of (2.5.7) which evidently satisfy $\phi^{(0)} = \phi^{\star(0)} = 0$, the on-shell condition (2.5.16a) for $\Delta \phi^{(1)}$ becomes

$$\int d^4y \left( S_0^{-1}(x, y) + \left[ \frac{\tilde{\phi}^2 \kappa^{(1)}}{\delta \phi^\dagger(x) \delta \phi(y)} \right]_0 \right) \Delta \phi(y)^{\text{(1)}} = 0.$$  \hfill (8.1.10)

We note in passing that, when we consider the ground state $|0\rangle$ or the vacuum state defined as $\hat{\phi}(x)|0\rangle = 0$ (no Fermi sea exists), many of the diagrams in $\kappa^{(1)}$ do not contribute to the result.\(^\text{6}\) This is because the situation does not allow anti-particles. The electron propagator $\langle 0 | T \hat{\phi}(x) \hat{\phi}^\dagger(y) | 0 \rangle$, which is graphically represented by a line with an arrow, is proportional to $\theta(t_x - t_y)$ when $J = 0$. So the diagrams including the propagators in opposite (time) directions vanish. Also the electron loops become equal to zero by the normal ordered form of (8.1.1). These properties drastically simplify the problem without approximations. In fact, one finds that the electron self-energy is not present, that is $[\tilde{\phi}^2 \kappa^{(1)} / (\delta \phi^\dagger \delta \phi)]_0 = 0$ in (8.1.10). The on-shell condit-
tion now trivially coincides with the Schrödinger equation under the external potential,
\[
\left( i\partial_0 + \frac{\mathbf{p}^2}{2m} + v(x) \right) \Delta \phi(x) = 0.
\] (8.1.11)

Here we remark again that the result comes from the second derivative of \( \Gamma \), while the equation determining the expectation value of the field \( \phi \) is given by the first derivative of \( \Gamma \).

Let us look into the problem from a different point of view — the energy level is examined through electron-nucleon composite channel. Thereby the recoil effect of the nucleon can automatically be taken into account. The starting Hamiltonian \( \hat{H} \) is given by
\[
\hat{H} \equiv \int d^3x \tilde{\phi}^\dagger(t, x) \left( -\frac{\mathbf{p}^2}{2m} \right) \tilde{\phi}(t, x) + \int d^3x \tilde{\phi}_N^\dagger(t, x) \left( -\frac{\mathbf{p}^2}{2m_N} \right) \tilde{\phi}_N(t, x)
+ \frac{1}{2} \int d^3x d^3y \tilde{\phi}_c^\dagger(t, x) \tilde{\phi}_c^\dagger(t, y) V_{ee}(x - y) \tilde{\phi}(t, y) \tilde{\phi}(t, x)
+ \int d^3x d^3y \tilde{\phi}_c^\dagger(t, x) \tilde{\phi}_c(t, y) V_{en}(x - y) \tilde{\phi}_e(t, y) \tilde{\phi}(t, x)
+ \frac{1}{2} \int d^3x d^3y \tilde{\phi}_N^\dagger(t, x) \tilde{\phi}_N^\dagger(t, y) V_{nn}(x - y) \tilde{\phi}_N(t, y) \tilde{\phi}_N(t, x),
\] (8.1.12)

where \( \tilde{\phi}_N(x) \) is the nucleon field satisfying anti-commutation relation,
\[
[ \tilde{\phi}_N(t, x), \tilde{\phi}_N^{}(t, y) ]_+ = \delta^3(x - y), \quad (\text{others are zero})
\] (8.1.13)

and \( V_{ee}, V_{en} \) and \( V_{nn} \) represent the interaction of electron-electron, electron-nucleon, and nucleon-nucleon, respectively. The action functional \( \tilde{I} = \int dt \tilde{L} \) is written similarly as in (8.1.7),
\[
\tilde{I} = \int d^4x d^4y \left\{ \tilde{\phi}^\dagger(x) iS_0^{-1}(x, y) \tilde{\phi}(y)
- \frac{1}{2} \tilde{\phi}^\dagger(x) \tilde{\phi}^\dagger(y) V_{ee}(x - y) \delta(t_x - t_y) \tilde{\phi}(y) \tilde{\phi}(x)
+ \tilde{\phi}_c(x) iS_0^{\dagger}(x, y) \tilde{\phi}_c^\dagger(y) V_{en}(x - y) \delta(t_x - t_y) \tilde{\phi}_e(y) \tilde{\phi}_c(x)
- \tilde{\phi}^\dagger(x) \tilde{\phi}_c^\dagger(y) V_{en}(x - y) \delta(t_x - t_y) \tilde{\phi}_c(y) \tilde{\phi}(x) \right\},
\] (8.1.14)

\[
iS_0^{-1}(x, y) \equiv \left( i\partial_0 + \frac{\mathbf{p}^2}{2m} \right) \delta^4(x - y),
\] (8.1.15a)

\[
iS_0^{\dagger}(x, y) \equiv \left( i\partial_0 + \frac{\mathbf{p}^2}{2m_N} \right) \delta^4(x - y).
\] (8.1.15b)

The source terms,
\[ J_1(a)\phi(a) + \frac{1}{2i}J_2(a, b)\phi(a)\phi(b), \]  

(8.1.16)

are then introduced with \( \phi = [\hat{\phi}, \hat{\phi}^+, \hat{\phi}_N, \hat{\phi}^+_N] \) to define the generating functional \( W[J_1, J_2] \). As new variables of \( \Gamma \), we use \( \bar{G}_2(a, b) \) which is given in this case,

\[ \bar{G}_2(a, b) = 2i \frac{\partial W[J_1, J_2]}{\partial J_2(a, b)} - \langle a | b \rangle = \begin{bmatrix}
\langle \hat{\phi} \hat{\phi} \rangle & \langle \hat{\phi} \hat{\phi}_N \rangle & \langle \hat{\phi} \hat{\phi}^+_N \rangle \\
\langle \hat{\phi}_N \hat{\phi} \rangle & \langle \hat{\phi}_N \hat{\phi}^+ \rangle & \langle \hat{\phi}_N \hat{\phi}^+_N \rangle \\
\langle \hat{\phi}_N \hat{\phi} \rangle & \langle \hat{\phi}_N \hat{\phi}^+ \rangle & \langle \hat{\phi}_N \hat{\phi}^+_N \rangle \\
-\bar{S} & -\bar{S}^t & \bar{S}^t \\
-\bar{S} & -\bar{S}^t & \bar{S}^t \\
-\bar{S} & -\bar{S}^t & \bar{S}^t \\
\end{bmatrix}_{ab} \]  

(8.1.17)

\( \bar{S} \) and \( \bar{S}_N \) in (8.1.17) indicate the connected part of the full propagator for electron and nucleon field, respectively. With these preliminaries, effective action \( \Gamma \) is defined and obtained as follows (see Appendix C),

\[ \Gamma[\phi, \phi^+, \phi_N, \phi^+_N, \bar{G}_2] = W[J_1, J_2] - J_1(a) \frac{\partial W}{\partial J_1(a)} - J_2(a, b) \frac{\partial W}{\partial J_2(a, b)} \]

\[ = \int d^4x d^4y \ iS_0^{-1}(x, y)(\phi^+(x)\phi(y) - \bar{S}(y, x)) \]

\[ + \int d^4x d^4y \ iS_N^{-1}(x, y)(\phi^+_N(x)\phi_N(y) - \bar{S}_N(y, x)) \]

\[ + \frac{i}{2} \text{Trln} \bar{G}_2 - i\kappa^{(2)}. \]  

(8.1.18)

Here \( \kappa^{(2)} \) represents the sum of 1,2PI (one and two-particle irreducible) vacuum diagrams constructed out of \( \langle a |, \bar{G}_2 \) (propagator), and the original two-body instantaneous interactions in (8.1.14).

As a solution of stationary condition \( (J_1 = J_2 = 0) \), we get \( \bar{S}_0^{(0)} = S_0 \) and \( \bar{S}_N^{(0)} = S_{N0} \) under our choice of the vacuum \( \hat{\phi}_N|0\rangle = 0 \). The solutions for other channels, \( \langle \hat{\phi} \hat{\phi} \rangle \) or \( \langle \hat{\phi}^+_N \hat{\phi}_N \rangle \) for instance, can be set to zero. The mode-determining equation for one-electron atom is then obtained as the on-shell condition for \( \phi_N\phi \)-channel,

\[ \int d^4wd^4z \left[ \frac{\partial^2 \Gamma}{\partial \phi_N \phi^+_N \phi_N \phi^+_N \phi_N \phi^+_N} \right] \Delta \langle \phi_N(w) \phi(z) \rangle^{(1)} = 0 \]

(8.1.19)

or, by using (8.1.18),

\[ \left[ (i\partial_\omega + \frac{P^2}{2m_N})(i\partial_\omega + \frac{P^2}{2m_N}) - iV_{en}(y-x)\delta(t_y - t_x) \right] \Delta \langle \phi_N(x)\phi(y) \rangle^{(1)} = 0. \]

(8.1.20)

The independent variables for the channels we are examining are conveniently written as \( \langle \phi_N \phi \rangle \) and \( \langle \phi^+_N \phi^+_N \rangle \) (instead of using \( \langle \hat{\phi} \hat{\phi}_N \rangle \) and \( \langle \hat{\phi}_N^+ \hat{\phi}_N^+ \rangle \) or other combinations). The first term of (8.1.20) comes from the second derivative of \( \text{Trln} \bar{G}_2 \) in (8.1.18), which is written in terms of \( \bar{G}_2 \) as \( \bar{G}_2^{-1}(\hat{\phi}_N, \phi_N)\bar{G}_2^{-1}(\phi^+ \phi) \). The explicit form of \( \bar{G}_2^{-1}(a, b) \) for \( J_1 = J_2 = 0 \) is given in the form,
\[ \begin{bmatrix} 0 & -\left( S^{(0)} \right)^{-1} t & 0 & 0 \\ S^{(0)} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\left( S_N^{(0)} \right)^{-1} t \\ 0 & 0 & S_N^{(0)} & 0 \end{bmatrix}_{ab} \] (8.1.21)

The second term of (8.1.20) is obtained from the diagram of \( \kappa^{(0)} \) shown in Fig. 8.1. Other diagrams do not contribute because of the property of the vacuum.

As we expect, the result is obtained in the form of Bethe-Salpeter wave equation, which has two independent time variables \( t_x \) and \( t_y \). To see the relation between (8.1.20) and the Schrödinger equation for hydrogen-like atoms, let us examine the equation satisfied by the equal-time component \( \Delta\langle \tilde{\phi}_N(t, x)\tilde{\phi}(t, y) \rangle^{(1)} \) of on-shell variation. For this purpose, first we Fourier transform (8.1.20) in terms of time coordinates and get the following formal expression,

\[
\Delta\phi^{(1)}(E, \omega, x, y) = \int dt_x dt_y d(t_x - t_y) e^{iE(t_x + t_y) + i\omega(t_y - t_x)} \Delta\langle \tilde{\phi}_N(x)\tilde{\phi}(y) \rangle^{(1)}
\]

\[
= \frac{1}{2E + \frac{\nabla_x^2}{2m_N} + \frac{\nabla_y^2}{2m}} \left[ \frac{1}{E + \omega + \frac{\nabla_x^2}{2m_N} + i\epsilon} + \frac{1}{E - \omega + \frac{\nabla_y^2}{2m} + i\epsilon} \right]
\]

\[
\times i V_{en}(y - x) \Delta\phi^{(1)}(E, t_x = t_y, x, y),
\] (8.1.22)

where we have restored \( i\epsilon(e \to 0+) \) in the denominator of the Green's function.\(^5\) Now (8.1.22) is integrated over \( \omega \) to achieve the limits \( (t_x - t_y) \to \pm 0 \). In both limits, \( \omega \)-integration is easily evaluated to get

\[
\left( i \frac{\partial}{\partial t} + \frac{\nabla_x^2}{2m_N} + \frac{\nabla_y^2}{2m} - V_{en}(y - x) \right) \Delta\langle \tilde{\phi}_N(t, x)\tilde{\phi}(t, y) \rangle^{(1)} = 0 ,
\] (8.1.23)

which shows that the equal-time component of the on-shell variation satisfies ordinary Schrödinger equation for one-electron atom.

8.1.2. Helium atom

Returning to the model (8.1.1), the same argument as above can be made for the non-relativistic two-electron atoms. Let us take the nucleus as a static source of Coulomb field. The starting effective action and on-shell condition for two-electron channel are then summarized as follows,

Fig. 8.1. Diagram of \( \kappa^{(0)} \) giving rise to (8.1.20).

Internal broken line represents the Coulomb potential.

Fig. 8.2. Diagram of \( \kappa^{(0)} \) giving rise to (8.1.26).
\[
\Gamma[\phi, \phi^*, \tilde{G}_2] = \int d^4x d^4y \ i S_{0}^{-1}(x, y)(\phi^*(x)\phi(y) - \bar{S}(y, x)) + \frac{i}{2} \text{Tr} \ln \tilde{G}_2 - i \kappa^{(2)}, \tag{8\cdot1\cdot24}
\]

\[
\int d^4zd^4z \left( \frac{1}{2} \bar{S}^{(0)-1}(x, z) \bar{S}^{(0)-1}(y, w) - \left[ \frac{\bar{s}_K^{(2)}}{\delta \phi^* \phi^{(0)}(x)} \right]_0 \right) \Delta \phi^* \phi \phi \psi = 0, \tag{8\cdot1\cdot25}
\]

where we have assumed the electron number conserving solutions \(\phi^{(0)} = \phi^{* (0)} = \langle \phi^{(0)} \phi^{(0)} \rangle = \langle \phi^* \phi \rangle^{(0)} = 0\). The field component \(a\) or \(b\) of \(\tilde{G}_2(a, b)\) represents \(\phi\) and \(\phi^*\) in this case. By the property of the chosen vacuum \(\bar{\phi}(x)\rangle = 0\), \(\bar{S}^{(0)}\) does not include self-energy corrections and the non-zero contributions of \([\delta^2 K^{(2)} / \delta \phi^* \phi \phi \psi \phi \phi \psi]_0\) come only from the diagram shown in Fig. 8.2. Therefore we get

\[
(i \frac{\partial}{\partial t} + \frac{\vec{p}_x}{2m} + v(x))(i \frac{\partial}{\partial y} + \frac{\vec{p}_y}{2m} + v(y)) \Delta \phi \phi \psi = i V(y - x) \delta(t_y - t_x) \Delta \phi \phi \psi \phi \psi \psi. \tag{8\cdot1\cdot26}
\]

Only the ladder-type diagrams remain in the result.

The relation between (8·1·26) and the Schrödinger equation is now obvious. By using the same technique used above, the equal-time component of \(\Delta \phi \phi \psi \phi \psi \psi \psi \phi \) is easily confirmed to satisfy

\[
\left( i \frac{\partial}{\partial t} + \frac{\vec{p}_x}{2m} + \frac{\vec{p}_y}{2m} + v(x) + v(y) - V(y - x) \right) \Delta \phi \phi \psi = 0. \tag{8·1·27}
\]

### 8.1.3. Lithium atom

For the case of lithium-like atoms, we start from the effective action including 3-body channel (see Appendix C),

\[
\Gamma[\phi, \phi^*, \tilde{G}_2, C_3] = \int d^4x d^4y \ i S_{0}^{-1}(x, y)(\phi^*(x)\phi(y) - \bar{S}(y, x)) + \frac{i}{2} \sum_{\{a, b, c\}} \epsilon^{P(a, b, c : a', b', c')} C_3(a, b, c) \tilde{G}_2(a, a') \tilde{G}_2(b, b') \tilde{G}_2(c, c') \tilde{G}_3(a', b', c') + \frac{i}{2} \text{Tr} \ln \tilde{G}_2 - i \kappa^{(3)}, \tag{8\cdot1\cdot28}
\]

where \(\kappa^{(3)}\) represents 1, 2, 3PI vacuum diagrams. We get the on-shell condition for three-electron channel, \(^2\)}
\[ \int d^4x'd^4y'd^4z' \left( \frac{1}{3!} \tilde{S}^{(0)-1}(x, x') \tilde{S}^{(0)-1}(y, y') \tilde{S}^{(0)-1}(z, z') \right. \]
\[ \left. - \left[ \frac{\delta}{\delta \tilde{\phi}^+(x) \tilde{\phi}^+(y) \tilde{\phi}^+(z)} \right] \delta \langle \tilde{\phi}(x') \tilde{\phi}(y') \tilde{\phi}(z') \rangle^{(1)} \right] = 0. \]

(8.1.29)

The stationary solutions \( \langle \tilde{\phi} \tilde{\phi} \tilde{\phi} \rangle^{(0)} = 0 \),
\( \langle \tilde{\phi}^+ \tilde{\phi}^+ \tilde{\phi}^+ \rangle^{(0)} = 0 \), etc., have been chosen in (8.1.29). Also in this case, only the diagram shown in Fig. 8.3 contributes to the result. So we find

\[ \left( i \partial_x + \frac{\vec{P}_x^2}{2m} + v(x) \right) \left( i \partial_y + \frac{\vec{P}_y^2}{2m} + v(y) \right) \left( i \partial_z + \frac{\vec{P}_z^2}{2m} + v(z) \right) \delta \langle \tilde{\phi}(x) \tilde{\phi}(y) \tilde{\phi}(z) \rangle^{(1)} \]
\[ = \left[ iV(y-x) \delta(t_y-t_x) \left( i \partial_x + \frac{\vec{P}_x^2}{2m} + v(x) \right) \right. \]
\[ + \text{(cyclic permutation of } x, y \text{ and } z ) \delta \langle \tilde{\phi}(x) \tilde{\phi}(y) \tilde{\phi}(z) \rangle^{(1)}. \]

(8.1.30)

The equivalence to the Schrödinger equation can also be confirmed and we obtain,

\[ \left[ i \frac{\partial}{\partial t} + \frac{\vec{P}_t^2}{2m} + V(x) + V(y) + V(z) - V(x-y) - V(y-z) - V(z-x) \right] \]
\[ \times \delta \langle \tilde{\phi}(t, x) \tilde{\phi}(t, y) \tilde{\phi}(t, z) \rangle^{(1)} = 0. \]

(8.1.31)

8.1.4. \textit{N-electron atom}

In order to extend the present approach to general \( N \)-electron atoms, it seems that we need an explicit form of the effective action \( \Gamma' \) as a functional of the expectation value \( \langle 0 | T \tilde{\phi}(x_1) \cdots \tilde{\phi}(x_N) | 0 \rangle \) in the presence of the source \( J \) coupled to the product operator \( \tilde{\phi}(x_1) \cdots \tilde{\phi}(x_N) \). It is not known at present.

However on-shell expansion scheme also tells us that it is not necessary to use the complete expression of the effective action in order to study the excited modes — what we need is the information of \( \Gamma' \) only in the vicinity of \( J = 0 \), which can be evaluated straightforwardly. This fact enables us to derive the general \( N \)-body bound state equation both in relativistic and non-relativistic theories. From this standpoint, we have discussed the formal derivation of the relativistic \( N \)-body wave equation in Chapter V. Below the non-relativistic version of \( N \)-body wave equation is studied. It contains an aspect which is interesting from a theoretical point of view.

In order to study the problem, we first introduce \( W[J_1, J_2, \ldots, J_N] \) as in (5.1.2),

\[ \exp i W[J_1, J_2, \ldots, J_N] = \int[d\phi \bar{\phi} \psi \bar{\psi}] \exp i I_{J_1, J_2} [\phi, \phi^*], \]

(8.1.32)

\[ I_{J_1, J_2} [\phi, \phi^*] = I[\phi, \phi^*] + \sum_{k=1}^{N} \int d^4x_1 \cdots d^4x_k J_k(x_1, \ldots, x_k) \phi(x_1) \cdots \phi(x_k) \]
\[ + \sum_{k=1}^{N} \int d^4x_1 \cdots d^4x_k J_k(x_1, \ldots, x_k) \phi^*(x_1) \cdots \phi^*(x_k) \]
\[ \equiv I[\phi, \phi^+] + \sum_{k=1}^{N} J_k \phi_k + \sum_{k=1}^{N} \bar{J}_k \phi_k^+ , \quad (8.1.33) \]

\[ \langle \tilde{\phi}^{(t)}(x_1) \cdots \tilde{\phi}^{(t)}(x_k) \rangle \equiv \frac{\delta W[J_1, \cdots, J_N, \bar{J}_1, \cdots, \bar{J}_N]}{\delta \bar{J}_k(x_1, \cdots, x_k)} \equiv \phi_k^{(t)} . \quad (8.1.34) \]

In the above formulas we have used the same notation \( \psi \) or \( \psi^+ \) for the path integral variables which will not cause any confusion, instead of \( \Psi \) or \( \Psi^+ \) introduced in § 2.5.

For odd number of \( i \), the source \( \bar{J}_i \) (and also \( \phi_i^{(t)} \)) is the Grassmann variable. Effective action is then defined by

\[ \Gamma[\phi_1, \phi_1^+, \cdots, \phi_N, \phi_N^+] \equiv W[J_1, \bar{J}_1, \cdots, J_N, \bar{J}_N] - \sum_{i=1}^{N} J_i \phi_i - \sum_{i=1}^{N} \bar{J}_i \phi_i^+ . \quad (8.1.35) \]

It satisfies

\[ \frac{\delta}{\delta \phi_i^{(t)}} = -\bar{J}_i . \quad (8.1.36) \]

As stated above, in order to determine the energy levels of atoms, it is enough to see the quadratic part of \( W \) or \( \Gamma \). It takes the following diagonalized form because of the electron number conservation which assures the absence of the term like \( J_n J_m \) or \( \phi_n^+ \phi_m \) where \( n \neq m \).

\[ W \approx J_1 c_1 \bar{J}_1 + J_2 c_2 \bar{J}_2 + \cdots + J_N c_N \bar{J}_N , \quad (8.1.37) \]

\[ \Gamma_N \approx -[(1) \phi_1^+(c_1)^{-1} \phi_1 + (1)^2 \phi_2^+(c_2)^{-1} \phi_2 + \cdots + (1)^N \phi_N^+(c_N)^{-1} \phi_N] , \quad (8.1.38) \]

where we have deleted all the indices including space-time coordinate.

The meaning of \( c_i \)'s is simple. Graphically, they are represented by the sum of diagrams which have \( i \) electron lines with possible insertion of electron-electron interaction.

The propagator \( \langle 0|T \tilde{\phi}(x) \tilde{\phi}^+(y)|0 \rangle \) is proportional to \( \theta(t_x - t_y) \), because the ground state \( |0 \rangle \) satisfies \( \tilde{\phi}(x)|0 \rangle = 0 \). This leads to the fact that \( c_i \) includes only the ladder type diagrams. See Fig. 8.4 as an example where we have represented \(-V(x-y)\) by a wavy line. Recall moreover that electron loops and self-energy are not present. Once \( c_i \) is obtained, we can derive on-shell condition (2.5.16a) or fermionic analog of (5.2.36) for \( \Delta \phi_i \),

\[ (c_i)^{-1} \Delta \phi_i = 0 . \quad (1 \leq i \leq N) \quad (8.1.39) \]

The general procedure to take the inverse of \( c_i \) has been explained in § 5.4. Although the formula (5.3.16) is for Hermite scalar field, it holds for any system and in the case considered here it becomes simple due to the non-relativistic character of electron system. Take the case \( i \leq 4 \), for simplicity. The result of \( c_i^{-1} \) is shown graphically in Fig. 8.4 where the slash indicates the amputation of electron propagator \( S_F \) which is represented by a line with an arrow and its inverse \( S_F^{-1} \) is equal to \( S_0^{-1} \). Therefore if an electron line has two slashes it signifies \( S_0^{-1} \). It is easy to see that Eq. (8.1.39) agrees with (8.1.10), (8.1.26) and (8.1.30) respectively. For \( i = 4 \), we need special care.
Note here that the operation of anti-symmetrization of the external legs are absorbed in $\Delta \phi_i$ in (8.1.39). Similarly the sign factors caused by the contraction of the interaction part are included in each rung of the ladder diagrams; $-iV$. These results, of course, coincide with the one derived by using the full order form of the corresponding effective action $\Gamma_i$ ($i \leq 4$). (For $i \leq 3$, see Appendix C. For the case $i = 4$, one can derive the explicit form of $\Gamma_4$ with the help of the Legendre transformation rule given by De Dominicis and Martin.) As we have discussed in Chapter V, the three types of second-order interaction diagrams which have the factor $(-iV)^2$ in Fig. 8.4 are required as the elements of $(c_4)^{-1}$ in order to reproduce the diagrams of $c_4$ in proper weight. Recall that the graph of $c_4$ shown in Fig. 8.5 is doubly counted if we calculate it from $(c_4)^{-1}$ considering only the first-order interaction graphs of Fig. 8.4. These facts have been explained in (iii) of § 5.4.

The multi-time Schrödinger equation for general $N$-electron system can systematically be derived from (5.3.16). It includes $l$-th power of potential $(-iV)^l$ with $1 \leq l \leq N/2$ if $N$ is even and $1 \leq l \leq (N-1)/2$ if $N$ is odd.

8.1.5. $N$-electron system — ordinary Schrödinger equation —

It seems to be strange that $(c_i)^{-1}$ in Fig. 8.4, or $(c_N)^{-1}$ in general, contains the graphs which are quadratic in $-iV$, whereas the Schrödinger equation is linear in the potential. But this is not strange in fact, as is shown below. The essential point is the role played by the equal time projection.

Ordinary Schrödinger equation is derived by taking equal time limit of (8.1.39). Instead of doing this job, we start afresh by introducing the source $J$ which refers to single time $t$. Thus we change the action,

$$ S \longrightarrow \mathcal{S} + \sum_{k=1}^{N} \int dt dx_1 dx_2 \ldots dx_h J_k(t; x_1, x_2, \ldots, x_h) \hat{\phi}(t, x_1) \hat{\phi}(t, x_2) \ldots \hat{\phi}(t, x_h) $$

$$ + (J \rightarrow \mathcal{J}, \hat{\phi} \rightarrow \hat{\phi}^+) $$

(8.1.40)
Now our on-shell equation for general \( N \) becomes

\[
\int dt \, d^3x_1 \cdots d^3x_N (|c_N|^{-1})_{\tau, \tau_1, \cdots, \tau_N; \tau', \tau_1, \cdots, \tau_N} \Delta \langle \hat{\phi}(t', x_1) \cdots \hat{\phi}(t', x_N) \rangle = 0, \tag{8.1.41}
\]

where the notation \(|c_N|\) is defined as taking the equal time limit of \( c_N \),

\[
|c_N|_{\tau, \tau'} = \lim_{t_1, t_2, \cdots t_N \to \tau; t_1, t_2, \cdots t_N \to \tau'} c_N. \tag{8.1.42}
\]

Here the space coordinates are suppressed. In (8.1.41), we emphasize that the notation \(|c_N|^{-1}\) implies that the inverse has to be taken after the equal time projection.

The explicit form of \(|c_N|\) and its inverse are obtained by using the property of the diagrams specific to non-relativistic theory. In fact the equal time projection contains many aspects which are interesting from theoretical point of view. Leaving the details to Ref. 4), we state the result that (8.1.41) reduces to

\[
\left[ i \frac{\partial}{\partial t} + \sum_{i=1}^{N} \frac{p_{x_i}^2}{2m} + \sum_{i=1}^{N} v(x_i) - \sum_{i,j=1 (i < j)}^{N} V(x_i - x_j) \right] \Delta \langle \hat{\phi}(t, x_1) \cdots \hat{\phi}(t, x_N) \rangle = 0. \tag{8.1.43}
\]

Thus the following identification of the Schrödinger wave function \( \Psi(t, x_1, x_2 \cdots x_N) \) can be made

\[
\Delta \langle \hat{\phi}(t, x_1, x_2 \cdots x_N) \rangle = \langle 0 | \hat{\phi}(t, x_1) \hat{\phi}(t, x_2) \cdots | N \rangle = \Psi(t, x_1, x_2 \cdots x_N). \]

Here the state \(|N\rangle\) is a general \( N \)-particle state.

We stress here that \( N \)-body bound state kernel \((c_N)^{-1}\) derived from \( c_N \) takes the form of (5.4.16), or of Fig. 8.4 for non-relativistic electrons, which contains infinite powers of the potential \( V \), while the equal time projection leads to the fact that \(|c_N|^{-1}\) in (8.1.41) only includes the first order term in \( V \), thus reproducing the correct Schrödinger wave equation.\(^3\)

\section{8.2. Density functional theory by Legendre transformation}

The density functional theory is now one of the most commonly used methods in discussing various many particle systems.\(^6\) In this formalism the energy of the system is written as a functional of the density which is a function of single variable \( \rho \) instead of \( N \) coordinates \( \{x_i\} \) of \( N \) particles. In spite of the usefulness, its theoretical formulation is rather involved and sometimes difficult to achieve a systematic approximation scheme.

The purpose of this section is to present a clear formulation of the density functional theory in terms of full use of the Legendre transformation.\(^7\) It presents a theoretical basis of the density functional formalism which is both exact and systematic including the way to get excitation spectra. These statements can be achieved by a straightforward application of our technique presented above. For some explicit calculations using auxiliary field, known as Stratonovich-Hubbard transformation,\(^8,9\) see Ref. 7).
8.2.1. Atomic system with N electrons

Let us take an atomic system whose Hamiltonian is the same as (8.1.1) except for adding spin index of electron and introducing the source term coupled to the density operator,

$$\hat{H} = \int d^3 x \hat{\phi}^\dagger_\alpha(x) \left( -\frac{\nabla^2}{2m} - v(x) - \mu \right) \hat{\phi}_\alpha(x) + \frac{e^2}{2} \int d^3 x \int d^3 y \hat{\phi}^\dagger_\alpha(x) \hat{\phi}^\dagger_\beta(y) \frac{1}{|x-y|} \hat{\phi}_\beta(y) \hat{\phi}_\alpha(x),$$  
(8.2.1)

$$\hat{H}_J = \hat{H} - \int d^3 x J(t, x) \hat{\phi}^\dagger_\alpha(x) \hat{\phi}_\alpha(x).$$  
(8.2.2)

Here we use the Schrödinger representation and μ is the chemical potential, the presence of which enables us to discuss the problem as a function of electron number N. We have introduced the spin indices α, β and the sum over repeated index is implied.

It is only for convenience that we have introduced both μ and J(t, x). The total number is either obtained by differentiating by μ or by functionally differentiating through J(t, x) which is then integrated over whole space, see (8.2.7) below. More detailed Hamiltonian with relativistic corrections such as L-S coupling can be treated in a similar way therefore we restrict ourselves to the form (8.2.1) in the following. We repeat below for ease of reference the arguments presented up to now by specifying the notations used in this section.

Consider the case where J is time independent then the kernel defined in the time interval $t_f - t_i = T$ is given by

$$K = \langle 0 | \exp(-i\hat{H}_J T) | 0 \rangle_J = \langle \exp(-i\hat{H}_J T) \rangle_J = \exp(iW[J]).$$  
(8.2.3)

We assume in the following that the ground state $|0\rangle_J$ is not degenerate. If it is degenerate, a weak external field is assumed to be present to lift the degeneracy. We have in mind the magnetic field, which is set to be zero in the end of calculation.

Taking the limit $t_i \to -\infty$, $t_f \to +\infty$, we get the path integral formula which is particularly suited for the diagrammatic expansion. In case the source J is time dependent, K is defined by the time ordered form,

$$K = \left\langle \exp\left( -i \int_{-\infty}^\infty dt \hat{H}_J \right) \right\rangle = \int [d\phi^\dagger d\phi] \exp\left( i \int_{-\infty}^\infty dt L_J \right) = \exp(iW[J]),$$  
(8.2.4)

where $L_J$ is the Lagrangian derived from $H_J$ and $\int [d\phi^\dagger d\phi]$ implies of course the Grassmanian functional path integral. We have used the same notation $\phi$ or $\phi^\dagger$ as the operator field of the electron for the functional integration variables. This corresponds to $\Psi$ or $\Psi^\dagger$ of § 2.5. Explicit form of $L_J$ is shown below,

$$L = i \int d^3 x \phi^\dagger_\alpha(x) \partial_t \phi_\alpha(x) - \int d^3 x \phi^\dagger_\alpha(x) \left( -\frac{\nabla^2}{2m} - v(x) - \mu \right) \phi_\alpha(x)$$
$$- \frac{e^2}{2} \int d^3 x \int d^3 y \phi^\dagger_\alpha(x) \phi^\dagger_\beta(y) \frac{1}{|x-y|} \phi_\beta(y) \phi_\alpha(x),$$  
(8.2.5)
where \( x = (t, \mathbf{x}) \) and \( J(x) = J(t, \mathbf{x}) \). The sum over spin indices \( \alpha, \beta \) is implied. Note that in (8.2.5), \( y \) stands for \( y = (t, \mathbf{y}) \). Strictly speaking, as has been stressed in Chapter I, the ground state \( |0\rangle \), in the presence of time dependent source is not definable but we always set \( J \) to be zero after taking the (functional) derivative with respect to \( J \). Therefore the notation \( |0\rangle \) does not cause any ambiguities. Or we can alternatively assume that \( J \) vanishes sufficiently fast and smoothly as \( t \to \pm \infty \).

Now we make the functional Legendre transformation by introducing the expectation value of the density \( n(x) \) and introduce action functional, i.e., effective action, \( \Gamma[n] \),

\[
\Gamma[n] = W[J] - \int d^4 x J(x) \frac{\delta W[J]}{\delta J(x)} .
\]

Here as usual, \( J \) has to be written as a functional of \( n \) by solving (8.2.7). The question whether \( E(n) \) exists as the density functional is the question about the possibility of inverting (8.2.7), which is discussed later in connection with the Hohenberg-Kohn theorem. In Chapter XI this invertibility is shown by diagrammatic expansion in full order (taking QED theory as an example).

The density \( n(x) \) as a function of \( x \) is determined by the stationarity requirement

\[
\frac{\delta \Gamma[n]}{\delta n(x)} = -J(x) = 0 .
\]

Since the ground state is stationary, we look for the time-independent solution \( n(x) = n^{(0)}(x) \) of (8.2.9) which represents the density of the ground state in the absence of the source \( J \),

\[
n^{(0)}(x) = \langle 0 | \phi^\dagger(x) \phi_\alpha(x) | 0 \rangle ,
\]

where \( |0\rangle = |0\rangle_{J=0} \). The energy \( E(n) \) as a density functional is obtained by assuming that \( n(x) \) is a function of the space variables \( \mathbf{x} \) only. In this case \( \Gamma[n] \) acquires a factor corresponding to the whole time interval \( t_f - t_i = \int_{-\infty}^{\infty} dt \) with the coefficient \( E[n] \),

\[
\Gamma[n] = -E[n] \times \int_{-\infty}^{\infty} dt .
\]

The above static solution \( n^{(0)}(x) \) can also be found by solving

\[
\frac{\delta E[n]}{\delta n(x)} = 0 .
\]

If a time-dependent external field is actually present, the solution \( n(x) \) to (8.2.9) is also time dependent which describes time dependence of the density in such a situation. In this case our \( \Gamma[n] \) is the time-dependent density functional defined in a
different way from Ref. 11), see also Ref. 6).

8.2.2. Spin density functional

All the above discussions are applicable to the spin density functional $I'[n_s]$ or $E[n_s]$ ($a = \uparrow, \downarrow$). We have only to introduce two independent sources $J_\uparrow(x)$ and $J_\downarrow(x)$ in $\tilde{H}_I$ of (8.2.2),

$$\tilde{H}_I = \tilde{H} - \int d^3x \sum_{a=\uparrow, \downarrow} J_a(x) \tilde{\psi}_a^\dagger(x) \tilde{\psi}_a(x).$$

Then $W[J_s]$ is defined as in (8.2.4) and $I'[n_s]$ by

$$I'[n_s] = W[J_s] - \int d^4x \sum_{\beta = \uparrow, \downarrow} J_\beta(x) \frac{\delta W[J_s]}{\delta J_\beta(x)},$$

$$n_\beta(x) = \frac{\delta W[J_s]}{\delta J_\beta(x)}.$$

The spin density is determined by solving

$$\frac{\delta I'[n_s]}{\delta n_\beta(x)} = 0. \quad (\beta = \uparrow, \downarrow) \quad (8.2.13)$$

8.2.3. Hohenberg-Kohn theorem

The relation of our approach to the Hohenberg-Kohn theorem\textsuperscript{10} is pointed out here. We discuss two theorems below which are the fundamental starting points of their approach.

(i) Existence theorem

The theorem states that the density functional $E[n]$ exists. As has been pointed out the validity of this theorem is converted, in our case, to the question whether the defining equation of $n(x)$ as a functional of $J(x)$ is invertible or not. If this is possible the Legendre transformation from $W[J]$ to $I'[n]$ can be done and hence $E[n]$ exists. In the quantized field theory the above inversion process has been extensively studied in diagrammatical terms, see Chapter VI or Appendix C. For the case of density variable the introduction of the auxiliary field corresponding to the density operator by Stratonovich-Hubbard transformation\textsuperscript{80,81} is particularly convenient. Then as a result of the Legendre transformation the concept of one particle irreducible (1PI) vacuum diagrams naturally appears. Note here that the diagrammatical expansion in our case is the expansion in powers of the electron repulsion. In Chapter XI, the inversion is performed diagrammatically without recourse to the Stratonovich-Hubbard transformation. The density functional $E[n]$ therefore exists in diagrammatical sense.

(ii) Universality theorem

The second theorem states that $E[n]$ can be written as a sum of two terms, $E[n] = E^0[n] + E^I[n]$ where $E^0[n]$ is a universal functional independent of the nuclear potential $v$ and $E^I[n]$ is given explicitly by

$$E^I[n] = \int d^3x v(x)n(x).$$

(8.2.14)
The proof of this theorem is rather trivial in our formalism since it is a well-known consequence of the Legendre transformation. We discuss the problem using the Hamiltonian (8·2·2) and the definition (8·2·3). Recall here that $W[J]$ is a functional of $v + J$ therefore, writing $\int_{-\infty}^{\infty} dt = T$,

$$-E[n] T = W[v + J] - \int d^3 x J(x) \frac{\delta W[v + J]}{\delta J(x)}$$

$$= W[v + J] - \int d^3 x (J(x) + \nu(x)) \frac{\delta W[v + J]}{\delta J(x)} + \int d^3 x \nu(x) \frac{\delta W[v + J]}{\delta J(x)} .$$

(8·2·15)

However if we invert the relation

$$n(x) T = \frac{\delta W[v + J]}{\delta J(x)} ,$$

(8·2·16)

$v + J$ is given as a functional of $n$ which is independent of $\nu$. Since the first and second terms on the right-hand side of (8·2·15) are written by $n$ only, the theorem is proved;

$$E[n] = E[n]_{\nu=0} - \int d^3 x \nu(x) n(x) .$$

8.2.4.  Excitation spectrum

One of the great advantages of the present formalism is that it provides a unified way of studying the excitation spectrum as opposed to the usual density functional theory. This is achieved by on-shell expansion scheme which is reproduced below restricting ourselves to the density variable.

Let $n^{(0)}(x)$ be a solution to the stationarity equation (8·2·9) and assume that $n^{(0)}(x)$ is independent of time since it corresponds to the ground state. In order to discuss the excitation levels above the ground state thus determined, we look for another solution of (8·2·9) in the vicinity of $n^{(0)}(x)$ by writing

$$n(x) = n^{(0)}(x) + \Delta n(x) .$$

Then, up to first order in $\Delta n(x)$, we get

$$0 = \frac{\delta \Gamma^{(n)}}{\delta n(x)}|_{n=n^{(0)}+\Delta n}$$

$$= \left( \frac{\delta \Gamma^{(n)}}{\delta n(x)} \right)_0 + \int d^4 y \left( \frac{\delta^2 \Gamma^{(n)}}{\delta n(x) \delta n(y)} \right)_0 \Delta n(y) + \cdots .$$

(8·2·17)

Here $(\cdots)_0$ implies the value of $(\cdots)$ evaluated at $n=n^{(0)}(x)$. Since the first term on the right-hand side of (8·2·17) vanishes by the definition of $n^{(0)}$, we arrive at the following result which we have called the mode determining equation or the on-shell condition,

$$\int d^4 y \Gamma^{(0)}(x, y)_{\nu} \Delta n(y) = 0 ,$$

(8·2·18)

$$\Gamma^{(0)}(x, y) = \frac{\delta^2 \Gamma^{(n)}}{\delta n(x) \delta n(y)} .$$
Regarding $x$ and $y$ as indices specifying rows and columns, Eq. (8.2.18) has the form of zero eigenvalue equation of the matrix of the second derivative of $\Gamma$. As an equation of the excitation energy $\omega$, it is a nonlinear eigenvalue equation which is seen as follows. The second derivative of $\Gamma$, if it is evaluated at the static solution $n^{(0)}$, is a function of difference $t - t'$ of the time coordinate of $x$ and $y$, therefore Eq. (8.2.18) takes the form

$$\int d^3 y dt' \Gamma^{(2)}(x, y, t - t') \Delta n(y, t') = 0.$$  

(8.2.19)

In Fourier space it becomes

$$\int d^3 y \Gamma^{(2)}(x, y, \omega) \Delta n(y, \omega) = 0.$$  

(8.2.20)

In this form it is easy to see that a non-trivial solution to $\Delta n$ exists only for such values of $\omega$ for which the matrix $\Gamma^{(2)}(x, y, \omega)$ has zero eigenvalue. Let one of such $\omega$ be $\omega_i$, assuming that it lies in a discrete spectrum, then Eq. (8.2.20) determines both eigenvalue $\omega$ and the wave function $\Delta n(y, \omega)$ corresponding to that mode, see Chapter II. It is easy to see that $\omega_i$ is the excitation energy $\pm |E_i - E_0|$ of the $i$-th excited state $|i\rangle$ where $E_i$ or $E_0$ is the energy eigenvalue of the state $|i\rangle$ or $|0\rangle$ respectively and $\Delta n$ is given by

$$\Delta n(x, \omega_i) = \begin{cases} 
\langle i | \hat{\varphi}^*_a(x) \hat{\varphi}_a(x) | 0 \rangle & \text{if } \omega_i = -(E_i - E_0), \\
\langle 0 | \hat{\varphi}^*_a(x) \hat{\varphi}_a(x) | i \rangle & \text{if } \omega_i = E_i - E_0.
\end{cases}$$  

(8.2.21)

Another way of deriving (8.2.18) and (8.2.21) is given as follows. We first note the following identity of the Legendre transformation (see (A.8) of Appendix A),

$$\int d^4 y \frac{\delta^2 \Gamma[n]}{\delta n(x) \delta n(y)} \frac{\delta^2 W[J]}{\delta J(y) \delta J(z)} = - \delta^4(x - z).$$  

(8.2.22)

We see that, by looking for the zero of the second derivative of $\Gamma$, we are at the same time searching for the pole of the second derivative of $W$, which is the connected part of the causal correlation function of densities,

$$\frac{\delta^2 W[J]}{\delta J(x) \delta J(y)} = \langle 0 | T \hat{\varphi}_a^*(x) \hat{\varphi}_a(x) \hat{\varphi}_a^*(y) \hat{\varphi}_a(y) | 0 \rangle.$$  

(8.2.23)

Let us rewrite (8.2.22) in Fourier representation in the time difference $t_x - t_y$ after setting $J = 0$,

$$\int d^3 y \Gamma^{(2)}(x, y, \omega) W^{(2)}(y, z, \omega) = - \delta^3(x - z).$$  

(8.2.24)

Now, by inserting the complete set $|j\rangle$ as usual, $W^{(2)}$ has the representation

$$W^{(2)}(y, z, \omega) = i \sum_f \left( \frac{n_f^+(y) n_f(z)}{\omega - \omega_f + i \varepsilon} - \frac{n_f^+(z) n_f(y)}{\omega + \omega_f - i \varepsilon} \right),$$  

$$n_f(y) = \langle j | \hat{\varphi}^*_a(y, 0) \hat{\varphi}_a(0) | 0 \rangle, \quad \omega_f = E_f - E_0.$$  

(8.2.25)
Here $\ast$ denotes the complex conjugation and $\epsilon$ is the positive infinitesimal quantity. Selecting particular $\omega_i$ we multiply $\omega + \omega_i$ on both side of (8.2.24) and take the limit $\omega \to -\omega_i$. Then using (8.2.25) we get

$$\int d^3 y \Gamma^{(2)}(x, y, \omega_i) n_i(y) = 0.$$  \hspace{1cm} (8.2.26)

In obtaining the above equation we have assumed that $n_i^*(x) \neq 0$ and that the level $\omega_i$ is not degenerate or if it is degenerate each state can be characterized by different symmetry. If we multiply $\omega - \omega_i$ and take the limit $\omega \to \omega_i$, the results (8.2.20), (8.2.21) together with the identification $\Delta n_i = n_i(y)$ or $n_i^*(y)$ are obtained. (In the above arguments, Heisenberg and Schrödinger representations are assumed to coincide at $t=0$.)

Note that in order to study the excitation levels the time-dependent probe is required. In this sense the energy functional $E[n]$, which is obtained by a static probe, does not contain any information on the excitation; we have to use the effective action $\Gamma[n]$. Since our formalism enables us to determine both the ground state, by (8.2.9), and the excited state, by (8.2.18), in a systematic way, both of them can be studied by the same approximation scheme because once the starting $\Gamma[n]$ is fixed all the calculations go through according to the above guideline.

It is straightforward to generalize the above arguments to the spin density functional. After solving (8.2.13), the excitation spectrum with the spin content specified is given by solving the following $2 \times 2$ (in spin space) coupled zero eigenvalue equation,

$$\sum_{\tau} \int d^3 y \left( \frac{\delta^2 \Gamma[n_1, n_1]}{\delta n_\tau(x) \delta n_\tau(y)} \right)_{\omega} \Delta n_\tau(y) = 0.$$  \hspace{1cm} (8.2.27)

We have discussed in (8.2.17) up to the term which is linear in $\Delta n$. As discussed in Chapter II, higher-order terms correspond to the scattering matrix elements among the modes determined by (8.2.18).\(^{12,13}\)

8.2.5. Method of auxiliary field

As has been pointed out, Legendre transformation for the density variable can most conveniently be done by introducing the auxiliary operator field $\bar{\sigma}(x)$ for the density $\bar{n}(x)$, which is a composite operator bilinear in electron field. The auxiliary field method, known as the Stratonovich-Hubbard transformation,\(^{8,9}\) enables us to treat the density operator as if it is an elementary field variable. This is done most conveniently in functional path integral formalism. For details of Legendre transformation after the introduction of auxiliary field, see Ref. 7).

§ 8.3. Generalization: ionization and affinity energy

In our formalism, the operator $\bar{O}$ which is probed by introducing the source term $f\bar{O}$ into the Hamiltonian is completely arbitrary. Therefore we can take not only $\int d^3 x f_\tau(x) \bar{\phi}_\tau(x) \bar{\phi}_\sigma(x)$ as a probe of the density but also any other operator $f\bar{O}$ as long as $\bar{O}$ does not change the electron number. Even if the operator $\bar{O}$ changes the electron number, all the procedures presented above go through. For instance we
arrive at the equation of the type (8.2.20) with $\Delta n$ replaced by $\langle i|\hat{D}|0\rangle$. This is the equation of the excitation spectrum determining the energy difference of the excited states $|i\rangle$ and $|0\rangle$ which differ in electron number. Furthermore the operator $\hat{D}$ can be non-local in the sense that it refers to two different space-time points. These examples are given below.

8.3.1. Ionization (Affinity) energy

As an example, let us consider an atom with $N$ electrons and add two source terms $-\int d^3 x\eta_a^\dagger(t, x)\bar{\phi}_a(x)$ and $-\int d^3 x\eta_a^\dagger(x)\eta_a(t, x)$ to the Hamiltonian with $\eta_a, \eta_a^\dagger$ being c-number Grassmann variables. These operators change one electron number. Let us consider

$$\hat{H}_{J, \eta, \eta'} = \hat{H} - \int d^3 x J(t, x)\bar{\phi}_a(x)\eta_a(x) - \int d^3 x\eta_a^\dagger(t, x)\bar{\phi}_a(x) - \int d^3 x\eta_a(x)\eta_a(t, x).$$

(8.3.1)

In the last term, the order of $\bar{\phi}_a^\dagger$ and $\eta$ is reversed compared with (2.5.1). Then $W[J, \eta, \eta']$ is defined as

$$\exp(iW[J, \eta, \eta']) = \int [d\phi^\dagger d\phi] \exp\left(i\int_0^\infty dt L_{J, \eta, \eta'}\right),$$

(8.3.2)

where $L_{J, \eta, \eta'}$ is the Lagrangian derived from $H_{J, \eta, \eta'}$,

$$L_{J, \eta, \eta'} = \int d^3 x J(x)\bar{\phi}_a(x)\bar{\phi}_a(x) + \int d^3 x\eta_a^\dagger(x)\phi_a(x) + \int d^3 x\eta_a(x)\phi_a(x).$$

(8.3.3)

Now we introduce the expectation values

$$n(x) = -\frac{\delta W}{\delta J(x)} = \langle \bar{\phi}_a^\dagger(x)\bar{\phi}_a(x)\rangle_{J, \eta, \eta'},$$

(8.3.4)

$$\Psi_a(x) = -\frac{\delta W}{\delta \eta_a^\dagger(x)} = \langle \bar{\phi}_a(x)\rangle_{J, \eta, \eta'}, \quad \bar{\Psi}_a^\dagger(x) = -\frac{\delta W}{\delta \eta_a(x)} = \langle \bar{\phi}_a^\dagger(x)\rangle_{J, \eta, \eta'}.$$

(8.3.5)

Since the probes $\eta_a, \eta_a^\dagger$ (and also $\Psi_a, \bar{\Psi}_a^\dagger$) are the Grassmann variables, we have to distinguish the left and right derivatives. The definitions of them are given for any Grassmann variable $\xi$ by

$$F[\xi + \delta \xi] - F[\xi] = \delta \xi \frac{\delta F[\xi]}{\delta \xi} = \frac{\delta F[\xi]}{\delta \xi} \delta \xi.$$

(8.3.6)

See (2.5.5). Then effective action defined in (8.2.8) is extended to the case of three variables,

$$\Gamma[n, \Psi, \bar{\Psi}^\dagger] = W[J, \eta^\dagger, \eta]$$

$$- \int d^4 x J(x)n(x) - \int d^4 x\eta_a^\dagger(x)\Psi_a(x) - \int d^4 x\Psi_a^\dagger(x)\eta_a(x).$$

(8.3.7)
Because the chemical potential \( \mu \) is kept fixed in the above Legendre transformation, we have the relation, which relates \( \mu \) to the total electron number \( N \),

\[
\frac{\partial \Gamma}{\partial \mu} = -\frac{\partial W}{\partial \mu} = \int d^4x \langle \tilde{\phi}^\dagger(x) \tilde{\phi}(x) \rangle_I, \eta^*, \eta \longrightarrow \int dt^* \ N \ . \ \text{(as \( I, \eta^*, \eta \rightarrow 0 \)) (8.3.8)}
\]

This condition determines \( \mu \) as a function of \( N \) and the vacuum state \(|0\rangle \) becomes the ground state of the system with \( N \) electrons, \( \mu = \mu(N), |0\rangle = |N\rangle \). There are now three stationary requirements

\[
\frac{\delta \Gamma}{\delta n(x)} = -J(x) = 0 , \ \text{(8.3.9)}
\]

\[
\frac{\delta \Gamma}{\delta \Psi_\pm^*(x)} = -\eta^\dagger(x) = 0 , \ \text{and} \ \frac{\delta \Gamma}{\delta \Psi_\pm(x)} = -\eta(x) = 0 , \ \text{(8.3.10)}
\]

and we write the solutions as

\[
n(x) = n^{(0)}(x) = \langle N | \tilde{\phi}^\dagger(x) \tilde{\phi}(x) | N \rangle , \ \text{(8.3.11)}
\]

\[
\Psi_\pm(x) = \Psi_\pm^{(0)}(x) = \langle N | \tilde{\phi}_\pm(x) | N \rangle = 0 ,
\]

\[
\Psi_\pm^*(x) = \Psi_\pm^{*(0)}(x) = \langle N | \tilde{\phi}_\pm^*(x) | N \rangle = 0 . \ \text{(8.3.12)}
\]

As in § 8.2.4, we look for other solutions to (8.3.9) and (8.3.10) in the vicinity of \( n^{(0)}(x) \), \( \Psi^{(0)}_\pm(x) \) and \( \Psi^{*(0)}_\pm(x) \) by writing \( n(x) = n^{(0)}(x) + \Delta n(x) \), \( \Psi_\pm(x) = \Psi^{(0)}_\pm(x) + \Delta \Psi_\pm(x) \), \( \Psi^{*(0)}_\pm(x) + \Delta \Psi^{*(0)}_\pm(x) \). Taking into account the electron number conservation law, which states for instance that

\[
\left( \frac{\delta \Gamma}{\delta \Psi_\pm(x)} \right)_{\delta n(x)} = 0 ,
\]

we get three mode-determining equations; one of them is identical to (8.2.18) and the other two take the form,

\[
\int d^4y \left( \frac{\delta \Gamma}{\delta \Psi_\pm^*(y)} \left( \frac{\delta \Gamma}{\delta \Psi_\pm(x)} \right) \right)_{\delta n(x)} \Delta \Psi_\pm^*(y) = 0 , \ \text{(8.3.13)}
\]

\[
\int d^4y \left( \frac{\delta \Gamma}{\delta \Psi_\pm(y)} \left( \frac{\delta \Gamma}{\delta \Psi_\pm^*(x)} \right) \right)_{\delta n(x)} \Delta \Psi_\pm(y) = 0 , \ \text{(8.3.14)}
\]

where \((\cdots)_{\delta n(x)}\) implies the value of \((\cdots)\) evaluated at the stationary solutions (8.3.11) and (8.3.12).

Now let us investigate the meaning of these wave equations. Using simple extension of the identity of the Legendre transformation (8.2.22), Eqs. (8.2.18), (8.3.13) and (8.3.14) can be seen to be the equation determining the pole of the Green's functions \( \langle N | T \tilde{n}(x) \tilde{n}(y) | N \rangle_{\delta n} \), \( \langle N | T \tilde{\phi}_\pm(x) \tilde{\phi}_\pm^*(y) | N \rangle_{\delta n} \) and \( \langle N | T \tilde{\phi}_\pm(x) \tilde{\phi}_\pm(y) | N \rangle_{\delta n} \) respectively. Inserting the complete set between \( \tilde{n}(x) \) and \( \tilde{n}(y) \) of \( \langle N | T \tilde{n}(x) \tilde{n}(y) | N \rangle_{\delta n} \), we see that only the states with \( N \) electrons contribute. So the eigenvalues of (8.2.18) are given as the difference of the energy between arbitrary excited levels and the ground state both with the same number \( N \) of the
electrons. On the other hand, if we insert the complete set between $\tilde{\phi}_a(x)$ and $\tilde{\phi}_b(y)$ of $\langle N | T \tilde{\phi}_a(x) \tilde{\phi}_b(y) | N \rangle$, only the states with $N \pm 1$ (for $t_x \equiv t_y$) electrons contribute. So the eigenvalues of Eq. (8.3.13) are given as the difference between the energy of the excited levels $\langle N | N \rangle$ of the system with $N \pm 1$ electrons and the ground state energy of the system with $N$ electrons. This is the ionization or the affinity energy. Equation (8.3.13) or (8.3.14) separately yields two different sets of mode each of which belongs to the channel defined by different electron number. However, we can easily distinguish between the affinity energy and the ionization energy, if we keep track of the sign of the time difference $t_x - t_y$ in (8.3.13) in the course of calculation. Equation (8.3.14), of course, gives the same eigenvalues as in (8.3.13), but there is a difference between $\Delta \Psi_a(y)$ and $\Delta \Psi_a(y)$. By the arguments leading to (8.2.26), the wave function $\Delta \Psi_a(y)$ can be written as

$$\Delta \Psi_a(y) = \langle N + 1 | \phi_a(y) | N \rangle_0 \quad \text{or} \quad \langle N | \phi_a(y) | N - 1 \rangle,$$

while $\Delta \Psi(y)$ has the form

$$\Delta \Psi(y) = \langle N - 1 | \phi_a(y) | N \rangle_0 \quad \text{or} \quad \langle N | \phi_a(y) | N + 1 \rangle.$$

In the following the explicit form of the mode determining equation is examined. Let us take Eq. (8.3.14) and consider, for simplicity, the case where we do not perform the Legendre transformation with regard to $J$ or disregard the $J$ dependence altogether. The effective action in such a case is given by (see Appendix C),

$$\Gamma[\Psi, \Psi^*] = \int d^4x \Psi_a^\dagger(x) \left( i \frac{\partial}{\partial t} + \frac{p^2}{2m} + V(x) + \mu \right) \Psi_a(x)$$

$$- \frac{e^2}{2} \int d^4x \int d^4y \Psi_a^\dagger(x) \Psi_a^\dagger(y) U_0(x - y) \Psi_a(y) \Psi_a(x) - i \kappa^{(1)},$$

where $\kappa^{(1)}$ represents all the one-particle irreducible vacuum graphs. In the above formula, we have included in $\kappa^{(1)}$ the one-loop vacuum diagrams represented by Trln.

Fig. 8.6. Diagrams contributing to the last term of (8.3.18) up to $e^4$. A solid line here represents the electron propagator, $i(i \frac{\partial}{\partial t} + (p^2/2m) + V(x) + \mu(N))^{-1} \delta(x - y) \delta_{ab}$. The potential between electrons is denoted by a broken line. The slashes indicate the amputation of the corresponding propagator lines.
So Eq. (8.3.14) becomes
\[
\int d^4y \left[ \left( i \frac{\partial}{\partial t} + \frac{p^2}{2m} + V(x) + \mu(N) \right) \delta^4(x - y) \delta_{a,s} - i \left( \frac{\delta}{\delta \Psi^s(y)} \left( \frac{\delta^{(1)}}{\delta \Psi^a(x)} \right) \right) \right] \Delta \Psi^s(y) = 0. \tag{8.3.18}
\]

This is the wave equation which determines the ionization or the affinity energy. In Fig. 8.6, we write down the last term of (8.3.18) up to the second order in $\epsilon^2$. The first or second term in Fig. 8.6 corresponds to Fock or Hartree term respectively. Let us study the relationship between our approach and the conventional independent particle approximation. For this purpose a new propagator $\Delta_{HF}$ is defined which is the electron propagator including Hartree and Fock term. It is a solution of the integral equation shown in Fig. 8.7 where a thick solid line is $\Delta_{HF}$. Then using $\Delta_{HF}$ we find that the last term of (8.3.18) can be written as in Fig. 8.8 and if we keep the first and second graph of Fig. 8.8 as an approximation, then Eq. (8.3.18) is seen to coincide with the Hartree-Fock equation. Recall here Koopman's theorem\(^\text{149}\) about Hartree-Fock equation:

The energy eigenvalue of the Hartree-Fock equation is equal to the work required to remove the electron from the system, or the negative of the binding energy obtained by independent particle approximation.

This statement agrees with the meaning of our equation (8.3.18). Moreover, since Eq. (8.3.18) determines the ionization (affinity) energy in full order, our approach generalizes Koopman’s theorem in exact form beyond the Hartree-Fock approximation.

Loosely speaking, $\Delta \Psi^s(y)$ or $\Delta \Psi^s_{\text{sp}}(y)$ is the wave function of the electron which is deleted or added. However such a picture does not hold in a strict sense, of course, since all the electrons are identical quantum mechanically. Combining (8.2.18),
(8.3.13) and (8.3.14) and surveying all the atomic number $Z$, we can obtain in principle any of the levels of atomic system. Detailed study of (8.3.18) is an interesting subject.

8.3.2. Multiple ionization (affinity) energy and Schrödinger equation

The above arguments can be generalized by adding the following source term to the Hamiltonian $\hat{H}$ (for notational clarity, the spin indices are suppressed),

$$-\int d^3x_1\cdots d^3x_k\eta^+(x_1, x_2, \cdots, x_k) \bar{\phi}(x_1) \bar{\phi}(x_2) \cdots \bar{\phi}(x_k) + \text{c.c.},$$

where c.c. implies the conjugate operation and the notation $x_j=(t, x_j)$ is used. The $c$-number variable $\eta$ or $\eta^+$ is completely antisymmetric in its arguments and it is a Grassmann number if $k$ is odd. This term corresponds to the source term

$$\int d^4x_1\cdots d^4x_k\eta^+(x_1, x_2, \cdots, x_k)\phi(x_1)\phi(x_2)\cdots\phi(x_k) + \text{c.c.},$$

which is to be added to $L$ of (8.2.5). In this form, we are probing the operator $\bar{\phi}(x_1)\bar{\phi}(x_2)\cdots\bar{\phi}(x_k)$ where $\bar{\phi}(x_j)$ is the electron field operator in Heisenberg representation. Now $W[\eta^+, \eta]$ is defined as usual and $\Gamma[\Psi, \Psi^+]$ is introduced as follows,

$$\Gamma[\Psi, \Psi^+]=W[\eta^+, \eta] - \int d^4x_1\cdots d^4x_k\left\{ \eta^+(x_1, \cdots, x_k)\Psi(x_1, \cdots, x_k) + \Psi^+(x_1, \cdots, x_k)\eta(x_1, \cdots, x_k) \right\},$$

$$\Psi(x_1, \cdots, x_k)=\frac{\partial}{\partial \eta^+(x_1, \cdots, x_k)} W[\eta^+, \eta],$$

$$\Psi^+(x_1, \cdots, x_k)=\frac{\partial}{\partial \eta(x_1, \cdots, x_k)} W[\eta^+, \eta].$$

The ground state is characterized of course by $\Psi^{(0)}=\Psi^{+(0)}=0$ and the excitation levels are determined by

$$\int d^4y_1\cdots d^4y_k\left( \frac{\partial}{\partial \Psi(y_1, \cdots, y_k)} \left( \frac{\partial}{\partial \Psi^+(y_1, \cdots, y_k)} \right) \right) \Delta \Psi(y_1, \cdots, y_k)=0$$

and its conjugate equation. The total energy $\omega=\sum_{i=1}^{N} \omega_i$, where $\omega_i$ is the energy Fourier component in the channel specified by $x_i$, is given as an eigenvalue of (8.3.19). It is the ionization (affinity) energy where $k$ electrons are removed from (added to) the $N$-electron atom ($N$ comes in through the chemical potential $\mu$).

The Schrödinger equation itself for $N$-electron system is derived in our formalism as follows. Take $k=N$ in (8.3.19) and $\mu=0$. Then it can be shown (see § 8.1.5 and Ref. 4) that Eq. (8.3.19) is nothing but the Schrödinger equation if we identify $\Delta \Psi(x_1, x_2, \cdots, x_N)=\Delta \Psi(t, x_1, t, x_2, t, \cdots, x_N)$ with the Schrödinger wave function $\Psi(t, x_1, \cdots, x_N)$,

$$\Delta \Psi(t, x_1, t, x_2, \cdots, t, x_N)=\Psi(t, x_1, x_2, \cdots, x_N)$$

$$=\langle 0 | \bar{\phi}(t, x_1) \bar{\phi}(t, x_2) \cdots \bar{\phi}(t, x_N) | N \rangle.$$
In this sense the energy eigenvalue of $N$-electron system is viewed in our formalism as the negative of the ionization energy required in the process of removing $N$-electrons from $N$-electron system.

8.3.3. Non-local density

As an electron number conserving operator, we can generalize the local density operator $\hat{n}(x) = \hat{\phi}^\dagger(x)\hat{\phi}(x)$ to “non-local density” operator $\hat{n}(x, y) = \hat{\phi}^\dagger(x)\hat{\phi}(y)$. This operator can equally be used in place of $\hat{n}(x)$ since $\hat{n}(x, y)$ has the same quantum number, i.e., zero-electron number, as $\hat{n}(x)$. Or we can generalize still further to consider the operator $\hat{n}(x, y) = \hat{\phi}^\dagger(x)\hat{\phi}(y)$ which is non-local in time also. Here $\hat{\phi}(x) = \hat{\phi}(t, x)$ is the Heisenberg field operator of the electron at time $t$. In order to get the effective action of $\hat{n}(x, y)$, we add the term $\int d^4x' d^4y' \int f(x, y) \hat{\phi}^\dagger(x)\hat{\phi}(y)$ to (8.2.5) and $W[J]$ is defined as in (8.2.4). Then as an argument of the effective action $\Gamma[n]$, we define

$$n(x, y) = \frac{\delta W[J]}{\delta f(x, y)} = \langle \hat{\phi}^\dagger(x)\hat{\phi}(y) \rangle_1$$

and $\Gamma[n]$ is given by

$$\Gamma[n] = W[J] - \int d^4x \int d^4y f(x, y) n(x, y).$$

The stationary solution $n^{(0)}(x, y)$ to the equation $\delta \Gamma/\delta n(x, y) = 0$ is the propagator function in this case,

$$n^{(0)}(x, y) = \langle N| T \hat{\phi}^\dagger(x)\hat{\phi}(y)|N \rangle_0$$

and the mode determining equation has the form,

$$\int d^4x' \int d^4y' \left( \frac{\delta^2 \Gamma[n]}{\delta n(x, y) \delta n(x', y')} \right)_0 \Delta n(x', y') = 0, \quad (8.3.20)$$

which determines the energy $\omega = \sum_{i=1}^2 \omega_i$, corresponding to the sum of energy of the channel specified by $x$ and $y$ (or $x'$ and $y'$). The energy $\omega$ thus determined is the same as is given by using the local density operator $\hat{n}(x)$.

Although $n(x, y)$ formalism looks more complicated than $n(x)$ it has an advantage that the Feynman rule of $\Gamma$ using $n(x, y)$ is more transparent than $n(x)$. It is known that $\Gamma[n]$ is given by the formula (Appendix C),

$$\Gamma[n] = \text{Tr} D_0(x - y)n(x, y) - \text{Tr} \ln n(x, y) + \kappa^{(2)}[n],$$

where $D_0(x - y)$ is defined by

$$D_0(x - y) = \left[ i\partial_t + \frac{p^2}{2m} + \mu + v(x) \right] \delta^4(x - y).$$

Here Tr implies the functional trace and $\kappa^{(2)}[n]$ is the sum of all 2PI (two particle irreducible) vacuum diagrams where the propagator is $n(x, y)$ and the vertices are dictated from the Lagrangian (8.2.5). Here 2PI means that the diagram is not separated into two disconnected parts if two propagator lines (each represented by
\( n(x, y) \) are cut at the same time. Examples are shown in Fig. 8.9. Equation (8.3.20) is the BS-type equation in relativistic field theory and various techniques developed there will be useful in solving (8.3.20). Another advantage of using \( n(x, y) \) is that, since the probe \( J(x, y) \) depends on \( x \) and \( y \) independently, we get more information about the ground state and excited levels. For example, the \( i \)-th level \( |i\rangle \) corresponds to \( \Delta n(x, y) = \langle N| T \phi^*(x) \phi(y)|N\rangle_0 \) therefore it contains the information about the dependence of the wave function on the relative coordinate of the particle-hole pair.

§ 8.4. **S-matrix approach of atomic scattering by effective action**

Effective action can also be applied to the scattering problem of atomic physics. In this formalism, the bound state wave function is clearly separated from the diagrams contributing to the scattering among bound states. Necessary diagrams are enumerated straightforwardly by taking appropriate derivatives of the effective action. Let us explain the relation between the scattering matrix element and the effective action.

In Appendix D, we have derived the scattering matrix element which is written in terms of connected Green’s function \( W^{(n)} \). The relation between \( W^{(n)} \) and \( \Gamma^{(n)} \) has been obtained in Appendix A. Neglecting all the indices \((A \cdot 27)\) can be written as follows,

\[
(W^{(2)})^{-1}(W^{(2)})^{-1} \cdots (W^{(2)})^{-1} W^{(N)} = \Gamma^{(N)} - \Gamma^{(N-1)}(\Gamma^{(2)})^{-1} \Gamma^{(3)} + \Gamma^{(N-2)}(\Gamma^{(2)})^{-1} \Gamma^{(3)}(\Gamma^{(2)})^{-1} \Gamma^{(3)} + \cdots. \tag{8.4.1}
\]

In the above expansion formula all the possible tree diagrams with \( N \) external lines appear which are constructed by vertices \( \Gamma^{(n)} \) with \( n \geq 3 \) and propagator \(- (\Gamma^{(2)})^{-1}\). The reason why only tree graphs emerge is because we are using exact \( \Gamma^{(n)} \) which
includes all the loop corrections. The formula of the scattering matrix element in terms of $\Gamma$ can readily be obtained by inserting tree expansion (8.4.1) into the formula for the scattering matrix element derived in Appendix D; (D-48), (D-53) and (D-73).

As a prototype example, we show the way how the scattering of two Hydrogen atoms is discussed in the lowest approximation of the effective action. The Hamiltonian in this case is given by (8.1.12) and since we are interested in two particle bound state we take the effective action $\Gamma$ of (8.1.18) setting $\langle \hat{\phi} \rangle = \langle \hat{\phi}^\dagger \rangle = \langle \hat{\phi}_N \rangle = \langle \hat{\phi}_N^\dagger \rangle = 0$. Thus $\Gamma$ is a function of $\bar{G}_2$ only,

$$\Gamma[\bar{G}_2] = -i \text{Tr}[S_0^{-1} \bar{S}] - i \text{Tr}[S_N^{-1} \bar{S}_N] + \text{Tr} \ln \bar{G}_2 - i \kappa^{(2)}.$$  \hspace{1cm} (8.4.2)

Here $\kappa^{(2)}$ is the sum of all the 2PI vacuum diagrams where the propagator is $\bar{G}_2$.

As an illustration of our approach, $\kappa^{(2)}$ is neglected and the lowest order discussion is given below. The tilde over $G_2$ can be deleted since the difference between $\bar{G}_2$ and $G_2$ vanishes because of $\langle \hat{\phi} \rangle = \langle \hat{\phi}_N \rangle = \cdots = 0$ when we set $J = 0$. We use the notation $G_2$ below.

In order to make expressions concise, the space time variables are omitted which can easily be recovered. For example

$$G(e', e) = \langle T \hat{\phi}^\dagger(x') \hat{\phi}(x) \rangle, \quad G(N', N) = \langle T \hat{\phi}_N^\dagger(x') \hat{\phi}_N(x) \rangle, \quad \text{etc.,} \hspace{1cm} (8.4.3)$$

where $T$ is the time ordering operator. According to the formula (8.4.1), the scattering matrix element of two hydrogen atoms requires fourth and third derivatives of the effective action. In the following the derivative is written, for example, as

$$\Gamma^{(4)}_{G(e', e)} = \frac{\delta \Gamma}{\delta G(e', e)}.$$  \hspace{1cm} (8.4.4)

Now neglecting the term $\kappa^{(2)}$ in (8.4.2) corresponds to the tree approximation where only the rearrangement of the constituent particle, electron or proton, is taken into account. The Coulomb interaction between bound states comes from higher-order terms contained in $\kappa^{(2)}$ but the effect of Coulomb interaction which is responsible for making up bound state is fully retained. The situation is similar to the QCD case studied in Chapter IV.

With these preliminaries we get

$$\Gamma^{(4)}_{G(e, e'), G(e', e'')} = -i G^{-1}(e', e') G^{-1}(e'', e),$$
$$W^{(3)}_{G(e, e'), G(e', e'')} = -i G(e, e'') G(e', e'),$$
$$\Gamma^{(4)}_{G(e, e'), G(e', e'')} W^{(3)}_{G(e', e''), G(e'', e''')} = -\delta_{e, e'} \delta_{e'', e''''}.$$ \hspace{1cm} (8.4.5)

Here $\delta$ is the Dirac $\delta$-function with the specified space-time index and similar equations hold for nucleon. For higher derivatives, we have expressions,

$$\Gamma^{(4)}_{G(N, e), G(e', N'), G(N', e'), G(e'', N'')}$$
$$= -i G^{-1}(e', e) G^{-1}(N', N') G^{-1}(e', e') G^{-1}(N', N)$$
$$- i G^{-1}(e', e) G^{-1}(N', N') G^{-1}(e'', e') G^{-1}(N'', N'),$$ \hspace{1cm} (8.4.6)
\[ \Gamma^{(3)}_{\tilde{c}(N,e), G(e', N'), G(e', e')} = -i G^{-1}(e', e) G^{-1}(e', e') G^{-1}(N', N), \quad (8.4.7) \]
\[ \Gamma^{(3)}_{\tilde{c}(N,e), G(e', N'), G(N', N')} = -i G^{-1}(N', N) G^{-1}(N', N') G^{-1}(e', e). \quad (8.4.8) \]

Now the Hydrogen scattering amplitude, denoted by \( A \), requires both \( \Gamma^{(3)} \) and \( \Gamma^{(4)} \),
\[
A = \frac{1}{4} \Gamma^{(4)}_{\tilde{c}(N,e), G(e', N'), G(N', e'), G(e', N')} \\
+ \frac{1}{2} \Gamma^{(3)}_{\tilde{c}(N,e), G(e', N'), G(e', e')} W^{(2)}_{\tilde{c}(e', e'), G(e', e')} \Gamma^{(3)}_{\tilde{c}(e', e'), G(e', N'), G(N', e')} \\
+ \frac{1}{2} \Gamma^{(3)}_{\tilde{c}(e', N'), G(N,e), G(N', N', N')} W^{(2)}_{\tilde{c}(N', N'), G(N', N'), G(N', N')} \Gamma^{(3)}_{\tilde{c}(N', N'), G(e', N'), G(N', e')}.
\quad (8.4.9) \]

Here the sum over variables which have double or triple primes are implied. We see a clear rearrangement process contained in (8.4.9). After substituting (8.4.6) \sim (8.4.8), the above expression turns out to be combined into two terms,
\[
A = \frac{i}{4} \left\{ G^{-1}(e', e) G^{-1}(N', N') G^{-1}(e', e') G^{-1}(N', N) \\
+ G^{-1}(e', e) G^{-1}(N', N') G^{-1}(e', e') G^{-1}(N', N) \right\}. \quad (8.4.10) \]

This is multiplied by the product of four Hydrogen wave functions
\[
\Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)} \Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)} \Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)} \Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)}, \quad (8.4.11) \]
where \( \Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)} \) and \( \Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)} \) represent incoming Hydrogens and the others outgoing ones. The above situation is illustrated in Fig. 8.10, where the inverse propagator \( G^{-1} \) is represented by a line and the wave function by a circle.

However it turns out that the two terms of (8.4.10) give the same contribution and the scattering matrix element becomes
\[
A = \frac{i}{2} G^{-1}(e', e) G^{-1}(N', N') G^{-1}(e', e') G^{-1}(N', N) \\
\times (8.4.11). \quad (8.4.12) \]

An alternative expression of \( A \) emerges if we use the BS-type Schrödinger equation (8.1.20) satisfied by \( \Delta \langle \tilde{\phi}_N^* \tilde{\phi} \rangle^{(1)}, \)
\[
\left( i \hat{\partial}_x + \frac{\hat{\mathbf{p}}_x^2}{2m} \right) \left( i \hat{\partial}_y + \frac{\hat{\mathbf{p}}_y^2}{2m_N} \right) \Delta \langle \tilde{\phi}_N(y) \tilde{\phi}(x) \rangle^{(1)} \\
= i V_{en}(x - y) \delta(t_x - t_y) \Delta \langle \tilde{\phi}_N(y) \tilde{\phi}(x) \rangle^{(1)}.
\quad (8.4.13) \]
By this process, we arrive at a concise formula (8.4.24) below which involves only equal time wave function — the Schrödinger wave function. Now the inverse of the propagator is given by
\[ iG^{-1}(e', e) = \left( i\partial_x + \frac{\nabla_x^2}{2m} \right) \delta^4(x - y). \] (8.4.14)

It is convenient to write (8.4.13) as shown in Fig. 8.11 where the circle with two lines indicates \( \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} \). Now ordering the factors in accordance with space-time variables, the following identities are obtained from (8.4.13),

\[
G^{-1}(N^t, N) \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} G^{-1}(e, e^t) = iV_{eN} \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)},
\]

\[
G^{-1}(e, e^t) \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} G^{-1}(N^t, N) = iV_{eN} \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)}. \quad (8.4.15)
\]

Now we write \( A \) as

\[
A = \frac{i}{2} \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} G^{-1}(e, e^t) \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} G^{-1}(N^t, N^t, N')
\]

\[
\times \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} G^{-1}(e', e^t) \Delta \langle \hat{\phi}_N^+ \hat{\phi}_N \rangle^{(1)} G^{-1}(N^t, N), \quad (8.4.16)
\]

and insert functional identity operator \( G^{-1}G \) in four places in such a way that we can utilize (8.4.15). Then we get the following form,

---

**Fig. 8.10.** Illustration of \( A \) of (8.4.10) multiplied by (8.4.11). Inverse propagator is represented by a line and the wave function by a circle.

---

**Fig. 8.11.** Graphical representation of wave equation (8.4.13). Wavy line implies the Coulomb interaction.
\[ A = \frac{i}{2} \left( iV_{en} \Delta \phi_{N} \phi^{(1)} \right)_{\xi} G(e^1, e_\xi) \times \left( iV_{en} \Delta \phi_{N} \phi^{(1)} \right)_{\kappa} G(N_{\xi}, N^{\kappa}_{\xi}) \times \left( iV_{en} \Delta \phi_{N} \phi^{(1)} \right)_{\eta} G(e^{\eta}_{\xi}, e^{\eta}_{\xi}) \times \left( iV_{en} \Delta \phi_{N} \phi^{(1)} \right)_{\rho} G(N_{\eta}, N^{\rho}_{\eta}) \cdot \]

\[ (8.4.17) \]

Here we have inserted indices for clarity and the result is shown in Fig. 8.12. Let us use the representation
\[
G(e, e^\dagger) = \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^0 - \frac{p^2}{2m} + i\epsilon} e^{ip(x-y)},
\]

where \( p(x-y) = p_0(x_0 - y_0) - p^0(x-y) \) with \( x_0 \) or \( y_0 \) denoting the time coordinate of \( x \) or \( y \). This is inserted into \( A \) which becomes
\[
A = \frac{i}{2} \int \cdots \left[ \int V_{en}(x-y) \delta(t_x - t_y) \Delta \phi_{N}(x) \phi(y)^{(1)} \int \frac{d^4p}{(2\pi)^4} \frac{i}{p^0 - \frac{p^2}{2m} + i\epsilon} e^{-ip(y-y')} \right.
\]
\[
\times V_{en}(y' - x') \delta(t_{y'} - t_{x'}) \Delta \phi_{N}(y') \phi_{N}(x')^{(1)} \int \frac{d^4q}{(2\pi)^4} \frac{i}{q^0 - \frac{q^2}{2m} + i\epsilon} e^{-iq(x-x')}
\]
\[
\times V_{en}(u - v) \delta(t_u - t_v) \Delta \phi_{N}(u) \phi(v)^{(1)} \int \frac{d^4p'}{(2\pi)^4} \frac{i}{p^0 - \frac{p^2}{2m} + i\epsilon} e^{-ip(u-v)}
\]
\[
\times V_{en}(v' - u') \delta(t_{v'} - t_{u'}) \Delta \phi_{N}(v') \phi_{N}(u')^{(1)} \int \frac{d^4q'}{(2\pi)^4} \frac{i}{q^0 - \frac{q^2}{2m} + i\epsilon} e^{-iq(u'-x)}
\]

\[ (8.4.18) \]

Here four dimensional integrations over \( x, x', y, y', u, u', v, v' \) are implied by the symbol \( \int \cdots \int \).

The advantage of (8.4.18) is, as has been announced above, that only the equal time wave function, the Schrödinger wave function, appears. It satisfies
\[
\left( i\partial_t + \frac{\vec{p}^2}{2m_N} + \frac{\vec{p}^2}{2m} - V_{en}(y-x) \right) \Delta \phi_{N}(t, x) \phi(t, y)^{(1)} = 0.
\]

\[ (8.4.19) \]

Using the delta function of time variable in (8.4.18), we define
\[
t_{y'} = t_x = t_1, \quad t_{v'} = t_{v} = t_2, \quad t_u = t_{v'} = t_3, \quad t_{u'} = t_u = t_4.
\]
Due to the presence of \(i\varepsilon\) with \(\varepsilon > 0\), the integrations over \(p^0, p^0, q^0, q^0\) lead to the following constraint,

\[ t_3, t_4 < t_1, t_2. \quad (8.4.20) \]

Now we assume that incoming (labeled by 3, 4) or outgoing (labeled by 1, 2) four Hydrogen atoms are eigenstate of (8.4.19) given by

\[ \Delta \langle \hat{\phi}_n(t_i, x) \hat{\phi}(t_i, y) \rangle^{(1)} = f_i(x, y)e^{-iE_{ni}t_i}, \quad (i = 3, 4) \]
\[ \Delta \langle \hat{\phi}_n^\dagger(t_i, x) \hat{\phi}_n^\dagger(t_i, y) \rangle^{(1)} = f_i^*(y, x)e^{iE_{ni}t_i}. \quad (i = 1, 2) \quad (8.4.21) \]

Here the first argument of \(f_i\) refers to proton. In this way, we get for the scattering amplitude,

\[ A = \frac{i}{2} \int d^3x \cdots d^3y' \int \frac{d^3p}{(2\pi)^3} \cdots \frac{d^3q'}{(2\pi)^3} \int dt_1 \cdots dt_4 \]
\[ \times V_{en}(x - y)f_3(x, y)e^{-i\mathbf{p}' \cdot \mathbf{x} - i\mathbf{p}' \cdot \mathbf{y}} \times V_{en}(y' - x')f_3(x', y')e^{i\mathbf{p}' \cdot \mathbf{x}' + i\mathbf{p}' \cdot \mathbf{y}'} \]
\[ \times V_{en}(u - v)f_4(u, v)e^{-i\mathbf{p} \cdot \mathbf{u} - i\mathbf{p} \cdot \mathbf{v}} \times V_{en}(v' - u')f_4(u', v')e^{i\mathbf{p} \cdot \mathbf{u}' + i\mathbf{p} \cdot \mathbf{v}'} \]
\[ \times \exp(i\sum t_iB_i), \quad (8.4.22) \]

where \(t_i\) integration is performed in the region (8.4.20) and \(B_i\) is defined by

\[ B_1 = E_1 - \frac{p^2}{2m} - \frac{q^2}{2m_N} + i\varepsilon, \quad B_2 = E_2 - \frac{p^2}{2m} - \frac{q^2}{2m_N} + i\varepsilon, \]
\[ B_3 = -E_3 + \frac{p^2}{2m} + \frac{q^2}{2m_N} - i\varepsilon, \quad B_4 = -E_4 + \frac{p^2}{2m} + \frac{q^2}{2m_N} - i\varepsilon. \quad (8.4.23) \]

The integrations by \(t_1 \sim t_4\) produce the factor,

\[-2\pi i\delta(E_1 + E_2 - E_3 - E_4)\frac{B_1 + B_2}{B_1 B_2 B_3 B_4} = 2\pi i\delta(E_1 + E_2 - E_3 - E_4)\frac{B_3 + B_4}{B_1 B_2 B_3 B_4}, \]

where we have used \(E_1 + E_2 - E_3 - E_4 = B_1 + B_2 + B_3 + B_4\). By eliminating \(V_{en}\) from expression (8.4.22) through the Schrödinger equation (8.4.19), we arrive at a compact formula for \(A\):

\[ A = \frac{1}{2} \int d^3x \int d^3y \int d^3u \int d^3v 2\pi \delta(E_1 + E_2 - E_3 - E_4) \]
\[ \times \left( E_1 + E_2 - \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{p'}^2}{2m} - \frac{\mathbf{V}^2}{2m_N} - \frac{\mathbf{V'}^2}{2m_N} \right) f_3(x, y)f_3(u, y)f_4(u, v)f_4(x, v) \]
\[ = \frac{1}{2} \int d^3x \int d^3y \int d^3u \int d^3v 2\pi \delta(E_1 + E_2 - E_3 - E_4) \]
\[ \times (E_1 + E_2)f_3(x, y)f_3(u, y)f_4(u, v)f_4(x, v). \quad (8.4.24) \]

We have neglected the surface terms in arriving at the last expression. This is the formula for the scattering of two Hydrogen atoms due to the exchange of the constituent particles of each atom. It clearly shows that such an effect comes about
when the wave functions overlap with each other, a short range effect.

In the actual calculation, center of mass $\mathbf{R}$ and relative coordinate $\mathbf{r}$ are introduced as

$$
\mathbf{R} = \frac{m_N \mathbf{x} + m_N \mathbf{y}}{m_N + m}, \quad \mathbf{r} = \mathbf{y} - \mathbf{x},
$$

$$
f_i(\mathbf{x}, \mathbf{y}) = e^{i \mathbf{p} \cdot \mathbf{r}} f_i(\mathbf{r}), \quad E_i = \frac{1}{2(m_N + m)} \mathbf{P}^2 + E_i^r.
$$

Here $\mathbf{P}$ is the total momentum, $f_i(\mathbf{r})$ is the relative wave function and $E_i^r$ is the relative energy. The application of (8.4.24) and numerical evaluation is left as a future study.

We have neglected $\kappa^{(2)}$ of (8.4.2) which includes the effect of Coulomb interaction other than the rearrangement of electron or nucleon. It has a graphical expansion and the lowest one is given in Fig. 8.13. To write down the mathematical expressions of these diagrams are straightforward.

§ 8.5. $Z^{-1}$ expansion

The purpose of this section is to show that our diagrammatic expansion scheme presented above is equivalent to the expansion in powers of $Z^{-1}$ where $Z$ is the atomic number. As is well-known, there are several ways of the proof but the following may be a transparent method.

8.5.1. Energy levels

Let us consider an atom of atomic number $Z$ with $\mathbf{R}$ and $\mathbf{r}_i$ the coordinates of nucleus and electrons respectively. We introduce here the rescaled coordinates by

$$
\mathbf{R} = a \bar{\mathbf{R}}, \quad \mathbf{r}_i = a \bar{\mathbf{r}}_i,
$$

$$
a = \frac{\hbar}{Z m e^2}.
$$

In terms of rescaled variables, the Schrödinger equation of energy $E_\pi$ becomes
\[
\left\{-\sum_{i} \frac{1}{2} \frac{\partial^{2}}{\partial \vec{r}_{i}^{2}} + Z^{-1} \sum_{i \neq j} \frac{1}{|\vec{r}_{i} - \vec{r}_{j}|} - \sum_{i} \frac{1}{|\vec{r}_{i} - \vec{R}|}\right\}\phi = \bar{E}_{n} \phi ,
\]

(8.5.3)

\[
\bar{E}_{n} = \frac{\hbar^{2}}{Z^{2}m_{e}c} E_{n} .
\]

(8.5.4)

We have neglected the kinetic energy term of nucleus. The eigenvalue \(\bar{E}_{n}\) is a function of \(Z^{-1}\) only and has the expansion in powers of \(Z^{-1}\) while \(\phi\) is a function of \(\vec{r}_{i}, \vec{R}\) and \(Z^{-1}\).

Since the diagrammatic expansion corresponds to the expansion in terms of electron repulsion, which has a factor \(Z^{-1}\) in the rescaled expression, it is the expansion scheme by \(Z^{-1}\).

8.5.2. Scattering matrix element

The diagrammatic expansion of scattering matrix element discussed in § 8.4 is also an expansion by \(Z^{-1}\) as is seen below. Suppose we take a scattering diagram of two atoms each having atomic number \(Z\). Consider another diagram describing the same scattering but with one more Coulomb interaction between two electron lines. The latter graph has one extra Coulomb term \(e^{2} V(r_{i} - r_{j})\) and two more electron propagators. Mathematical expression of this extra factor is

\[
Y = e^{2} \int dt \int dt' \int dr_{i} \int dr'_{j} \frac{1}{|r_{i} - r_{j}|} \delta(t - t') G(x_{i} - x_{k}) G(x'_{j} - x_{i}) ,
\]

(8.5.5)

where \(G\) is the propagator appearing in (8.4.17). It is the inverse of (8.4.14). We have introduced \(x_{i} = (t, r_{i})\), etc., and \(x_{k}\) is some space-time point connected with the point \(x_{i}\) or \(x_{j}\) respectively.

Let us rescale as in (8.5.1) and (8.5.4) and redefine \(x\) and \(p\) (appearing in the Fourier representation of \(G(x_{i} - x_{k})\), etc.) as

\[
p = \frac{1}{a} \bar{p} , \quad t = \frac{a}{Ze^{2} \bar{r}} .
\]

(8.5.6)

Then \(Y\) becomes \(Z^{-1}\) times the same \(Y\) expressed now by the variables with bar. Thus the diagram with one more Coulomb interaction between electrons is down by one factor of \(Z^{-1}\).

The Coulomb interaction involving nucleus seems to produce one extra factor of \(Z\) but as is well known, due to the shielding property of neutral atom, such a factor is not present actually.

References

1) For a textbook of atomic system, see
Chapter VIII. Atomic System

5) See, for example, the textbook by
6) For the textbook or the review, see
14) T. Koopman, Physica 1 (1933), 104.

For a textbook, see for example, I. Lindgren and J. Morrison, Atomic Many-Body Theory (Springer-Verlag, 1982).
Chapter IX. Superconductivity by Inversion Method

From a field theoretical point of view, the superconducting system is particularly interesting because of its spontaneous breaking of the symmetry which is realized in the Hamiltonian. The symmetry that is broken is of course the one associated with the electron number conservation.

Up to now, three approaches seem to be present to investigate the properties of superconductivity. The variational calculation, starting from BCS and Bogoliubov, is of course the oldest one. The Green's function approach, initiated by Gorkov and further exploited by Nambu is widely used for most of arguments because of its convenience especially in describing the case with the spatial variation of the system due to external electromagnetic field. The third approach is the one based on the functional integral accompanied by the auxiliary field method known as the Hubbard-Stratonovich transformation. This method makes it possible to evaluate the correction terms of the mean-field result by using the method of steepest descent.

One of the purpose of this chapter is to show that the discussions based on inversion method can be regarded as the fourth approach for the theory of superconductivity. Along this line, equilibrium superconductivity is first discussed in § 9.1 based on the BCS Hamiltonian. Section 9.2 is devoted to the second purpose of our study, i.e., to apply the inversion method to non-equilibrium systems. In principle, the extension can straightforwardly be accomplished by introducing the time-dependent source term which is introduced to probe the time-dependent superconducting order of the system. Hence the main difference compared with § 9.1 lies in the method how to evaluate the original series of order parameter as a perturbation expansion in a time-dependent situation.

Although there exist several methods for non-equilibrium theory, we use recently introduced formalism in which $3 \times 3$ rather than $2 \times 2$ matrix form of the contour-ordered real time Green's function appears. It has an advantage that the initial time $t_i$ when the density matrix is prepared is explicitly taken into account. (Formal discussions on the non-equilibrium theory based on inversion method is given in Chapter XII.)

As a model Hamiltonian of non-equilibrium superconductivity, we take the one which explicitly contains phonon degrees of freedom. This is essential for the discussion of dissipative effects in superconductor.

§ 9.1. Application to equilibrium system

9.1.1. Hamiltonian

We first discuss the application of inversion method to the equilibrium superconductivity. Let $\hat{a}_\alpha(k)$ and $\hat{a}_\alpha^\dagger(k)$ be the annihilation and creation operators of electron in the Schrödinger representation, whose momentum is $k$ and spin $\alpha$. Then the BCS Hamiltonian is expressed as a sum of two parts: the kinetic energy of electrons
\[ \hat{H} = \hat{H}_0 + \hat{H}_I, \quad (9.1.1) \]
\[ \hat{H}_0 = \int \frac{d^3k}{(2\pi)^3} \varepsilon_k \hat{a}_\sigma^\dagger(k) \hat{a}_\sigma(k), \quad (9.1.2) \]
\[ \hat{H}_I = -\frac{1}{2} \int \frac{d^3k d^3p d^3q}{(2\pi)^9} \nu(q) \hat{a}_\sigma^\dagger(k+q) \hat{a}_\sigma^\dagger(p-q) \hat{a}_\beta(p) \hat{a}_\beta(k). \quad (9.1.3) \]

Here \( \varepsilon_k = (k^2/2m) - \mu \) is the energy of the free electron with momentum \( k \), measured from the level of the chemical potential \( \mu \). The interaction Hamiltonian among electrons \( \hat{H}_I \) is assumed to be instantaneous and is regarded as the perturbation in what follows. In addition, here we assume \( \nu(q) > 0 \) in (9.1.3) so that the Cooper instability occurs at low temperature. (Throughout in this chapter, the unit \( \hbar = k_B = c = 1 \) is used and we employ the summation convention with respect to spin indices \( \sigma, \beta \) and the one in the Nambu space\(^{11} \) \( \mu, \nu \) appearing below.) On the basis of the above Hamiltonian, the results of applying inversion method to the equilibrium superconductivity\(^{2,3} \) are first presented.

Since each term in (9.1.1) contains the same number of the annihilation and the creation operators, the BCS Hamiltonian has the following first kind gauge symmetry which is related to the electron number conservation,
\[ \hat{a}_\sigma(k) \rightarrow e^{i\theta} \hat{a}_\sigma(k), \quad \hat{a}_\sigma^\dagger(k) \rightarrow e^{-i\theta} \hat{a}_\sigma^\dagger(k), \quad (9.1.4) \]
where \( \theta \) is some real and constant parameter. The superconducting state is known as the one where the above symmetry is spontaneously broken so that we choose the source term \( \hat{H}_J \) as to break the symmetry (9.1.4):
\[ \hat{H}_J = -\int \frac{d^3k}{(2\pi)^3} J(k) \{ \hat{a}_\sigma^\dagger(k) \hat{a}_\sigma^\dagger(-k) + \hat{a}_\sigma(-k) \hat{a}_\sigma^\dagger(k) \} \]
\[ -\int \frac{d^3k}{(2\pi)^3} \chi[J](k) \hat{a}_\sigma^\dagger(k) \hat{a}_\sigma(k), \quad (9.1.5) \]

where, owing to the Hermiticity of the Hamiltonian, the source field \( J(k) \) is chosen to be a real function. The second term on the right-hand side of (9.1.5) is related to the renormalization of the chemical potential due to \( \hat{H}_I \) and is added to get rid of \( J(k) \) dependence of the Hartree-Fock potential due to the interaction between electrons. Since the source term has to vanish when the source becomes zero, we also demand the function \( \chi[J](k) \) vanishes as \( J(k) \rightarrow 0 \). Explicit form of \( \chi[J](k) \) will be determined below. This source term \( \hat{H}_J \) probes the pairing correlation between electrons.

9.1.2. Thermodynamics of superconductor

Let us now consider the thermodynamical properties of the superconductors in the absence of external magnetic field. The order parameter \( \phi(k) \) is chosen as the expectation value of the local product of annihilation operators with opposite spins and momentum:
\[ \phi(\mathbf{k}) \equiv \frac{1}{V} \langle \hat{a}^\dagger(\mathbf{k}) \hat{a}^\dagger(-\mathbf{k}) + \hat{a}_i(-\mathbf{k}) \hat{a}^\dagger_i(\mathbf{k}) \rangle, \quad (9.1.6) \]

where \( \langle \cdots \rangle \) designates the thermal average defined by the Hamiltonian \( \hat{H} + \hat{H}_J \). In order to evaluate this expectation value, it is convenient to introduce the Gibbs type free energy \( W[J] \) as

\[ \exp[-\beta W[J]] = \text{Tr} \exp[-\beta(\hat{H} + \hat{H}_J)], \quad (9.1.7) \]

where \( 1/\beta \) is the temperature of the system. The order parameter is then given by a simple functional differentiation,

\[ \phi(\mathbf{k}) = -\frac{(2\pi)^3}{V} \frac{\partial W[J]}{\partial J(\mathbf{k})}. \quad (9.1.8) \]

According to Ref. 2), the perturbation series for \( W[J] \) is obtained by introducing the functional integral (holomorphic) representation and its explicit form up to linear term in \( v(q) \) is as follows,

\[
W[J]/V = -\beta^{-1} \int \frac{d^3p}{(2\pi)^3} \ln\left[ 4e^{-\frac{\beta q^2}{2}} \cosh\left( \frac{\beta \omega_k}{2} \right) \right] \\
- \int \frac{d^3k d^3p}{4(2\pi)^6} \left[ 2v(0) - v(\mathbf{k} - \mathbf{p}) \right] \left[ 1 - \text{sgn}(\varepsilon_k) \tanh\left( \frac{\beta \varepsilon_k}{2} \right) \right] \\
\times \left[ 1 - \text{sgn}(\varepsilon_p) \tanh\left( \frac{\beta \varepsilon_p}{2} \right) \right] \\
- \int \frac{d^3k d^3p}{4(2\pi)^6} v(\mathbf{k} - \mathbf{p}) j(\mathbf{k}) j(\mathbf{p}) \tanh\left( \frac{\beta \omega_k}{2} \right) \tanh\left( \frac{\beta \omega_p}{2} \right) + O(v^2), \quad (9.1.9)
\]

where \( \text{sgn}(x) \equiv \theta(x) - \theta(-x) \) is the sign function and

\[ \omega_k = \sqrt{\varepsilon_k^2 + J^2(\mathbf{k})}, \quad j(\mathbf{k}) = \frac{J(\mathbf{k})}{\omega_k}, \quad j_3(\mathbf{k}) = \frac{\varepsilon_k}{\omega_k}. \quad (9.1.10) \]

In deriving (9.1.9), we have chosen \( \chi[J](\mathbf{k}) \) as

\[
\chi[J](\mathbf{k}) \equiv - \int \frac{d^3p}{4(2\pi)^3} \left[ 2v(0) - v(\mathbf{k} - \mathbf{p}) \right] \left[ 1 - j_3(\mathbf{p}) \tanh\left( \frac{\beta \varepsilon_p}{2} \right) \right] \\
- \frac{1 - \text{sgn}(\varepsilon_k) \tanh\left( \frac{\beta \varepsilon_k}{2} \right)}{1 - j_3(\varepsilon_k) \tanh\left( \frac{\beta \varepsilon_k}{2} \right)} \\
\times \int \frac{d^3p}{4(2\pi)^3} \left[ 2v(0) - v(\mathbf{k} - \mathbf{p}) \right] \left[ 1 - \text{sgn}(\varepsilon_p) \tanh\left( \frac{\beta \varepsilon_p}{2} \right) \right].
\]

If the \( v(\mathbf{k}) \to 0 \) limit is taken in (9.1.9), one immediately finds that the first term on the right-hand side corresponds to the free energy given by the Hamiltonian \( \hat{H}_0 + \hat{H}_J \). On the other hand, since
\[
\frac{1}{2} \left\{ 1 - \text{sgn}(\varepsilon_h) \tanh \left( \frac{\beta \varepsilon_h}{2} \right) \right\} = \Theta(\varepsilon_h) \frac{1}{\exp(\beta \varepsilon_h) + 1} + \Theta(-\varepsilon_h) \left\{ 1 - \frac{1}{\exp(\beta \varepsilon_h) + 1} \right\}
\]

is the particle (hole) number density when \( \varepsilon_h > 0 \) (\( \varepsilon_h < 0 \)), the second term of \( (9\cdot1\cdot9) \) represents the Hartree-Fock correction term due to \( \tilde{H}_f \) in the absence of \( \tilde{H}_i \).

With the help of \( (9\cdot1\cdot8) \) and \( (9\cdot1\cdot9) \), the original series of perturbation \( (7\cdot2\cdot2) \) for the order parameter turns out to be written as follows,

\[
\phi(h) = \phi_0(h) + \phi_1(h) + O(v^2),
\]

\[
\phi_0(h) = j(h) \tanh \left( \frac{\beta \omega_h}{2} \right),
\]

\[
\phi_1(h) = \left( \frac{1}{\omega_h} \right) \left[ j_2(h) \tanh \left( \frac{\beta \omega_h}{2} \right) + \frac{j_2^2(h)}{\cosh^2 \left( \frac{\beta \omega_h}{2} \right)} \right]
\times \int \frac{d^3p}{(2\pi)^3} v(h - p) j(p) \tanh \left( \frac{\beta \omega_p}{2} \right)
\]

\[
= \left[ \frac{d\phi_0(h)}{dJ(h)} \right] \int \frac{d^3p}{(2\pi)^3} v(h - p) \phi_0(p).
\]  \( (9\cdot1\cdot11) \)

Now we need the inverted series. Making use of inversion formulas \( (7\cdot2\cdot4) \) and \( (7\cdot2\cdot5) \), we can solve \( (9\cdot1\cdot11) \) in favour of \( J(h) \) by regarding \( \phi(h) \) on the left-hand side as a quantity of order unity, i.e., the quantity independent of \( v(h) \). The result is given in a very compact form:

\[
J(h) = \phi_0^{-1}[(\phi)(h)] - \int \frac{d^3p}{(2\pi)^3} v(h - p) \phi(p) + O(v^2), \tag{9\cdot1\cdot12}
\]

where \( \phi_0^{-1}[(\phi)] \) is the inverse function of \( \phi_0[J] \). The reason why such a simple formula is obtained is that the factor \( d\phi_0/dJ \) in the inversion formula \( (7\cdot2\cdot5) \) and that of \( \phi_1(h) \) shown above cancels out with each other and \( \phi_0 \) in the integrand becomes \( \phi \) because of \( (7\cdot2\cdot4) \).

In order to see that the equation of state, which is obtained from \( (9\cdot1\cdot12) \) by setting \( J(h) = 0 \), is equivalent to the well-known BCS gap equation, all we have to do is to eliminate \( \phi(h) \) from \( (9\cdot1\cdot12) \) by introducing \( \Delta(h) \) as

\[
\Delta(h) = \int \frac{d^3p}{(2\pi)^3} v(h - p) \phi(p). \tag{9\cdot1\cdot13}
\]

This is an example of the change of the order parameter from \( \phi \) to \( h_0(\phi) \) as discussed in the point (8) of § 7.2.1. Because of \( (9\cdot1\cdot10) \), \( (9\cdot1\cdot11) \) and \( (9\cdot1\cdot13) \), the relation between \( \phi(h) \) and \( \Delta(h) \) is

\[
\phi(h) = \frac{\Delta(h)}{\sqrt{\varepsilon_h^2 + \Delta^2(h)}} \tanh \left( \frac{\sqrt{\varepsilon_h^2 + \Delta^2(h)}}{2} \right), \tag{9\cdot1\cdot14}
\]

and it follows that \( \Delta(h) \) is determined by the following integral equation,
\[ \Delta(k) = \int \frac{d^3p}{(2\pi)^3} v(k-p) \frac{\Delta(p)}{\sqrt{\epsilon_\phi^2 + \Delta^2(p)}} \tanh \left( \frac{\beta \sqrt{\epsilon_\phi^2 + \Delta^2(p)}}{2} \right). \quad (9.1.15) \]

This is precisely the one we call the gap equation. The above result is also obtained of course by direct application of (7.2.4) and (7.2.5).

Next, let us consider the instability of the normal Fermi vacuum and the thermodynamics of the superconductor by using the thermodynamic potential \( \Gamma[\phi] \) defined as the Legendre transform of \( W[J] \),

\[ \Gamma[\phi] = W[J] + V \int \frac{d^3k}{(2\pi)^3} \phi(k) f(k), \quad (9.1.16) \]

where \( \phi(k) \) is given by (9.1.8). Once \( \Gamma[\phi] \) is calculated, various physical properties are discussed in a transparent manner. As already mentioned in Chapter VII, see (7.2.12), the explicit formula for the thermodynamic potential \( \Gamma[\phi] \) can be calculated by integrating (9.1.12) with respect to \( \phi(k) \) since \( \Gamma[\phi] \) satisfies

\[ \frac{\delta \Gamma[\phi]}{\delta \phi(k)} = \frac{V}{(2\pi)^3} f(k). \quad (9.1.17) \]

Differentiating with respect to \( \phi(k) \), it is not difficult to check that \( \Gamma[\phi] \) takes the form,

\[ \frac{\Gamma[\phi]}{V} = \frac{\Gamma[0]}{V} + \int \frac{d^3k}{(2\pi)^3} \phi(k) \phi^{-1}(k) \]

\[ -2\beta^{-1} \int \frac{d^3k}{(2\pi)^3} \left[ \ln \cosh \left( \frac{\beta \sqrt{\epsilon_\phi^2 + \phi^{-1}(k)^2}}{2} \right) \right] - \ln \cosh \left( \frac{\beta \epsilon_\phi}{2} \right) \]

\[ - \int \frac{d^3k d^3p}{4(2\pi)^6} v(k-p) \phi(k) \phi(p), \quad (9.1.18) \]

where the integration constant \( \Gamma[0] \) is nothing but \( W[J=0] \) which is the energy of the normal ground state. This is \( \Gamma[\phi] \) that we are looking for. With the help of \( \Gamma[\phi] \), it is possible to consider the stability of the state characterized by the solution of the equation of state, (9.1.12) with \( J(k)=0 \), by taking the second derivative of \( \Gamma[\phi] \).

Let \( \bar{\phi}(k) \) be a solution of (9.1.12), then the stability is discussed by considering the infinitesimal variation \( \Delta \phi(k) \) from \( \bar{\phi}(k) \). If there exists \( \Delta \phi(k) \) such that \( \Gamma[\phi + \Delta \phi] < \Gamma[\phi] \) or if \( \Delta \phi(k) \) renders the following expression negative,

\[ \Gamma^{(2)}[\Delta \phi] \equiv \frac{1}{2} \int d^2k d^3p \left[ \frac{\delta^2 \Gamma[\phi]}{\delta \phi(k) \delta \phi(p)} \right]_{\phi \to \bar{\phi}} \Delta \phi(k) \Delta \phi(p), \quad (9.1.19) \]

then the state characterized by \( \bar{\phi}(k) \) is unstable. \( \Gamma^{(2)}[\Delta \phi] \) is easily calculated by (9.1.12).

In order to discuss the stability of the normal Fermi vacuum, we choose \( \bar{\phi}(k)=0 \). Here we look for \( \Delta \bar{\phi}(k) \) which minimizes \( \Gamma^{(2)}[\Delta \phi] \) under the constraint,

\[ \int \frac{d^3k}{(2\pi)^3} (\Delta \phi(k))^2 = \text{const}. \]

Introducing the Lagrangian multiplier \( E \), the variation
\[ \Gamma^{(2)}[\Delta \phi] - EV \int \frac{d^3k}{(2\pi)^3} [\Delta \phi(k)]^2 \]

with respect to \( \Delta \phi(k) \) yields the following equation which determines \( \Delta \phi(k) \),

\[ \left\{ \varepsilon \coth\left( \frac{\beta \varepsilon_k}{2} \right) - 2E \right\} \Delta \phi(k) = g \int \frac{d^3p}{(2\pi)^3} \Delta \phi(p). \]  \hspace{1cm} (9.1.20)

We have assumed here that, for the sake of simplicity, the interaction between electrons is local, \( \nu(q) = 2g = \text{const.} \) This equation is equivalent to the eigenvalue equation of the coefficient matrix \( \delta^2 \Gamma/\delta \phi \delta \phi \) of (9.1.19). As is obvious the solution of (9.1.20) takes the form \( \Delta \phi \propto \left\{ \varepsilon \coth(\beta \varepsilon_k/2) - 2E \right\}^{-1} \), so that the Lagrange multiplier \( E \) is determined by the following equation:

\[ 1 = g \int \frac{d^3k}{(2\pi)^3} \left\{ \varepsilon \coth\left( \frac{\beta \varepsilon_k}{2} \right) - 2E \right\}^{-1}. \]  \hspace{1cm} (9.1.21)

By an explicit calculation, the minimum value of \( \Gamma^{(2)}[\Delta \phi] \) is given by

\[ \Gamma^{(2)}[\Delta \phi] = 2EV \int \frac{d^3k}{(2\pi)^3} [\Delta \phi(k)]^2. \]

Therefore we conclude that the normal Fermi vacuum is unstable when \( E < 0 \).

Differentiating both side of (9.1.21) with respect to \( T = \beta^{-1} \), one finds that \( E \) is the monotonically increasing function of \( T \) because

\[ T \frac{dE}{dT} = \left[ \int \frac{d^3p}{(2\pi)^3} \left\{ \varepsilon \coth\left( \frac{\beta \varepsilon_p}{2} \right) - 2E \right\}^{-2} \right]^{-1} \]

\[ \times \int \frac{d^3p}{(2\pi)^3} \frac{\varepsilon_p^2}{\sinh^2(\beta \varepsilon_p/2)} \left\{ \varepsilon \coth\left( \frac{\beta \varepsilon_p}{2} \right) - 2E \right\}^{-2} > 0. \]

It follows that Eq. (9.1.21) allows negative \( E \) when the temperature becomes lower than the superconducting transition temperature \( T_c = \beta_c^{-1} \) defined by (9.1.15) with \( \nu(q) = 2g, \Delta(\mathbf{k}) = 0. \) It is easy to see that (9.1.21) with \( E = 0 \) coincides with (9.1.15) in this case.

We point out here that (9.1.21) is a generalization of Cooper's equation to finite temperature. In fact, when we take the limit \( T \to 0 \), Eq. (9.1.21) coincides with the well-known Cooper's instability equation.

Up to now, the instability of the normal Fermi vacuum is discussed. Now we are going to investigate several thermodynamic quantities characterizing the superconducting state to show that (9.1.18) is applicable to any of the equilibrium phenomena.

For our purpose, it is convenient to change the variable of \( \Gamma[\phi] \) to \( \varphi(\mathbf{k}) = \phi^{-1}[\phi](\mathbf{k}) \). We use \( \varphi(\mathbf{k}) \) for \( \Delta(\mathbf{k}) \) in order to avoid confusion; the energy gap \( \Delta(\mathbf{k}) \) is defined by the stationary condition: \( \delta \Gamma[\varphi]/\delta \varphi(\mathbf{k}) = 0 \) at \( \varphi(\mathbf{k}) = \Delta(\mathbf{k}) \). For simplicity, \( \varphi(\mathbf{k}) \) is hereafter assumed to be independent of \( \mathbf{k} \). Then \( \Gamma[\varphi] \equiv \Gamma[\varphi(\mathbf{k})] \) takes the form,

\[ \Gamma[\varphi]/V = \Gamma[0]/V + \int \frac{d^3k}{(2\pi)^3} \frac{\varphi^2}{\sqrt{\varepsilon_k^2 + \varphi^2}} \tanh\left( \frac{\beta \sqrt{\varepsilon_k^2 + \varphi^2}}{2} \right) \]
\[-2\beta^{-1}\int \frac{d^3k}{(2\pi)^3} \left\{ \ln \left[ \cosh \left( \frac{\beta \sqrt{\varepsilon_k^2 + \varphi^2}}{2} \right) \right] - \ln \left[ \cosh \left( \frac{\beta \varepsilon_k}{2} \right) \right] \right\} \]
\[-\frac{1}{2}g \int \frac{d^3k d^3p}{(2\pi)^6} \frac{\varphi^2}{\sqrt{\varepsilon_k^2 + \varphi^2 \varepsilon_p^2 + \varphi^2}} \times \tanh \left( \frac{\beta \sqrt{\varepsilon_k^2 + \varphi^2}}{2} \right) \tanh \left( \frac{\beta \sqrt{\varepsilon_p^2 + \varphi^2}}{2} \right) . \tag{9.1.22} \]

In order to see that Eq. (9.1.22) is exactly the thermodynamic potential, let us now consider the temperature near the critical value $T_c$. Since the normal-super phase transition is second order, it is allowed to expand $\Gamma[\varphi]$ with respect to $\varphi$ looking upon $\varphi$ as small:

\[
\Gamma[\varphi]/V = \Gamma[0]/V + \frac{1}{2} \{ 1 - g A(\beta) \} A(\beta) \varphi^2
+ \frac{1}{8} \{ 3 - 4 g A(\beta) \} B(\beta) \varphi^4 + O(\varphi^6), \tag{9.1.23} \]

where the coefficients $A(\beta)$ and $B(\beta)$ are expressed by familiar integrals, \textsuperscript{4)

\[
A(\beta) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\varepsilon_k} \tanh \left( \frac{\beta \varepsilon_k}{2} \right) = \frac{1}{\beta \pi^2} \sum_{s=-\infty}^{\infty} \int \frac{k^2 dk}{(2s+1)^2 \pi^2 \beta^{-2} + \varepsilon_k^2} = N_0 \ln \left( \frac{2 \beta \gamma \omega_0}{\pi} \right), \]

\[
B(\beta) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\varepsilon_k^3} \left[ \frac{(\beta \varepsilon_k)}{2 \cosh^2 \left( \frac{\beta \varepsilon_k}{2} \right)} - \tanh \left( \frac{\beta \varepsilon_k}{2} \right) \right]
= - \frac{2}{\beta \pi^2} \sum_{s=-\infty}^{\infty} \int \frac{k^2 dk}{((2s+1)^2 \pi^2 \beta^{-4} + \varepsilon_k^2)^2} = - \frac{7 \xi(3) \beta^2}{4 \pi^2} N_0 . \]

Here $N_0 = m k_F / \pi^2$ is the density of states at the Fermi level, $k_F$ the Fermi momentum, $\ln \gamma C = 0.577\ldots$ Euler's constant, $\omega_0$ the Debye energy (so as to cut-off the energy integral) and $\xi(3)$ Riemann's zeta function.

The critical temperature $T_c$ defined by (9.1.15) with $\Delta(\mathbf{k}) = 0$ and $\nu(\mathbf{k} - \mathbf{p}) = 2g$ is evaluated as

\[
T_c = \frac{2 \gamma \omega_0}{\pi} \exp \left( \frac{1}{g N_0} \right) , \]

and Eq. (9.1.23) can be expressed as

\[
\Gamma[\varphi]/V = \Gamma[0]/V + \frac{1}{2} \left\{ a(T) \varphi^2 + \frac{1}{4} \beta(T) \varphi^4 \right\} , \tag{9.1.24} \]

where the definitions of $a(T)$ and $\beta(T)$ are

\[
a(T) = - N_0 (1 + g N_0 \ln(T_c/T)) , \]
\[\beta(T) = \frac{7 \xi(3)}{4 \pi^2 T^2} N_0 (1 + 4 g N_0 \ln(T_c/T)) . \tag{9.1.25} \]
Expanding (9.1.24) up to first order of $T_c - T$, it coincides with the function what we call the Ginzburg-Landau free energy without spatial derivative term.

The formula for the energy gap at $T \lesssim T_c$ is easily obtained by the stationary condition of $\Gamma[\varphi]$ at $\varphi = \Delta$, we have

$$\Delta^2 = \frac{8\pi^2 T^2}{7\xi(3)} \left( \frac{1 + gN_0 \ln(T_c/T)}{1 + 4gN_0 \ln(T_c/T)} \right) \ln(T_c/T). \quad (9.1.26)$$

This result is, of course, equivalent to the one obtained by (9.1.15). The difference of the free energy between superconducting ($\varphi = \Delta$) and normal ($\varphi = 0$) state is evaluated from (9.1.24) and (9.1.25),

$$\frac{\Gamma[\Delta]}{V} - \frac{\Gamma[0]}{V} = -\frac{2\pi^2 T^2}{7\xi(3)} N_0 \left( \frac{1 + gN_0 \ln(T_c/T)}{1 + 4gN_0 \ln(T_c/T)} \right)^2 \ln(T_c/T)^2. \quad (9.1.27)$$

If we expand (9.1.26) and (9.1.27) up to first order of $T_c - T$, they precisely coincide with those of the formulae evaluated by the conventional BCS variational approach.

§ 9.2. Application to non-equilibrium system

9.2.1. Hamiltonian

In this section, the time-dependent phenomenon is discussed within our formalism. We adopt a model Hamiltonian which contains explicitly the phonon degrees of freedom. The reason why the electron-phonon Hamiltonian is employed rather than the BCS Hamiltonian of previous section is to take into account of the inelastic collisions between electron and phonon, which plays the most important role in dissipation and the decay of an elementary excitation. In order to see this, let us recall that the decay rate of an elementary excitation $\gamma_p$ is expressed as the imaginary part of the self-energy of the retarded Green’s function, $\Sigma_R(\epsilon_p, \mathbf{p})$,

$$\gamma_p = 2|\text{Im} \Sigma_R(\epsilon_p, \mathbf{p})|,$$

where $\epsilon_p$ is the energy of an elementary excitation with momentum $\mathbf{p}$. However, if one assumes the BCS Hamiltonian as a low energy effective theory, then the lowest Hartree-Fock diagrams, which explain most of the equilibrium properties, do not give rise to the dissipative effect because the first order self-energy is a real function in this approximation. On the other hand, it is possible to discuss the dissipative phenomena by using the electron-phonon Hamiltonian and by taking one-phonon exchange diagram into account. This is an important point because we have in mind the application of inversion method in the lowest order form.

In the following discussions, the reminiscence of the initial correlation can also be well described by the electron-phonon Hamiltonian in the first order perturbative calculation while the BCS Hamiltonian cannot. This is also due to the fact that the interaction between electrons occurs at single time in the lowest order of BCS Hamiltonian whereas the electron-phonon Hamiltonian produces the lowest order self-energy which is non-local in time.

Consider the Hamiltonian under the external electromagnetic field,
\[ \tilde{H}(t) = \tilde{H}_{el} + \tilde{H}_{ph} + \tilde{H}_{em}(t) + \tilde{H}_{int}, \]  

where \( \tilde{H}_{el}, \tilde{H}_{ph}, \tilde{H}_{em}(t) \) and \( \tilde{H}_{int} \) represent the Hamiltonians for non-interacting electrons, non-interacting phonons, interaction between electron and external electromagnetic field and interaction between electron and phonon, respectively.

Besides electron operators \( \tilde{a}_a(\mathbf{k}) \) and \( \tilde{a}_a^+(\mathbf{k}) \) \((a=\text{up or down})\), let us introduce the annihilation and creation operators of (longitudinal) phonon with momentum \( \mathbf{k} \), by \( \tilde{b}(\mathbf{k}) \) and \( \tilde{b}^+(\mathbf{k}) \). The explicit form of \( \tilde{H}_{el} \) and \( \tilde{H}_{ph} \) are written as follows,

\[ \tilde{H}_{el} = \int \frac{d^3k}{(2\pi)^3} \varepsilon_k \tilde{a}_a^+(\mathbf{k}) \tilde{a}_a(\mathbf{k}) , \]  

\[ \tilde{H}_{ph} = \int \frac{d^3k}{(2\pi)^3} \omega_k \tilde{b}^+(\mathbf{k}) \tilde{b}(\mathbf{k}) , \]  

where \( \varepsilon_k = (k^2/2m) - \mu \) and \( \omega_k = |\mathbf{k}| \) \((u \text{ is the velocity of sound})\) are the energy of a free electron and phonon with momentum \( \mathbf{k} \), respectively. Here, as in § 9.1, the level of the chemical potential \( \mu \) is chosen as the zero of the energy of free electron and, for the time being, all operators are defined in the Schrödinger representation.

In our discussion, the system is brought into the non-equilibrium state by changing the external electromagnetic field so that the time evolution of the system is governed by the interaction Hamiltonian between electrons and the external electromagnetic field, \( \tilde{H}_{em}(t) \). Introducing the vector and scalar potentials as \( A(\mathbf{k}, t) \) and \( A_\theta(\mathbf{k}, t) \), the explicit form of \( \tilde{H}_{em}(t) \) is written as follows,

\[ \tilde{H}_{em}(t) = -\int \frac{d^3k d^3p}{(2\pi)^6} f(\mathbf{k}, \mathbf{p}; t) \tilde{a}_a^+(\mathbf{k}) \tilde{a}_a(\mathbf{p}) , \]  

\[ f(\mathbf{k}, \mathbf{p}; t) = - eA_\theta(\mathbf{k} - \mathbf{p}, t) + \frac{e}{2m} (\mathbf{k} + \mathbf{p}) \cdot A(\mathbf{k} - \mathbf{p}, t) \]  

\[ -\frac{e^2}{2m} \int \frac{d^3q}{(2\pi)^3} A(\mathbf{k} - \mathbf{q}, t) \cdot A(\mathbf{q} - \mathbf{p}, t) . \]  

Here, as in the most discussions on the electromagnetic properties of superconductors, the electromagnetic field is not quantized but is treated as a purely classical object in order to make the discussion simple.

The interaction Hamiltonian between electron and phonon, that is regarded as the perturbation in what follows, is of course

\[ \tilde{H}_{int} = \int \frac{d^3k d^3p}{(2\pi)^6} \lambda(\mathbf{k} - \mathbf{p}) \tilde{a}_a^+(\mathbf{k}) \tilde{a}_a(\mathbf{p})(\tilde{b}^+(\mathbf{k} - \mathbf{p}) + \tilde{b}(\mathbf{p} - \mathbf{k})) , \]  

where \( \lambda(\mathbf{k}) \) is the electron-phonon coupling constant.

Just as in the case of BCS Hamiltonian (9.1.1), Eq. (9.2.1) has the first kind gauge symmetry (9.1.4) and this symmetry is broken spontaneously in the superconducting state. Moreover, here we want to consider the time-dependent, spatially varying superconducting order of the system. It is therefore necessary to choose the source term as to break the translational symmetry in space-time as well as the symmetry (9.1.4). Thus the following form of the source term is chosen:
\[ \tilde{H}(t) = -\int \frac{d^3k d^3p}{(2\pi)^6} \{ J(\mathbf{k}, \mathbf{p}; t) \tilde{\alpha}^\dagger(\mathbf{k}) \tilde{\alpha}^\dagger(-\mathbf{p}) + J^*(\mathbf{p}, \mathbf{k}; t) \tilde{\alpha}_i(-\mathbf{p}) \tilde{\alpha}_i(\mathbf{k}) \}, \]  

(9.2.7)

where the complex conjugate of \( J^*(\mathbf{k}, \mathbf{p}; t) \) coincides with \( J(\mathbf{p}, \mathbf{k}; t) \) in order to make \( \tilde{H}(t) \) Hermitian.

9.2.2. Perturbation series for contour-ordered Green's function

Let us now consider the contour-ordered Green's function in the Nambu representation defined by

\[ \langle T_c \tilde{\Psi}_\mu(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \rangle = \frac{\text{Tr}[T_c \tilde{\Psi}_\mu(\mathbf{k}_1, \tau_1) \tilde{\Psi}_\nu^\dagger(\mathbf{k}_2, \tau_2)]}{\text{Tr}[\tilde{U}_c(t_i - i\beta, t_i)]}, \]  

(9.2.8)

where \( \tau_1 \) and \( \tau_2 \) specify the points on the contour defined below. Here the contour ordering operator \( T_c \) emerges as a generalization of the time ordering operator and it orders operators in a sense of the contour, which starts at \( \tau = t_i \) and runs along the real time axis to \( \tau = t_F \) (\( t_F > \max(\text{Re} \tau_1, \text{Re} \tau_2) \)) and returns to \( \tau = t_i \) parallel to the real time axis and then continues to \( \tau = t_i - i\beta \) along the imaginary time axis (Fig. 9.1). Here \( \beta^{-1} = T \) is the temperature of the system at initial time which is assumed to be in the equilibrium state.

The quantities \( \tilde{\Psi}_\mu(\mathbf{k}_1, \tau_1) \) and \( \tilde{\Psi}_\nu^\dagger(\mathbf{k}_2, \tau_2) \) are the Nambu pseudo spinors in the “Heisenberg” representation given by

\[ \tilde{\Psi}_\mu(\mathbf{k}, \tau) = \tilde{U}_c^{-1}(\tau, t_i)(\tilde{\alpha}_\mu(\mathbf{k}) \tilde{\alpha}^\dagger(-\mathbf{k})), \]

\[ \tilde{\Psi}_\nu^\dagger(\mathbf{k}, \tau) = \tilde{U}_c^{-1}(\tau, t_i)(\tilde{\alpha}^\dagger(\mathbf{k}), \tilde{\alpha}_\nu(-\mathbf{k})), \]  

(9.2.9)

where \( \tilde{U}_c(\tau, t_i) \) stands for the “time evolution” operator defined along the contour:

\[ \tilde{U}_c(\tau, t_i) \equiv T_c \exp \left[ -i \int_c d\tau'(\tilde{H}(\text{Re}\tau')) \right. \]

\[ + \tilde{H}(\text{Re}\tau') \left] \right. \]  

(9.2.10)

The \( \tau' \)-integration in (9.2.10) is along a contour connecting the initial \( \tau' = t_i \) and an arbitrary point \( \tau' = \tau \) on the contour. The meaning of the notation \( \tilde{H}(\text{Re}\tau) \) is that if \( \tau \) is on the contour parallel to the imaginary-time axis then it takes the value \( \tilde{H}(t_i) \) otherwise \( \tilde{H}(\tau) \).

From (9.2.9) and (9.2.8), we find that \( \langle T_c \tilde{\Psi}_\mu(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \rangle \) and \( \langle T_c \tilde{\Psi}_\nu^\dagger(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \rangle \) represent the contour-ordered Green's

Fig. 9.1. The contour on the complex time plane. The label \( a \) takes the values 1, 2 and 3, which specify three segments of contour: from \( t_i \) to \( t_F \), \( t_F \) to \( t_i \) and \( t_i \) to \( t_i - i/T \).
function for up spin electrons and down spin holes, respectively. On the other hand, the off-diagonal (i.e., $\mu \neq \nu$) components $G_{12}(k_1, \tau_1; k_2, \tau_2)$ and $G_{21}(k_1, \tau_1; k_2, \tau_2)$ are the anomalous Green's functions describing the superconducting order. This is seen as follows. Consider the equal-time limit of (9.2.8)

$$\lim_{\tau_2-\tau_1 \to 0} G_{\mu \nu}(k_1, \tau_1; k_2, \tau_2) = \langle \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_1) \rangle = \begin{pmatrix} \langle \tilde{a}_+(k_1, \tau_1) \tilde{a}_+^*(k_2, \tau_1) \rangle & \langle \tilde{a}_+(k_1, \tau_1) \tilde{a}_-(k_2, \tau_1) \rangle \\ \langle \tilde{a}_-(k_1, \tau_1) \tilde{a}_+^*(k_2, \tau_1) \rangle & \langle \tilde{a}_-(k_1, \tau_1) \tilde{a}_-(k_2, \tau_1) \rangle \end{pmatrix}_{\mu \nu}, \quad (9.2.11)$$

where $\epsilon$ is the infinitesimal positive quantity and

$$\tilde{a}_+^*(k, \tau) \equiv U_c^{-1}(\tau, t_i) \tilde{a}_+^*(k) U_c(\tau, t_i).$$

If $\tau_1$ is on the branch parallel to the real time axis, i.e., $t_1 \leq \text{Re} \tau_1 \leq t_\tau$, then the off-diagonal components of (9.2.11) give the expectation value of the local product of annihilation or creation operators at $\tau_1$, while if it is on the branch parallel to the imaginary time axis, i.e., $-\beta \leq \text{Im} \tau_1 \leq 0$ then, because of the cyclic invariance of trace, Eq. (9.2.11) gives the expectation value of the same operators at initial time $t_i$.

In practical calculations, it is often more convenient to use matrix representation of the contour-ordered Green's function rather than (9.2.8) itself. In order to give its explicit definition, let us introduce the index of Keldysh space $a, b, \cdots$ in order to specify the three segments of the contour: the branch starting from $t=t_i$ to $t=t_\tau$ corresponds to $a=1$, and that from $t=t_\tau$ to $t=t_i$ corresponds to $a=2$ and that from $t=t_i$ to $t=t_i - i\beta$ to $a=3$. Since the contour-ordered Green's function has two "time" arguments, there are nine distinct possibilities to classify these two parameters. The matrix representation of the contour-ordered Green's function is introduced by mapping each of nine possibilities onto a corresponding component of $3 \times 3$ matrix:

$$G^{ab}_{\mu \nu}(k_1, \tau_1; k_2, \tau_2) = \begin{pmatrix} \langle T \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) \rangle & \langle \tilde{\Psi}_\mu^*(k_2, \tau_2) \tilde{\Psi}_\mu(k_1, \tau_1) \rangle & i\langle \tilde{\Psi}_\mu^*(k_2, \tau_2) \tilde{\Psi}_\mu(k_1, \tau_1) \rangle \\ -\langle \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) \rangle & \langle T \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) \rangle & -i\langle \tilde{\Psi}_\mu^*(k_2, \tau_2) \tilde{\Psi}_\mu(k_1, \tau_1) \rangle \\ -i\langle \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) \rangle & i\langle \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) \rangle & \langle T \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) \rangle \end{pmatrix}^{ab}, \quad (9.2.12)$$

where the row index denotes the position of $\tau_1$ while the column index refers to the position of $\tau_2$. Operators $T$ and $\bar{T}$ stand for the ordinary time ordering and the anti-time ordering operator defined by

$$\bar{T} \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) = \theta(\tau_2-\tau_1) \tilde{\Psi}_\mu(k_1, \tau_1) \tilde{\Psi}_\nu^*(k_2, \tau_2) - \theta(\tau_1-\tau_2) \tilde{\Psi}_\nu^*(k_2, \tau_2) \tilde{\Psi}_\mu(k_1, \tau_1), \quad (9.2.13)$$

respectively, while $T_r$ denotes the $r$-ordering operator. In (9.2.12), we have introduced, for the sake of notational convenience, Heisenberg and Matsubara representation defined by
\( \tilde{\Psi}_{\mu}(k, t) \equiv \tilde{U}(t, t_i) \tilde{\Theta}_{\mu}(k) \tilde{U}(t, t_i) \),

\( \tilde{\Theta}_{\mu}(k, \tau) \equiv \tilde{\rho}^{-1}(\tau, 0) \tilde{\Theta}_{\mu}(k) \tilde{\rho}(\tau, 0) \), \hspace{1cm} (9.2.14)

where \( \tilde{\rho}(\tau, \tau') \) and \( \tilde{U}(t, t') \) are the density matrix and the time evolution operator, respectively, whose definitions are

\[ \tilde{U}(t, t') \equiv \text{Exp} \left[ -i \int_{t'}^{t} dt'' (\tilde{H}(t'') + \tilde{H}_f(t'')) \right], \]  

\[ \tilde{\rho}(\tau, \tau') \equiv \text{Exp} \left[ -(\tau - \tau')(\tilde{H}(t_i) + \tilde{H}_f(t_i)) \right] \]  

with \( t_i \leq t, t' \leq t_f \) and \( 0 \leq \tau, \tau' \leq \beta \). In addition, \( \langle \cdots \rangle \) represents the ensemble average given by the density matrix \( \tilde{\rho}(\beta, 0) \). In (9.2.14), we have employed the same symbol “\( \dagger \)” to express the Matsubara representation of \( \tilde{\Theta}_{\mu}(k) \), although \( \tilde{\Theta}_{\mu}(k, \tau) \) is no longer Hermitian conjugate of \( \tilde{\Theta}_{\mu}(k, \tau) \).

From (9.2.12), one may immediately observe that the left upper edge of the 2 × 2 submatrix coincides with the contour-ordered Green’s function in the Schwinger-Keldysh’s theory, \( a = b = 3 \) component represents familiar temperature Green’s function. The remaining components \( G_{a2}^{\mu\nu} \) and \( G_{22}^{\mu\nu} (a = 1, 2) \) are inherent to our theory, which describes the correlation between the operators defined at \( t = t_i \) and \( t \geq t_i \). If the adiabatic hypothesis is taken into account, all these components vanish in the limit \( t_i \to -\infty \). In such an occasion, the temperature Green’s function is no longer mixed with the 2 × 2 submatrix components in the perturbation series of the Green’s function, so that only the components of 2 × 2 submatrix emerge in the formulas of the expectation value of operators at \( t \gg t_i \sim -\infty \). This 3 × 3 representation of the contour-ordered Green’s function is nothing but the one introduced by Wagner\(^9\) and by Fukuda et al.,\(^9,10\) where they have extended the quantum transport theory of Keldysh to the case of arbitrary initial time \( t_i \). While the operator formalism is exclusively used in the original Wagner’s theory, it has been shown in Ref. 3) that the 3 × 3 representation of the contour-ordered Green’s function can be quite naturally obtained by calculating functional derivatives of the generating functional. This formalism has great advantages in two respects: the first is that it is possible to treat the real-time many-particle Green’s functions and the initial correlations on the same footing, and the second is that the well-known Feynman-Dyson perturbation theory can be utilized as discussed in detail by Fukuda et al.,\(^9,10\)

While the 3 × 3 matrix representation of the contour-ordered Green’s function introduced in (9.2.12) is most convenient for calculation, it is somewhat complicated to reduce it to the measurable quantities because of the appearance of the nine correlation functions. On the other hand, it is observed from (9.2.12) that all the components of the contour-ordered Green’s function are not linearly independent but there are only five independent matrix elements in it because

\[
G_{12}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -\theta(\tau_1 - \tau_2)G_{22}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2) - \theta(\tau_2 - \tau_1)G_{12}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[
G_{22}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -\theta(\tau_1 - \tau_2)G_{22}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2) - \theta(\tau_2 - \tau_1)G_{22}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[
G_{13}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -G_{23}^{\mu\nu}(k_1, \tau_1; k_2, \tau_2),
\]
\[ G^{31}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -G^{32}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2). \]  

(9.2.17)

It is therefore possible to transform this \(3 \times 3\) matrix so that the number of the non-vanishing matrix elements is minimized and we can remove part of redundancy. Such a transformation is easily achieved by introducing the following unitary transformation:

\[ X^{ab} \mapsto X^{ab} = (R^{-1}XR)^{ab}, \]  

(9.2.18)

where \(X^{ab}\) represents symbolically some element of the Keldysh space such as the contour-ordered Green's function or the self-energy part and so forth. Here the definition of the \(3 \times 3\) unitary matrix \(R\) is

\[ R = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}, \quad R^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}. \]  

(9.2.19)

In what follows we call this representation as the "physical" representation* because every component in this representation has a direct contact with measurable quantities.

Making use of (9.2.12) and (9.2.18), we find that the physical representation of the contour-ordered Green's function turns out to be given as follows,

\[ G^{ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \begin{pmatrix} G^{11}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & G^{12}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & G^{13}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) \\ G^{21}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & 0 & 0 \\ G^{31}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & 0 & G^{33}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) \end{pmatrix}^{ab}, \]  

(9.2.20)

where the explicit form of each component is

\[ G^{11}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \langle \varphi_{\mu}(k_1, \tau_1), \varphi_{\nu}^*(k_2, \tau_2) \rangle, \]
\[ G^{12}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \theta(\tau_1 - \tau_2) \langle \varphi_{\mu}(k_1, \tau_1), \varphi_{\nu}^*(k_2, \tau_2) \rangle, \]
\[ G^{13}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = i\sqrt{2} \langle \psi_{\mu}(k_2, \tau_2), \varphi_{\nu}^*(k_1, \tau_1) \rangle, \]
\[ G^{21}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -\theta(\tau_2 - \tau_1) \langle \varphi_{\mu}(k_1, \tau_1), \varphi_{\nu}^*(k_2, \tau_2) \rangle, \]
\[ G^{23}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -i\sqrt{2} \langle \psi_{\mu}(k_1, \tau_1), \varphi_{\nu}^*(k_2, \tau_2) \rangle, \]
\[ G^{31}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = -\langle \psi_{\mu}(k_1, \tau_1), \psi_{\nu}^*(k_2, \tau_2) \rangle. \]  

(9.2.21)

The correlation functions \(G^{12}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2), G^{13}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) and \(G^{33}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) are, of course, the retarded, advanced and temperature Green's functions, respectively. On the other hand, \(G^{11}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\), which is often called the Keldysh function, plays the essential role of the Keldysh's theory. Roughly speaking, this correlation function corresponds to the distribution function of the electron in the non-equilibrium state. The remaining functions describe the correlation of long time effect of particles in the initial density matrix. Although the representation of (9.2.20) still has

* This terminology is due to Chou et al., while in Ref. 8) is called the \textit{rak} representation.
more than five non-vanishing components, it seems to be the best form attainable. Since, in general, the Hermite conjugate of the retarded Green’s function is the advanced Green’s function, one observes that there are only five independent components in (9·2·20). In the following discussion, we use exclusively the contour-ordered Green’s function in the physical representation, so that overline above the correlation functions will be omitted.

Without specifying the explicit form of the electromagnetic potential $A_0(\mathbf{k}, t)$ and $\mathbf{A}(\mathbf{k}, t)$, even the leading term of the perturbation series, i.e., Green’s function in the absence of the electron-phonon interaction, cannot be obtained. Nevertheless, it is possible to define implicitly but uniquely the perturbation series for the contour-ordered Green’s function through an integral equation.

As shown in Refs. 3) and 5), the contour-ordered Green’s function for free electron (the source term, electromagnetic field and electron-phonon interaction are all absent) can be exactly obtained through the functional integral formalism. Explicit form of each component is written as follows,

\[
\begin{align*}
G_{11}(\mathbf{k}; \tau_1, \tau_2) = & (1 - \frac{i}{2} \Delta_{\mathbf{k}}(\mathbf{k})) [ \tau_1 \cos \varepsilon(\tau_1 - \tau_2) - i \tau_1 \sin \varepsilon(\tau_1 - \tau_2) ]_{\tau_1, \tau_2} , \\
G_{12}(\mathbf{k}; \tau_1, \tau_2) = & \theta(\tau_1 - \tau_2) [ \tau_1 \cos \varepsilon(\tau_1 - \tau_2) - i \tau_1 \sin \varepsilon(\tau_1 - \tau_2) ]_{\tau_1, \tau_2} , \\
G_{21}(\mathbf{k}; \tau_1, \tau_2) = & -\theta(\tau_2 - \tau_1) [ \tau_1 \cos \varepsilon(\tau_1 - \tau_2) - i \tau_1 \sin \varepsilon(\tau_1 - \tau_2) ]_{\tau_1, \tau_2} , \\
G_{13}(\mathbf{k}; \tau_1, \tau_2) = & \frac{i}{\sqrt{2 \cosh(\frac{\beta_{\mathbf{k}}}{2})}} \left\{ [ \tau_1 \cos \varepsilon(\tau_1 - \tau_2) - i \tau_1 \sin \varepsilon(\tau_1 - \tau_2) ] \right. \\
& \times \left[ \tau_1 \cosh \varepsilon(\frac{\tau_1 - \beta}{2}) - \tau_1 \sinh \varepsilon(\frac{\tau_1 - \beta}{2}) \right]_{\tau_1, \tau_2} , \\
G_{31}(\mathbf{k}; \tau_1, \tau_2) = & -\frac{i}{\sqrt{2 \cosh(\frac{\beta_{\mathbf{k}}}{2})}} \left\{ [ \tau_1 \cos \varepsilon(\tau_1 - \tau_2) - i \tau_1 \sin \varepsilon(\tau_1 - \tau_2) ] \\
& \times \left[ \tau_1 \cosh \varepsilon(\frac{\tau_1 - \beta}{2}) + i \tau_1 \sin \varepsilon(\tau_1 - \tau_2) \right]_{\tau_1, \tau_2} , \\
G_{33}(\mathbf{k}; \tau_1, \tau_2) = & -\frac{\theta(\tau_1 - \tau_2)}{2 \cosh(\frac{\beta_{\mathbf{k}}}{2})} \left[ \tau_1 \cosh \varepsilon(\tau_1 - \tau_2) - \tau_1 \sinh \varepsilon(\tau_1 - \tau_2) - \frac{\beta}{2} \right]_{\tau_1, \tau_2} \right. \\
& \left. + \frac{\theta(\tau_2 - \tau_1)}{2 \cosh(\frac{\beta_{\mathbf{k}}}{2})} \left[ \tau_1 \cosh \varepsilon(\tau_1 - \tau_2 + \frac{\beta}{2}) - \tau_1 \sinh \varepsilon(\tau_1 - \tau_2 + \frac{\beta}{2}) \right]_{\tau_1, \tau_2} , \\
G_{22}(\mathbf{k}; \tau_1, \tau_2) = & G_{33}(\mathbf{k}; \tau_1, \tau_2) = G_{23}(\mathbf{k}; \tau_1, \tau_2) = 0 .
\end{align*}
\]
Fermi distribution function, \( n_F(\mathbf{k}) = \frac{1}{\exp(\beta \varepsilon_b) + 1} \), appears only in the expression of the Keldysh function \( \mathcal{G}^{(1)}_{\mu \nu} \) is one of the evidence that this correlation function acts as a particle distribution function in our theory. Making use of \( \mathcal{G}_{\mu \nu}^{(2)}(\mathbf{k}_1, \mathbf{r}_1, \mathbf{r}_2) \), the contour-ordered Green's function in the absence of the electron-phonon interaction is given uniquely as a solution of the following integral equation corresponding to the Feynman diagram given in Fig. 9.2:

\[
G^{(0)ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{r}_1; \mathbf{k}_2, \mathbf{r}_2) = (2\pi)^3 \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}_2) \mathcal{G}^{(2)}_{\mu \nu}(\mathbf{k}_1, \mathbf{r}_1, \mathbf{r}_2) + i \int d\tau \int \frac{d^3q}{(2\pi)^3} \mathcal{G}^{ac}_{\mu \alpha}(\mathbf{k}_1, \mathbf{r}, \tau)f^{cd}_{\mu \alpha}(\mathbf{k}, \mathbf{q}, \mathbf{r})G^{(0)ab}_{\beta \nu}(\mathbf{q}, \mathbf{r}; \mathbf{k}_2, \mathbf{r}_2). \tag{9.2.23}
\]

Here, for the sake of notational convenience, we have introduced \( f^{ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{k}_2; \tau) \) defined by

\[
f^{ab}_{\mu \nu}(\mathbf{k}, \mathbf{p}; \tau) = \begin{pmatrix} 0 & f^{ab}_{\mu \nu}(\mathbf{k}, \mathbf{p}; \tau) & 0 \\ f^{ab}_{\mu \nu}(\mathbf{k}, \mathbf{p}; \tau) & 0 & 0 \\ 0 & 0 & i f^{ab}_{\mu \nu}(\mathbf{k}, \mathbf{p}; \tau) \end{pmatrix}, \tag{9.2.24}
\]

where \( f^{ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{k}_2; \tau) \) is expressed in terms of \( f(\mathbf{k}_1, \mathbf{k}_2; \tau) \) of \((9.2.5)\) and \( J^{(a)}(\mathbf{k}_1, \mathbf{k}_2; \tau) \) defined in \((9.2.7)\) as follows,

\[
f^{ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{k}_2; \tau) = \begin{pmatrix} f(\mathbf{k}_1, \mathbf{k}_2; \tau) & J(\mathbf{k}_1, \mathbf{k}_2; \tau) \\ J^{*}(\mathbf{k}_1, \mathbf{k}_2; \tau) & -f(-\mathbf{k}_2, -\mathbf{k}_1; \tau) \end{pmatrix}. \tag{9.2.25}
\]

In the \( 3 \times 3 \) matrix representation of contour-ordered Green's function, the region of \( r \)-integration depends on the position of \( \tau \) on the contour: if \( \tau \) is on the branch parallel to the real time axis then it extends from \( t_i \) to \( t_f \), while if it is on the \( a=3 \) branch it extends from 0 to \( \beta \). It follows that, in \((9.2.23)\), \( \tau \)-integration is performed in the range \([t_i, t_f]\) when \( c=1, 2 \) otherwise in the range \([0, \beta]\). Owing to the matrix structure of \( f^{ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{k}_2; \tau) \), i.e., \( f^{ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{k}_2; \tau) = f^{ab}_{\mu \nu}(\mathbf{k}_1, \mathbf{k}_2; \tau) = 0 \) \((a=1, 2)\), the region of the \( r \)-integration is consistently determined if we look at the index \( d \) instead.

Fig. 9.3. Diagrams representing the one-phonon exchange correction terms for the contour-ordered Green's function. \((a)\) represents the Hartree term which is insensitive for the superconducting state while \((b)\) corresponding to the Fock term, is responsible for the order parameter.
Now electron-phonon interaction is taken into account. Up to the order of one-phonon exchange, the correction term for contour-ordered Green's function is obtained by considering the Feynman diagrams given in Fig. 9.3. The physical meaning of (a) of Fig. 9.3 is of course the correction due to the Hartree approximation whereas the (b) corresponding to the Fock term. In what follows, just as in the investigations on the strong coupling superconductivity, the Hartree term will be neglected because the role of this term is only to give the energy shift of the electron. By a straightforward calculation, the result is expressed as follows:

\[
G^{(1)ab}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2)
= - \int \mathbf{d} \tau \int \mathbf{d} \tau' \int \frac{d^3 \mathbf{p}_1 d^3 \mathbf{p}_2}{(2\pi)^6} \left( G^{(0)ac}_{\rho\nu}(k_1, \tau_1; p_1, \tau) \right) \tau_3 \sum_{cd} \left( p_1, \tau \; p_2, \tau' \right) \times \tau_5 G^{(0)db}(p_2, \tau'; k_2, \tau_5) \right)_{\rho\nu} .
\]

(9.2.26)

Here the self-energy of the contour-ordered Green's function (in the physical representation) \( \Sigma^{ab}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) \) takes the following matrix form:

\[
\Sigma^{ab}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = \begin{pmatrix}
0 & \Sigma^{12}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) & 0 \\
\Sigma^{21}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) & \Sigma^{22}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) & \Sigma^{23}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) \\
0 & \Sigma^{32}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) & \Sigma^{33}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2)
\end{pmatrix}^{ab},
\]

(9.2.27)

and the explicit form of each component is written as:

\[
\Sigma^{12}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = \theta(\tau_2 - \tau_1) \tau_5 \Sigma^{\tau}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[
\Sigma^{21}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = - \theta(\tau_1 - \tau_2) \tau_5 \Sigma^{\tau}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[
\Sigma^{22}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = \Sigma^{\tau}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[
\Sigma^{23}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = -2 \int \frac{d^3 \mathbf{q}}{(2\pi)^3} |\lambda(\mathbf{q})|^2 D^{13}(\mathbf{q}; \tau_1, \tau_2) \Sigma^{013}_{\rho\nu}(k_1 - \mathbf{q}, \tau_1; k_2 - \mathbf{q}, \tau_2),
\]

\[
\Sigma^{32}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = -2 \int \frac{d^3 \mathbf{q}}{(2\pi)^3} |\lambda(\mathbf{q})|^2 D^{31}(\mathbf{q}; \tau_1, \tau_2) \Sigma^{031}_{\rho\nu}(k_1 - \mathbf{q}, \tau_1; k_2 - \mathbf{q}, \tau_2),
\]

\[
\Sigma^{33}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = 2 \int \frac{d^3 \mathbf{q}}{(2\pi)^3} |\lambda(\mathbf{q})|^2 D^{33}(\mathbf{q}; \tau_1, \tau_2) \Sigma^{033}_{\rho\nu}(k_1 - \mathbf{q}, \tau_1; k_2 - \mathbf{q}, \tau_2),
\]

(9.2.28)

where we have introduced \( \Sigma^{\tau}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) \) defined by

\[
\Sigma^{\tau}_{\rho\nu}(k_1, \tau_1; k_2, \tau_2) = - \int \frac{d^3 \mathbf{q}}{(2\pi)^3} |\lambda(\mathbf{q})|^2 \left[ D^{+}(\mathbf{q}; \tau_1, \tau_2) G^{011}_{\rho\nu}(k_1 - \mathbf{q}, \tau_1; k_2 - \mathbf{q}, \tau_2)
\right.
\]

\[
- D^{-}(\mathbf{q}; \tau_1, \tau_2) \left( G^{012}_{\rho\nu}(k_1 - \mathbf{q}, \tau_1; k_2 - \mathbf{q}, \tau_2)
\right.
\]

\[
- G^{031}_{\rho\nu}(k_1 - \mathbf{q}, \tau_1; k_2 - \mathbf{q}, \tau_2) \right] ,
\]
\[
\Sigma_{\mu\nu}(\mathbf{q}, \tau_1, \tau_2) = -\int \frac{d^3q}{(2\pi)^3} \lambda(q) |D^{-}(\mathbf{q}; \tau_1, \tau_2) G_{\mu\nu}^{(0)}(\mathbf{k}_1 - \mathbf{q}, \tau_1; \mathbf{k}_2 - \mathbf{q}, \tau_2) \\
- D^{+}(\mathbf{q}; \tau_1, \tau_2) [G_{\mu\nu}^{(0)}(\mathbf{k}_1 - \mathbf{q}, \tau_1; \mathbf{k}_2 - \mathbf{q}, \tau_2) - G_{\mu\nu}^{(0)}(\mathbf{k}_1 - \mathbf{q}, \tau_1; \mathbf{k}_2 - \mathbf{q}, \tau_2)] .
\] (9.2.29)

In (9.2.29), \(D^{-}(\mathbf{q}; \tau_1, \tau_2)\) and \(D^{+}(\mathbf{q}; \tau_1, \tau_2)\) stand for the spectral density (i.e., difference between the retarded and advanced Green's function) and Keldysh function of phonon, respectively, whose explicit forms are written as follows,

\[
D^{-}(\mathbf{q}; \tau_1, \tau_2) = -i \sin \omega_q (\tau_1 - \tau_2),
\]

\[
D^{+}(\mathbf{q}; \tau_1, \tau_2) = -(1 + 2n_B(\mathbf{k})) \cos \omega_q (\tau_1 - \tau_2).
\] (9.2.30)

\(D^{33}(\mathbf{q}; \tau_1, \tau_2)\) is the temperature Green's function of phonon. Explicit form of \(D^{13}\) and \(D^{31}\) are not required for our purposes.

Substituting (9.2.27) into the right-hand side of (9.2.26), one immediately observes that the physical meanings of \(\Sigma_{\mu\nu}^{33}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\), \(\Sigma_{\mu\nu}^{12}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\) and \(\Sigma_{\mu\nu}^{23}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\) are the self-energies of the retarded, advanced and temperature Green's functions, respectively. On the other hand, the Keldysh component of the self-energy \(\Sigma_{\mu\nu}^{\text{Kd}}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\) is generally a non-trivial object in non-equilibrium systems while, in equilibrium, it is a function of the difference \(\tau_1 - \tau_2\) and is related to the Fourier transform of \(\Sigma_{\mu\nu}^{\text{Kd}}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\), i.e., the difference between self-energies of retarded and advanced Green's function, through the following identity:*)

\[
\Sigma_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = \int d(\tau_1 - \tau_2) e^{+ip_0(\tau_1 - \tau_2)} \tanh \left( \frac{\beta p_0}{2} \right) \left[ \Sigma_{\mu\nu}^{12}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) - \Sigma_{\mu\nu}^{23}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \right]
\]

\[
= \int d(\tau_1 - \tau_2) e^{+ip_0(\tau_1 - \tau_2)} \tanh \left( \frac{\beta p_0}{2} \right) \Sigma_{\mu\nu}^{\text{Kd}}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) .
\]

The self-energies \(\Sigma_{\mu\nu}^{12}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\) and \(\Sigma_{\mu\nu}^{23}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\), which are inherent to our contour-ordered Green's function formalism, are in close connection with the time which characterize the memory of the initial correlation.

From (9.2.23) and (9.2.26), the equation we have to invert in the inversion process turns out to be as follows,

\[
G_{\mu\nu}^{ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = G_{\mu\nu}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) - \int d\tau \int d\tau' \int d^3p_1 d^3p_2 \left( \frac{G^{(0)ac}(\mathbf{k}_1, \tau_1; \mathbf{p}_1, \tau) \tau_3}{2\pi} \times \Sigma^{cd}(\mathbf{p}_1, \tau; \mathbf{p}_2, \tau') \tau_3 G^{(0)db}(\mathbf{p}_2, \tau'; \mathbf{k}_2, \tau_2) \right)_{\mu\nu} .
\] (9.2.31)

External probes are contained in \(G_{\mu\nu}^{(0)ab}\) and \(\Sigma_{\mu\nu}^{ab}\) which have to be expressed by \(G_{\mu\nu}^{ab}\).

9.2.3. \textit{Derivation of generalized Gorkov's equation}

Before applying the inversion method, it is convenient if we include the dissipative parts into zeroth order term of the perturbation series (9.2.31) and rewrite it in terms of new contour-ordered Green's function. For this purpose, let us introduce the "symmetric" and "anti-symmetric" part of the self-energy \(\Sigma_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)\) and

* This relation is a direct consequence of the fluctuation-dissipation theorem.
\(\Gamma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\), defined by

\[
\Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \frac{1}{2} \left[ \Sigma^{32}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) + \Sigma^{13}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) \right]
\]

\[
= -\frac{1}{2} \text{sgn}(\tau_1 - \tau_2) \Sigma^{-\nu}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[\Gamma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = i[\Sigma^{32}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) - \Sigma^{13}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)]
\]

\[= -i\Sigma^{-\nu}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2), \quad (9.2.32)\]

where \(\text{sgn}(\tau) \equiv \theta(\tau) - \theta(-\tau)\) stands for the sign function. These new quantities are well-known in the theory of the quantum transport equation, in which the generalized Boltzmann equation is derived from Keldysh's theory\(^7\) or from Kadanoff-Baym theory\(^6\) through the gradient expansion or the quasi-classical approximation\(^8,9,11,17-19\). As stated above, the physical significance of \(\Sigma^{32}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) and \(\Sigma^{13}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) are the self-energy of the retarded and advanced Green's functions, respectively, so that, in general, the diagonal \((\mu = \nu)\) part of \(\Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) describes the renormalization effects as well as the energy shift of electron due to the interaction. On the other hand, \(\Gamma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) is known to give the dissipative effects because this quantity is related to the width in the distribution of the spectral weight function. In what follows, we shall disregard the diagonal part of \(\Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) because not only energy shift but also renormalization effect are practically insensitive to the deviation from the equilibrium.\(^19,20\) This approximation leads to the situation where renormalization constant is unity. In the same spirit, we will also neglect the diagonal part of the self-energy of the temperature Green's function \(\Sigma^{33}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) because it describes the same effects at the initial time.

Then, let us decompose the self-energy into the dissipative part and the remainder which turns out below to describe the pairing correlation,

\[
\Sigma^{ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \Sigma^{(D)ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) + \Sigma^{(P)ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2),
\]

\[
\Sigma^{(D)ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \begin{pmatrix}
0 & \frac{i}{2} \Gamma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & 0 \\
-\frac{i}{2} \Gamma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & \Sigma^{++}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & \Sigma^{33}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) \\
0 & \Sigma^{32}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & 0 
\end{pmatrix}^{ab},
\]

\[
\Sigma^{(P)ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) = \begin{pmatrix}
0 & \Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & 0 \\
\Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) & 0 & 0 \\
0 & 0 & \Sigma^{33}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) 
\end{pmatrix}^{ab}. \quad (9.2.33)
\]

The reason why we call \(\Sigma^{(D)ab}_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)\) the dissipative part is that this part is in direct connection with essential quantities in the non-equilibrium state such as decay rate of the quasi-particles or the relaxation time of the initial correlation.
use of these definitions, we introduce new contour-ordered Green’s function 
\[ G^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \approx G^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \]
\[ - \int dt \int dt' \int \frac{d^3 p_1 d^3 p_2}{(2\pi)^3} (G^{(0)ac}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \tau_3 \Sigma^{(p)cd}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \times \tau_3 \Sigma^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2))_{\mu\nu} . \]  

Then Eq. (9·2·31) can be rewritten in terms of \[ \widetilde{G}^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \] as follows,
\[ G^{ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \]
\[ = \widetilde{G}^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \]
\[ + \int dt \int dt' \int \frac{d^3 p_1 d^3 p_2}{(2\pi)^3} \Sigma^{(p)cd}(\mathbf{p}_1, \tau; \mathbf{p}_2, \tau') \widetilde{G}^{(0)ab}_{\mu\nu}(\mathbf{p}_1, \tau; \mathbf{p}_2, \tau') \]
\[ \times \Sigma^{(p)cd}(\mathbf{p}_1, \tau; \mathbf{p}_2, \tau') G^{ab}_{\mu\nu}(\mathbf{p}_2, \tau'; \mathbf{h}_2, \tau_2) , \]  

where the higher-order terms are neglected. In deriving (9·2·35), we have used the fact that 
\[ \{r_3\}_{\mu\nu} \Sigma^{(p)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)(r_3)_{\nu\nu} = - \Sigma^{(p)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) , \]
which holds because \( \mu = \nu \) components of \( \Sigma^{(p)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) have been dropped. It is allowed to replace \( \widetilde{G}^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) by \( G^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) in the definition of \( \Sigma^{(p)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) or \( \Sigma^{(p)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) because it appears in the expression which is already second order in \( \lambda(h) \).

For our purpose, it is particularly convenient to use the following equation rather than (9·2·34) which is obtained by eliminating \( G^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) using (9·2·23) and (9·2·34):
\[ G^{(0)ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = (2\pi)^3 \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}_2) G^{ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \tau_2) + \int dt \int dt' \int \frac{d^3 q}{(2\pi)^3} \]
\[ \times G^{ac}_{\mu\nu}(\mathbf{k}_1, \tau; \tau') \Pi^{cd}_{\nu\nu}(\mathbf{k}_1, \tau; \mathbf{q}, \tau') \widetilde{G}^{(0)ab}_{\mu\nu}(\mathbf{q}, \tau'; \mathbf{k}_2, \tau_2) , \]  

where 
\[ \Pi^{ab}_{\nu\nu}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \equiv i \delta(\tau_1 - \tau_2) f^{ab}_{\mu\nu}(\mathbf{k}_1, \tau_1; \tau_2) - \{r_3\}_{\mu\nu} \Sigma^{(p)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)(r_3)_{\nu\nu} . \]

\[ (9·2·37) \]

Now, the inversion method is applied to the perturbation series (9·2·35), which is the original series (7·2·2). Hereafter, for the sake of notational convenience, we will use \( J_i(\mathbf{k}, \mathbf{p}; t) \) defined by
\[ J_i(\mathbf{k}, \mathbf{p}; t) \equiv \delta_{i_1} J(\mathbf{k}, \mathbf{p}; t) + \delta_{i_2} J^*(\mathbf{k}, \mathbf{p}; t) , \]  

in place of \( J(\mathbf{k}, \mathbf{p}; t) \) and \( J^*(\mathbf{k}, \mathbf{p}; t) \). Strictly speaking, the roles of the source term introduced for \( a = 1, 2 \) and for \( a = 3 \) are different: the former is to probe the superconducting order for the time \( t > t_i \) while the latter is to probe the order at \( t = t_i \). Hence, it is necessary to regard them as independent variables when the inversion method is
applied.

Suppose we invert \( (9 \cdot 2 \cdot 3) \) with respect to \( J_i(k, p; t) \), then the following inverted series \( (7 \cdot 2 \cdot 3) \) for \( J_i(k, p; t) \) is obtained

\[
J_i(k, p; t) = h_i^{(0)}(k, p; t) + h_i^{(1)}(k, p; t) + O(\lambda^4)
\]

for the source introduced into the branch \( a=1 \) and \( a=2 \). Similarly, for the probe of \( a=3 \) branch, we have the expansion

\[
J_i(k, p; t_i) = h_i^{(0)}(k, p; t_i) + h_i^{(1)}(k, p; t_i) + O(\lambda^4).
\]

Here \( h_i^{(0)}(k, p; t) \) and \( h_i^{(1)}(k, p; t) \) are the quantities of order \( \lambda^0 \) and \( \lambda^2 \), respectively. As stated in Chapter VII, when we solve \( (9 \cdot 2 \cdot 3) \) with respect to \( J_i(k, p; t) \), the contour-ordered Green's function \( G_{\mu\nu}^{ab}(k_1, k_2; \tau_1, \tau_2) \) on the left-hand side is regarded as a quantity independent of \( \lambda \), so that, in \( (9 \cdot 2 \cdot 39) \) and \( (9 \cdot 2 \cdot 40) \), both \( h_i^{(0)}(k, p; t) \) and \( h_i^{(1)}(k, p; t) \) are looked upon as its functionals: \( h_i^{(0)} = h_i^{(0)}[G_{\mu\nu}^{ab}] \) and \( h_i^{(1)} = h_i^{(1)}[G_{\mu\nu}^{ab}] \).

Making use of \( (7 \cdot 2 \cdot 4) \), \( h_i^{(0)}(k, p; t) \) is determined by solving

\[
G_{\mu\nu}^{ab}(k_1, k_2; \tau_1, \tau_2) = \hat{G}_{\mu\nu}^{ab}(k_1, k_2; \tau_1, \tau_2)|_{J_i = h_i^{(0)}}
\]

with respect to \( J_i(k, p; t) \) where \( |J_i = h_i^{(0)} \) implies that this is evaluated at the point \( J_i(k, p; t) = h_i^{(0)}(k, p; t) \) and \( J_i(k, p; t_i) = h_i^{(0)}(k, p; t_i) \). According to \( (9 \cdot 2 \cdot 36) \), Eq. \( (9 \cdot 2 \cdot 41) \) turns out to be equivalent to the following integral equation,

\[
G_{\mu\nu}^{ab}(k_1, k_2; \tau_1, \tau_2) = (2\pi)^3 \delta^{(3)}(k_1 - k_2) \hat{\Omega}_{\mu\nu}^{ab}(k_1, \tau_1, \tau_2) + \int d\tau \int d\tau' \int \frac{d^3q}{(2\pi)^3}
\]

\[
\times \hat{\Omega}_{\mu\nu}^{ab}(k_1, \tau_1, \tau) \hat{\Pi}_{\rho\sigma}^{ab}(k_1, \tau; q, \tau') G_{\rho\sigma}^{ab}(q, \tau'; k_2, \tau_2),
\]

where

\[
\hat{\Pi}_{\mu\nu}^{ab}(k_1, k_2; \tau_1, \tau_2) = \Pi_{\mu\nu}^{ab}(k_1, k_2, \tau_1, \tau_2)|_{J_i = h_i^{(0)}}.
\]

Equation \( (9 \cdot 2 \cdot 42) \) is too complicated to solve and get the functional relation \( h_i^{(0)} = h_i^{(0)}[G_{\mu\nu}^{ab}] \), even if the explicit form of the external electromagnetic field is specified. However, the explicit form is not necessary in our discussion. As discussed in Ref. 3, we observe from \( (9 \cdot 2 \cdot 42) \) that the non-trivial off-diagonal \( (\mu \neq \nu) \) components of the contour-ordered Green's function are obtained if and only if \( h_i^{(0)}(k, p; t) \) is not zero. Therefore, it is allowed to regard \( h_i^{(0)}(k, p; t) \) as a new order parameter in place of the off-diagonal components of the contour-ordered Green's function.\(^*\)

From this new point of view, Eq. \( (9 \cdot 2 \cdot 42) \) specifies the functional form of the contour-ordered Green's function \( G_{\mu\nu}^{ab} = G_{\mu\nu}^{ab}[h_i^{(0)}] \) as the functional of the new order parameter \( h_i^{(0)} \). This is an example of the point (8) in § 7.2.1.

Next, let us consider the lowest correction term \( h_i^{(1)} \) to get the functional form \( h_i^{(1)} = h_i^{(1)}[h_i^{(0)}] \). From \( (7 \cdot 2 \cdot 5) \), this term is obtained by solving the equation of the form,

\(*\) Here we note that, in inversion method, it is not necessary to choose the order parameter as a quantity like \( \langle \hat{O} \rangle \) even if the source term is in the form \( \hat{H}_f = J \cdot \hat{O} \).
\[
\frac{h_1(\varphi)}{df} \frac{df}{dJ} \bigg|_{J=\hbar_0[\varphi]} = -f_1[J] \bigg|_{J=\hbar_0[\varphi]}. 
\]

As stated above, here we have to regard the sources \(f_i(\mathbf{k}, \mathbf{p}; t)\) introduced in the branch \(a=1, 2\) and \(f_i(\mathbf{k}, \mathbf{p}; t_1)\) on \(a=3\) as three independent variables, so that the functional form of \(h_i^{(1)}\) is determined by solving the following equation:

\[
- \int dt' \frac{d^3 \mathbf{p} \, d^3 \mathbf{p}_2}{(2\pi)^3} \sum_{\rho \delta} \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} h_i^{(1)}(\mathbf{p}_1, \mathbf{p}_2; \tau)
\]

\[
= \sum_{i=1}^3 \int d^3 \mathbf{p}_1 \, d^3 \mathbf{p}_2 \left[ \int dt' \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} h_i^{(1)}(\mathbf{p}_1, \mathbf{p}_2; \tau) 
\right.
\]

\[
+ \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; t_1)} h_i^{(1)}(\mathbf{p}_1, \mathbf{p}_2; t_1) \bigg|_{J=\hbar_0[\varphi]} + O(\lambda^4). 
\]

(9.2.44)

As shown in Appendix E of Ref. 3, \(\delta G_{\rho\delta}^{(0)ab}/\delta f_i\) on the right-hand side of (9.2.44) can be expressed as follows,

\[
(2\pi)^6 \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} = iG_{\rho\sigma}^{(0)ac}(\mathbf{k}_1, \tau_1; \mathbf{p}_1, \tau) \left( \begin{array}{cc} 0 & \delta_{ij} \\ \delta_{ij} & 0 \end{array} \right) \frac{\delta_{ij}}{\rho_\sigma} \left( \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right) G_{\rho\sigma}^{(0)db}(\mathbf{p}_2, \tau; \mathbf{k}_2, \tau_2), 
\]

(9.2.45)

\[
(2\pi)^6 \frac{\delta G_{\rho\sigma}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; t_1)} = i \int dt' G_{\rho\sigma}^{(0)ac}(\mathbf{k}_1, \tau_1; \mathbf{p}_1, \tau) \left( \begin{array}{cc} 0 & \delta_{ij} \\ \delta_{ij} & 0 \end{array} \right) \frac{\delta_{ij}}{\rho_\sigma} \left( \begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array} \right) i G_{\rho\sigma}^{(0)db}(\mathbf{p}_2, \tau; \mathbf{k}_2, \tau_2). 
\]

(9.2.46)

Therefore, substituting (9.2.45) and (9.2.46) into the right-hand side of (9.2.44) and disregarding higher-order terms, Eq. (9.2.44) reduces to the following equation:

\[
- \int dt' \frac{d^3 \mathbf{p} \, d^3 \mathbf{p}_2}{(2\pi)^3} \sum_{\rho \delta} \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} 
\]

\[
= i \int dt' \frac{d^3 \mathbf{p} \, d^3 \mathbf{p}_2}{(2\pi)^3} \sum_{\rho \delta} \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{p}_1, \tau)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} \frac{\delta G_{\rho\delta}^{(0)ab}(\mathbf{k}_1, \tau_1; \mathbf{p}_1, \tau)}{\delta f_i(\mathbf{p}_1, \mathbf{p}_2; \tau)} \bigg|_{J=\hbar_0[\varphi]}. 
\]
\[
\begin{align*}
&\times \left\{ \begin{pmatrix} 0 & h_1^{(1)}(p_1, p_2; \tau) \\ h_2^{(1)}(p_1, p_2; \tau) \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_{\sigma'd} \right\} \\
&+ \left\{ \begin{pmatrix} 0 & h_1^{(1)}(p_1, p_2; t_1) \\ h_2^{(1)}(p_1, p_2; t_1) \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & i \end{pmatrix}_{\sigma'd} \right\} .
\end{align*}
\tag{9.2.47}
\]

Although Eq. (9.2.47) takes somewhat complicated form, it is possible to solve it and to get \( h_1^{(1)} = h_1^{(1)}[h_1^{(0)}] \) if one considers the weak coupling (or BCS) limit. We recall that in the weak coupling limit, the energy change of the electron due to collision is sufficiently small compared with the Debye energy \( \omega_D \). To see this, let us first investigate the Fourier transform of \( \text{sgn}(t-t') \mathcal{D}^\pm(k; t, t') \):

\[
\text{sgn}(t-t') \mathcal{D}^\pm(k; t, t') = \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} e^{-i\Omega(t-t')} \mathcal{D}^\pm(k; \Omega) .
\tag{9.2.48}
\]

From (9.2.30), explicit forms of \( \mathcal{D}^\pm(k; \Omega) \) are easily calculated by direct integration. The results are

\[
\begin{align*}
\mathcal{D}^-(k; \Omega) &= i \left\{ \frac{\omega_k}{(\Omega + i\epsilon)^2 - \omega_k^2} + \frac{\omega_k}{(\Omega - i\epsilon)^2 - \omega_k^2} \right\} , \\
\mathcal{D}^+(k; \Omega) &= -2i \left( 1 + 2n_s(k) \right) \mathcal{P} \left\{ \frac{\Omega}{\Omega^2 - \omega_k^2} \right\} ,
\end{align*}
\tag{9.2.49}
\]

where \( \mathcal{P} \) stands for the principal part of the integral.

Near the Fermi surface, the momentum transfer due to the electron-electron interaction is, in general, of the order of Fermi momentum \( p_F \). Then the energy of the lattice vibration is the quantity of order \( \omega_0 \) because \( \omega p_F \sim \omega_D \) (where \( u \) is the velocity of sound). Therefore, if one considers the weak coupling limit in which the energy transfer of the electron is sufficiently small compared with the energy of lattice vibration, it is allowed to use the following form of \( \text{sgn}(t-t') \mathcal{D}^\pm(k; t, t') \) which is obtained by expanding \( \mathcal{D}^\pm(k; \Omega) \) with respect to \( \Omega/\omega_k \) and by taking only the leading term:

\[
\begin{align*}
\text{sgn}(t-t') \mathcal{D}^-(k; t, t') &\approx - \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} e^{-i\Omega(t-t')} \left( \frac{2i}{\omega_k} \right) \\
&= -2i \frac{\omega_k}{\omega_k} \delta(t-t') , \\
\text{sgn}(t-t') \mathcal{D}^+(k; t, t') &\approx 2i \left( 1 + 2n_s(k) \right) \mathcal{P} \int_{-\infty}^{+\infty} \frac{d\Omega}{2\pi} e^{-i\Omega(t-t')} \left( \frac{\Omega}{\omega_k^2} \right) \\
&= 0 .
\end{align*}
\tag{9.2.50}
\]

Substituting (9.2.50) into the right-hand side of the first equation of (9.2.32), we

\* The following approximation corresponds to the instantaneous-exchange approximation in the theory of dynamical symmetry breaking at finite temperature.\textsuperscript{21,22}
obtain the following expression for $\Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2)$,

\[
\Sigma_{\mu\nu}(k_1, \tau_1; k_2, \tau_2) \approx \frac{1}{2} \int \frac{d^3q}{(2\pi)^3} |\lambda(q)|^2 \left\{ -\frac{2i}{\omega_k} \delta(\tau_1 - \tau_2) \right\} G_{\mu\nu}^{(0)}(k_1 - q, \tau_1; k_2 - q, \tau_2) \\
= -i g^2 \delta(\tau_1 - \tau_2) \int \frac{d^3q}{(2\pi)^3} G_{\mu\nu}^{(0)}(k_1 - q, \tau_1; k_2 - q, \tau_2),
\]

(9.2.51)

where $g^2 = |\lambda(k)|^2/\omega_k$.

Similarly, introducing the bosonic Matsubara frequency as $\nu_n = 2\pi n\beta^{-1}(n = 0, \pm 1, \pm 2, \cdots)$, $\mathcal{D}^{33}(k; \tau, \tau')$ is expressed as

\[
\mathcal{D}^{33}(k; \tau, \tau') = -\beta^{-1} \sum_n e^{-i\nu_n(\tau - \tau')} \left( \frac{\omega_k}{\nu_n^2 + \omega_k^2} \right).
\]

Therefore, in the same accuracy, we can use the following form of $\mathcal{D}^{33}(k; \tau, \tau')$ in the expression of $\Sigma_{\mu\nu}^{33}(k_1, \tau_1; k_2, \tau_2)$:

\[
\mathcal{D}^{33}(k; \tau, \tau') \approx -\beta^{-1} \sum_n e^{-i\nu_n(\tau - \tau')} \left( \frac{1}{\omega_k} \right) \\
= -\frac{1}{\omega_k} \delta(\tau - \tau').
\]

(9.2.52)

Then we obtain

\[
\Sigma_{\mu\nu}^{33}(k_1, \tau_1; k_2, \tau_2) \approx 2 \int \frac{d^3q}{(2\pi)^3} \left\{ -\frac{|\lambda(q)|^2}{\omega_k} \delta(\tau_1 - \tau_2) \right\} G_{\mu\nu}^{(33)}(k_1 - q, \tau_1; k_2 - q, \tau_2) \\
= -2g^2 \delta(\tau_1 - \tau_2) \int \frac{d^3q}{(2\pi)^3} G_{\mu\nu}^{(0)}(k_1 - q, \tau_1; k_2 - q, \tau_2).
\]

(9.2.53)

After substituting (9.2.51) and (9.2.53) into (9.2.47), the explicit form of $h_{1}^{(1)}$ turns out to be as follows,

\[
h_{1}^{(1)}(k_1, k_2; t) = g^2 \int \frac{d^3q}{(2\pi)^3} G_{12}^{(0)}(k_1 - q, t; k_2 - q, t) \\
= g^2 \int \frac{d^3q}{(2\pi)^3} G_{12}^{(1)}(k_1 - q, t; k_2 - q, t),
\]

\[
h_{2}^{(1)}(k_1, k_2; t) = g^2 \int \frac{d^3q}{(2\pi)^3} G_{21}^{(0)}(k_1 - q, t; k_2 - q, t) \\
= g^2 \int \frac{d^3q}{(2\pi)^3} G_{21}^{(1)}(k_1 - q, t; k_2 - q, t),
\]

\[
h_{1}^{(1)}(k_1, k_2; \tau) = -2g^2 \int \frac{d^3q}{(2\pi)^3} G_{12}^{(33)}(k_1 - q, \tau; k_2 - q, \tau) \\
= -2g^2 \int \frac{d^3q}{(2\pi)^3} G_{12}^{(3)}(k_1 - q, \tau; k_2 - q, \tau),
\]
\[ h_2^{(1)}(\mathbf{k}_1, \mathbf{k}_2; t_i) = -2g^2 \int \frac{d^3q}{(2\pi)^3} G_2^{(0)}(\mathbf{k}_1 - \mathbf{q}, \mathbf{r}; \mathbf{k}_2 - \mathbf{q}, \mathbf{r}) \bigg|_{J_i = h_i^{(0)}}. \]

\[ = -2g^2 \int \frac{d^3q}{(2\pi)^3} G_2^{(0)}(\mathbf{k}_1 - \mathbf{q}, \mathbf{r}; \mathbf{k}_2 - \mathbf{q}, \mathbf{r}), \tag{9.2.54} \]

where the relation (9.2.41) has been used. Equation (9.2.54) gives the functional form of \( h_i^{(1)} = h_i^{(1)}[h_i^{(0)}] \) through the functional relation \( G_2^{(0)} = G_2^{(0)}[h_i^{(0)}] \) defined as the solution of (9.2.42).

Finally, the self-consistency conditions for the order parameters \( h_i^{(0)} \) is obtained by substituting (9.2.54) into the right-hand side of (9.2.39) and (9.2.40) and then by setting \( J_i = 0 \). In this way, the result obtained from the inverted series of \( J_i(\mathbf{k}, \mathbf{p}; t) \), which is introduced as a probe into the segment parallel to the real time axis, is given as follows,

\[ h_1^{(0)}(\mathbf{k}_1, \mathbf{k}_2; t) = -g^2 \int \frac{d^3q}{(2\pi)^3} G_1^{(0)}(\mathbf{k}_1 - \mathbf{q}, t; \mathbf{k}_2 - \mathbf{q}, t), \]

\[ h_2^{(0)}(\mathbf{k}_1, \mathbf{k}_2; t) = -g^2 \int \frac{d^3q}{(2\pi)^3} G_2^{(0)}(\mathbf{k}_1 - \mathbf{q}, t; \mathbf{k}_2 - \mathbf{q}, t). \tag{9.2.55} \]

On the other hand, if we set \( J_i(\mathbf{k}, \mathbf{p}; t_i) = 0 \) for \( a = 3 \) branch, the result is

\[ h_1^{(0)}(\mathbf{k}_1, \mathbf{k}_2; t_i) = 2g^2 \int \frac{d^3q}{(2\pi)^3} G_1^{(0)}(\mathbf{k}_1 - \mathbf{q}, \mathbf{r}; \mathbf{k}_2 - \mathbf{q}, \mathbf{r}), \]

\[ h_2^{(0)}(\mathbf{k}_1, \mathbf{k}_2; t_i) = 2g^2 \int \frac{d^3q}{(2\pi)^3} G_2^{(0)}(\mathbf{k}_1 - \mathbf{q}, \mathbf{r}; \mathbf{k}_2 - \mathbf{q}, \mathbf{r}). \tag{9.2.56} \]

According to (9.2.21) and the cyclic invariance of trace, we find that there exists the following relation between \( G_1^{(0)}(\mathbf{k}_1, \mathbf{n}_1; \mathbf{k}_2, \mathbf{n}_2) \) and \( G_2^{(0)}(\mathbf{k}_1, \mathbf{n}_1; \mathbf{k}_2, \mathbf{n}_2) \) for \( \mu \neq \nu \),

\[ \lim_{t_i \to t_1} \lim_{t_i \to t_2} G_1^{(0)}(\mathbf{k}_1, \mathbf{n}_1; \mathbf{k}_2, \mathbf{n}_2) = 2\langle \overline{\psi}_\mu(\mathbf{k}_1, t_1) \overline{\psi}_\nu(\mathbf{k}_2, t_2) \rangle = -2\lim_{t_1 \to t_2} G_1^{(0)}(\mathbf{k}_1, \mathbf{n}_1; \mathbf{k}_2, \mathbf{n}_2) = -2\lim_{t_1 \to t_2} G_1^{(0)}(\mathbf{k}_1, \mathbf{n}_1; \mathbf{k}_2, \mathbf{n}_2). \tag{9.2.57} \]

so that the self-consistency condition (9.2.56) turns out to be included into (9.2.55).

Equation (9.2.42) and the self-consistency conditions (9.2.55) are a set of integral equations for five independent correlation functions of electron-phonon system. All the quantities appearing in this equation are expressed as functionals of the order parameter \( h_i^{(0)}(\mathbf{k}, \mathbf{p}; t) \). As stated above, the \( a\neq b = 3 \) component of contour-ordered Green's function corresponds to the temperature Green's function which describes the initial correlation of the system which is supposed to be in equilibrium. Hence, in our formalism, the question of whether the system at initial time is in superconducting state is automatically determined quite naturally by solving this component with the self-consistency condition (9.2.56) under some given electromagnetic field and temperature. The initial condition is already fixed to be the equilibrium so that there is no room for imposing any initial conditions for Green's function or order parameter, as the conventional treatment does.
In order to see whether \( a = b = 3 \) component of (9.2.42) with self-consistency condition (9.2.56) is equivalent to the well-known Gorkov's equation, it is much more convenient to convert it into a differential equation. Due to causality, the explicit form of \( a = b = 3 \) component of (9.2.42) turns out to be expressed in terms of only \( a = b = 3 \) component of the Green's function and self-energy:

\[
G_{\nu\rho}^{33}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = (2\pi)^3 \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}_2) \Pi_{\nu\rho}^{33}(\mathbf{k}_1; \tau_1, \tau_2)
+ \int d\tau' \int d\tau'' \int \frac{d^3q}{(2\pi)^3} \Delta^{33}(\mathbf{q}; \tau') \Pi_{\rho\sigma}^{33}(\mathbf{k}_1, \tau; \mathbf{q}, \tau') G_{\sigma\nu}^{33}(\mathbf{q}, \tau'; \mathbf{k}_2, \tau_2),
\]

(9.2.58)

where

\[
\Pi_{\nu\rho}^{33}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) = - \delta(\tau_1 - \tau_2) f_{\nu\rho}(\mathbf{k}_1, \mathbf{k}_2; t_1)
= - \delta(\tau_1 - \tau_2) \begin{pmatrix}
    f(\mathbf{k}_1, \mathbf{k}_2; t_1) & h^{(0)}(\mathbf{k}_1, \mathbf{k}_2; t_1) \\
    h^{(0)}(\mathbf{k}_1, \mathbf{k}_2; t_1) & - f(-\mathbf{k}_2, -\mathbf{k}_1; t_1)
\end{pmatrix}_{\nu\rho}. 
\]

(9.2.59)

On the other hand, by a direct differentiation of (9.2.22), it is found that \( Q_{\nu\rho}^{33}(\mathbf{k}; \tau_1, \tau_2) \) satisfies the following differential equation,

\[
\left\{ -\frac{\partial}{\partial \tau_1} - \frac{\partial}{\partial \tau_2} - \varepsilon_k \right\} \Delta_{\nu\rho}^{33}(\mathbf{k}; \tau_1, \tau_2) = \delta_{\nu\rho} \delta(\tau_1 - \tau_2). 
\]

(9.2.60)

Therefore, introducing Fourier transform of \( G_{\nu\rho}^{ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2) \) as

\[
G_{\nu\rho}^{ab}(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) = \int \frac{d^3k_1 d^3k_2}{(2\pi)^6} e^{i\mathbf{k}_1 \cdot \mathbf{x}_1 - i\mathbf{k}_2 \cdot \mathbf{x}_2} G_{\nu\rho}^{ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2),
\]

(9.2.61)

we find that \( G_{\nu\rho}^{ab}(\mathbf{x}_1, \tau_1; \mathbf{x}_2, \tau_2) \) satisfies the following differential equation, which exactly coincides with Gorkov's equation,

\[
\left\{ -\frac{\partial}{\partial \tau} + \frac{1}{2m} \left( \nabla_x - ie \varepsilon_3 A(x, t_1) \right)^2 - eA_0(x, t_1) + \mu \right\} \mathcal{D}^x + \begin{pmatrix} 0 & \Delta(x, t_1) \\
\Delta^*(x, t_1) & 0 \end{pmatrix}
\cdot \left( \Delta(x, t) \right)_{\nu\rho},
\]

(9.2.62)

where \( \nabla_x \equiv \partial/\partial x \) and \( \Delta^*(x, t) \) is defined as follows,

\[
\Delta(x, t) = \frac{1}{2} \int \frac{d^3k - \mathbf{p}}{(2\pi)^3} e^{i(k - p) \cdot x} h^{(0)}(\mathbf{k}, \mathbf{p}; t)
= g^2 \langle \tilde{a}_+(x, t) \tilde{a}_+(x, t) \rangle,
\]

\[
\Delta^*(x, t) = \frac{1}{2} \int \frac{d^3k - \mathbf{p}}{(2\pi)^3} e^{i(k - p) \cdot x} h^{(0)}(\mathbf{k}, \mathbf{p}; t)
= g^2 \langle \tilde{a}_+^\dagger(x, t) \tilde{a}_+^\dagger(x, t) \rangle.
\]

(9.2.63)

Since \( Q_{\nu\rho}^{33}(\mathbf{k}; \tau_1, \tau_2) \) satisfies the Kubo-Martin-Schwinger's anti-periodic boundary condition, \( Q_{\nu\rho}^{33}(\mathbf{k}; \tau_1 + \beta, \tau_2) = - Q_{\nu\rho}^{33}(\mathbf{k}; \tau_1, \tau_2) \), Eq. (9.2.62) has to be solved with this
boundary condition of course.

It is obvious that our result has much more ingredients than the conventional Gorkov's equation because $a=1$, $b=2$ component of (9.2·42) corresponds to the retarded Green's function which describes the dynamical properties of the system whereas the Keldysh function ($a=b=1$ component) contains the information of the time evolution of the distribution function. In this sense, Eq. (9.2·42) with the self-consistency condition (9.2·55) is regarded as a generalization of Gorkov's equation. We note here that $2 \times 2$ submatrix appearing in left upper edge of our result has a strong resemblance to the generalized Gorkov's equation of Larkin and Ovchinnikov\(^{23,24}\) in the absence of the impurity potential whereas our equation has a wide applicability in discussing the transient behavior of the system short time after the preparation or the initial time correlation.

The obtained results (9.2·42) and (9.2·55) are the fundamental equations describing not only dynamical but also static properties of the superconducting system, which constitute the starting basis of the further study in this area.

9.2.4. Effect of direct Coulomb repulsion

Considering the fact that the effective interaction between electrons is due to direct Coulomb repulsion as well as electron-phonon interaction, it is essential to investigate the effect of Coulomb repulsion. For this purpose, let us first examine the electron dielectric function $\kappa(q_0, q)$. Owing to the Migdal's theorem, the phonon correction to the electron dielectric function is negligible so that it is allowed to use Lindhard expression for dielectric function given by the random phase approximation. In addition, since the effect of dynamical electric screening emerges only for $q_0 \leq \varepsilon_F$ ($\varepsilon_F$ is Fermi energy), one can approximate $\kappa(q_0, q)$ to its static limit $\kappa(q) \equiv \kappa(0, q)$ and neglect its imaginary part (i.e., $\text{Im}(\kappa(0, q) \approx 0)$).

The effect of direct Coulomb interaction is then taken into account with the aid of the following procedure:

(i) Replace bare electron-phonon coupling constant $\lambda(q)$ by dressed (or renormalized) one given by $\lambda^\kappa(q) = \sqrt{\kappa(q)}$.

(ii) Replace bare phonon energy $\omega_k$ by dressed one given by $\omega_k^\kappa = \omega_k / \sqrt{\kappa(\mathbf{k})}$.

(iii) In order to get the dressed phonon Green's function, multiply renormalization factor $\sqrt{\kappa(\mathbf{k})}$ to the bare phonon Green's function:

$$\mathcal{D}^{ab}(\mathbf{k}; \tau_1, \tau_2) \rightarrow \sqrt{\kappa(\mathbf{k})} \mathcal{D}^{ab}(\mathbf{k}; \tau_1, \tau_2).$$

(iv) Add self-energy due to the direct Coulomb interaction.

Within this approximation, Eqs. (9.2·42) and (9.2·55) are modified to the following equations as calculated in Ref. 5,

$$G_{\mu\bar{\nu}}^{ab}(\mathbf{k}_1, \tau_1; \mathbf{k}_2, \tau_2)$$

$$= (2\pi)^3 \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}_2) \mathcal{D}^{ab}_{\mu\bar{\nu}}(\mathbf{k}_1; \tau_1, \tau_2)$$

$$+ \int d\tau \int d\tau' \int \frac{d^3q}{(2\pi)^3} \sqrt{\kappa(q)} \mathcal{D}^{ab}_{\mu\bar{\nu}}(\mathbf{k}_1; \tau_1, \tau) \mathcal{T}^{ab}_{\mu\bar{\nu}}(\mathbf{k}_1, \tau; \mathbf{q}, \tau') G_{\mu\bar{\nu}}^{ab}(\mathbf{q}, \tau'; \mathbf{k}_2, \tau_2),$$

(9.2·64)
\[ h_1^{(2)}(k_1, k_2; t) = -\int \frac{d^3q}{(2\pi)^3} \left( \hat{\sigma}^2(q) - CV(q) \right) G^{12}_0(q, t; k_1 - q, t), \]

\[ h_2^{(2)}(k_1, k_2; t) = -\int \frac{d^3q}{(2\pi)^3} \left( \hat{\sigma}^2(q) - CV(q) \right) G^{12}_0(q, t; k_2 - q, t), \]

(9.2.65)

where \( \hat{\sigma}^2(q) = \alpha^2(q)^2/\omega_{q} \) and the self-energy \( \Pi^{ab}_{\omega} \) is evaluated by using \( \omega_{q} \) and \( \lambda^k(k) \). Here \( CV(q) = V(q) / \alpha(q) \) with \( V(q) = 4\pi e^2 / |q|^2 \) standing for the screened Coulomb potential. As in the previous section, Hartree term due to the direct Coulomb repulsion as well as diagonal \((\mu = \nu)\) component of the self-energy is neglected. In addition, the instantaneous exchange approximation is also employed. In practical application of (9.2.64) and (9.2.65), it might be much efficient to use Coulomb pseudo potential\(^{12} - 15\) in place of screened Coulomb potential because, near Fermi surface, the effective Coulomb repulsion is known to be weaker than the true screened Coulomb interaction.

References

Chapter X. Hubbard Model by Inversion Method

As another exercise of inversion method, the Hubbard model is studied both in weak coupling and strong coupling region. The most salient feature of the approach is that a systematic improvement of the results is possible in a straightforward way. In the weak coupling expansion, for example, we can take into account the spin fluctuation systematically by diagrammatic technique à la Feynman-Dyson. This is illustrated for the ferromagnetic phase up to the second order of the inversion series. There is a possibility to get the linear Curie-Weiss law by taking first three terms of the inversion series. Analysis of the structure of the higher-order diagrams will be done in Chapter XI.

The strong coupling Hubbard model is then studied. In this case, the inversion series is constructed by the expansion in both the inverse powers of the coupling constant and the powers of the hopping parameter for the arbitrary filling factor. Our approach is an attempt at the strong coupling version of the mean field theory. Within the lowest approximation, it is shown that for large filling factor or for large electron correlation, the ferromagnetic phase is favored and there is a crossover to the antiferromagnetic state when these parameters are reduced.

In this chapter the imaginary time formalism is adopted. The relation between the real and imaginary time on-shell expansion is studied in § 12.3.3.

The present chapter is inserted with the hope that the reader become familiar with the inversion method and, without higher order contributions, the numerical result of § 10.2.3 has only a meaning of illustration.

§ 10.1. Ferromagnetic phase by weak coupling expansion

The Hubbard model is defined by\(^1,2\)

$$\mathcal{H} = \sum_{\mathbf{r}} \sum_{\sigma} t_{\mathbf{r}\mathbf{r}'} a_{\mathbf{r}\sigma}^\dagger a_{\mathbf{r}'\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}, \quad (10\cdot1\cdot1)$$

where the creation and annihilation operators for the electron of spin \(\sigma\) and \(\sigma'\) at the lattice site \(\mathbf{r}\) and \(\mathbf{r}'\) satisfy anti-commutation relations

$$\{a_{\mathbf{r}\sigma}, a_{\mathbf{r}'\sigma'}^\dagger\} = \delta_{\mathbf{r}\mathbf{r}'} \delta_{\sigma\sigma'}, \quad \text{etc.} \quad (10\cdot1\cdot2)$$

The number operator of the spin \(\sigma\) has been introduced as

$$n_{\mathbf{r}\sigma} = a_{\mathbf{r}\sigma}^\dagger a_{\mathbf{r}\sigma} \quad (10\cdot1\cdot3)$$

Furthermore \(t_{\mathbf{r}\mathbf{r}'}\) represents the hopping term and \(U\) the Coulomb interaction. Only the on-site Coulomb interaction will be considered in the following and we assume that \(t_{\mathbf{r}\mathbf{r}'}\) is a function of \(|\mathbf{r} - \mathbf{r}'|\). In the standard Hubbard model, only the hoppings of the electrons from one site to the nearest-neighbor sites are allowed. The Fourier transform of \(t_{\mathbf{r}\mathbf{r}'}\) is given by
for the $d$-dimensional analog of the square lattice. The lattice constant has been set to unity.

Since we have interest in the ferromagnetism at finite temperature, the variable of interest or the order parameter is the total spin operator

$$
\hat{S} = \sum_r \hat{S}(r) \quad \text{with} \quad \hat{S}(r) = \frac{1}{2} \tau_\sigma \sigma^\sigma \tau_{\sigma^\sigma},
$$

where $\tau$ is the usual $2 \times 2$ Pauli matrix ($\tau_x, \tau_y, \tau_z$). Three components of $\hat{S}$ form $SU(2)$ algebra and commute with the Hamiltonian (10.1.1). Thus the Hamiltonian has the continuous symmetry. The appearance of the ferromagnetism in the zero magnetic field implies the spontaneous breakdown of this continuous symmetry.

If we choose the source term as $\mathbf{H} \cdot \hat{S}$, then the breaking of the $SU(2)$ symmetry can be discussed. But in the following we first study the case of the $Z_2$ symmetric source where only the $z$-component of $\hat{H}$ has the nonzero value.

10.1.1. **Ferromagnetism by $Z_2$ symmetric inversion up to second order**

Let us introduce the source term $H_x \hat{S}_z$ which is $Z_2$-symmetric. The main concern of this section is to clarify rather technical aspect of the problem. Physical content of the inversion series will be examined in the following sections.

STEP 1—Introduction of the source

The grand canonical Hamiltonian for the $Z_2$-symmetric source takes the form ($H_x$ is written as $H$ for convenience)

$$
\mathcal{H} = \mathcal{H} - \mu \tilde{N} - H \hat{S}_x = \mathcal{H} - J_\sigma \tilde{N}_\sigma,
$$

where the summation over the repeated index $\sigma$ is implied as we will do below unless it is ambiguous. The $z$-component of the spin operator $\hat{S}_z$ and the total number of the electron $\tilde{N}$ are given by

$$
\hat{S}_z = \frac{1}{2} \sum_r (n_r, -n_r),
$$

$$
\tilde{N} = \sum_\sigma \tilde{N}_\sigma, \quad \tilde{N}_\sigma = \sum_r n_{r\sigma}.
$$

We introduce the total magnetization operator $\tilde{M}$ or its density $\tilde{m}$ by $\hat{S}_z = -\tilde{M} = -V \tilde{m}$, where $V$ is the volume of the system. (We have taken $\hbar$, and $\mu_b$, the Bohr magneton, to be unity.) The sources $J_\sigma$ and $\tilde{N}_\sigma$ in (10.1.6) are given by

$$
J_\sigma = \frac{\sigma}{2} H + \mu, \quad \tilde{N}_\sigma = \frac{\tilde{N}}{2} + \sigma \hat{S}_z.
$$

The chemical potential $\mu$ has been introduced as usual and here it is considered as a part of the source for convenience. The two sources $\mu$ and $H$ are combined into $J_\sigma$ as in (10.1.9). The spin index $\sigma$ is defined to take the value $(+1, -1)$ for $(\uparrow, \downarrow)$. Note that the original Hamiltonian defined in (10.1.1) has the $SU(2)$ symmetry while
the source terms in (10.1.6) reduce the symmetry down to the $Z_2$ invariance. The case where more general source term $H \cdot \mathcal{S}$ is introduced will be studied later.

STEP 2—Conventional perturbative calculation of the order parameter

The thermodynamical potential $\Omega(J^1, J^i)/\beta = -\frac{1}{\beta} \mathcal{O}(H, \mu)/\beta$ is defined here by

$$e^{-\beta \mathcal{O}(J^1, J^i)}/\beta = \text{Tr} e^{-\beta H},$$

where $\beta^{-1} k_b^{-1} = T$ is the temperature of the system. The expectation values $\phi_\sigma$ of the operators $\hat{N}_\sigma/V$ are considered as order parameters for convenience although the original order parameter of the present problem is the expectation value $m$ of the operator $\hat{m} = -\hat{S}_x/V$. The value $m$ is easily given by $m = (\phi_1 - \phi_2)/2$ once $\phi_\sigma$ is known. This is clear from the relation,

$$V\phi_\sigma = \langle \hat{N}_\sigma \rangle = \frac{1}{2} N + \sigma S_z = \frac{1}{2} N - \sigma M,$$

where $N$, $S_z$ and $M$ are the expectation values of the operators $\hat{N}$, $\hat{S}_z$ and $\hat{M}$ respectively. One can calculate $\phi_\sigma$ as a function of $J_\sigma$ by the conventional perturbation technique since $\phi_\sigma$ is given by

$$\beta V \phi_\sigma = -\frac{\partial \Omega}{\partial J_\sigma}.\quad (10.1.12)$$

The diagrammatic expansion according to the imaginary time formalism is done as follows. Since the source term $J_\sigma N_\sigma = \sum J_\sigma \sum a_\tau a_{\tau'} a_{\tau'} a_{\tau'}$ is quadratic, it can be absorbed into the propagator $G_\delta$,

$$[G^\delta]_{x x'} = G_{x x'} - \delta_{x x'} \delta_{\tau \tau'} J_\sigma$$

with

$$G_{x x'} = \delta_{\tau \tau'} \left( \delta_{x x'} \frac{\partial}{\partial x'} + t_{x x'} \right),\quad (10.1.14)$$

where $x$ and $x'$ denote the sets $(x, \tau)$ and $(x', \tau')$ respectively. Here $\tau$ represents the imaginary time variable. Specifically $\phi_\tau$ is given by the following graph in which the solid (dashed) line represents the propagator $G^1_\delta (G^1_\delta)$ and the factor $U$ is assigned to the 4-point vertex (see Appendix H for the Feynman-Dyson expansion including the symmetry factor),

$$\phi_\tau = \phi^{(0)}_\tau + \phi^{(1)}_\tau + \phi^{(2)}_\tau + \cdots,$$

where

$$-\beta V \phi^{(0)}_\tau(J^1, J^i) = \quad (10.1.16)$$

$$-\beta V \phi^{(1)}_\tau(J^1, J^i) = \quad (10.1.17)$$
\[-\beta V \phi^{(2)}(J, J) = \begin{array}{c}
\circ \longrightarrow \circ \\
\circ \longrightarrow \circ \\
\circ \longrightarrow \circ 
\end{array}, \quad (10.1.18)\]

and so on. Here and hereafter the \(n\)-th order of the quantity \(X\) is denoted not as \(U^n X^{(n)}\) but simply as \(X^{(n)}\). (This is different from the notation used in Chapter II but it is only for notational convenience and is limited to this section.) The black dot \(\bullet\) written at the place where two propagators meet corresponds to the derivative with respect to \(J\), since we have the relation

\[\frac{\partial G^i(y, z)}{\partial J} = \sum_x G^i(y, x) G^i(x, z),\]  \hspace{1cm} (10.1.19)

where \(\sum_x = \int dx \sum_r\).

We notice from (10.1.16) that \(\phi^{(0)}(J, J)\) depends only on \(J\), so we write it as \(\phi^{(0)}(J, J) = \phi_0(J)\);

\[\phi_0(J) = -\frac{1}{\beta V} \sum_x (G^{-1} - \delta_{xx} J)^{-1} \cdot \]  \hspace{1cm} (10.1.20)

Then \(\phi^{(0)}(J, J)\) can be written by using the same function, that is, \(\phi^{(0)}(J, J) = \phi_0(J)\).

By the conventional perturbation approach like the above (up to any finite order) one obtains \(\phi_1 = \phi_1\), which means \(m = 0\), if one sets \(H = 0\) \((J = J)\). This is easily understood if one notices that for the case \(H = 0\) the propagators \(G^i\) and \(G^i\) take the same value to result in \(\phi_1 = \phi_1\).

**STEP 3—Inversion of \(\phi = \phi(J)\) to obtain \(J = J(\phi)\)**

Let us discuss the graphical expressions of the inversion formulae (7.2.4) to (7.2.6). (We use them in a slightly different form with the notations appropriate to the problem here.) From (10.1.16) the 0-th order formula (7.2.4) becomes

\[-\beta V \phi_1 = \]  \hspace{1cm} (10.1.21)

where the line represents not \(G^i\) but \(G^{(0)}\) defined by

\[\left[ G^{(0)} \right]_{xx} = G^{-1} - \delta_{xx} J^{(0)}. \]  \hspace{1cm} (10.1.22)

Since (10.1.21) defines \(J^{(0)}\) implicitly we know that \(J^{(0)}(\phi)\) is a function of \(\phi\) which does not depend on \(\phi_0\). In other words \(J^{(0)}(\phi)\) is given by

\[\phi_0 = \phi_0(J^{(0)}) \quad \text{or} \quad J^{(0)} = \phi_0^{-1}(\phi_0). \]  \hspace{1cm} (10.1.23)

By noting that

\[\left. -\beta V \frac{\partial \phi^{(0)}(J, J)}{\partial J} \right|_{J = J^{(0)}} = -\beta V \frac{\partial \phi_1}{\partial J^{(0)}} = \delta_{1, \sigma} \]  \hspace{1cm} (10.1.24)
and by using Eq. (10.1.17), the first order formula (7.2.5) becomes

\[ J^{(1)} + J^{(1)} = 0. \] (10.1.25)

Here and hereafter the line represents not \( G' \) but \( G^{(0)} \) as in (10.1.21). Thus we get

\[ J^{(1)} = - \leftarrow \] (10.1.26)

or

\[ J^{(1)} = - G^{(0)}_{\sigma x} = \phi_0(J^{(0)}_x) = \phi_\sigma. \] (10.1.27)

We have used (10.1.23) and the fact that \( G^{(0)}_{\sigma x} \) does not depend on \( x \) (assuming the translational invariance). The graphs of the second order formula (7.2.5) are obtained by (10.1.16) to (10.1.18) through the way similar to the one of getting (10.1.25).

\[ J^{(1)} + J^{(1)} + J^{(1)} + J^{(1)} + J^{(1)} + J^{(1)} = 0. \] (10.1.28)

Inserting the graphic expression of \( J^{(1)} \) like (10.1.26) into this equation, we see that the third and the sixth graphs cancel out (taking the symmetry factor into account of course — see Appendix H). The second, fourth, fifth and the seventh graphs are also summed up to zero. Thus we have the simple result,

\[ - \leftarrow J^{(0)}_x = \rightarrow \] (10.1.29)

We can continue this course of study up to the desired order. The result for full order is already known to be given as a simple rule. This problem will be discussed in Chapter XI.

We have completed the inversion up to the second order. It is convenient to get the free energy from these results. The Helmholtz free energy \( F(M, N) \) is defined through Legendre transformation,

\[ F = \Omega + \beta V \sum_\sigma J_\sigma \phi_\sigma. \] (10.1.30)

Then \( F \) is actually a function of \( \phi_+ \) and \( \phi_- \) (or of \( M \) and \( N \)) with an identity,
\[ J_\sigma = \frac{1}{\beta V} \frac{\partial F}{\partial \phi_\sigma}. \] (10.1.31)

We introduce the \( n \)-th order of \( F \) in accordance with (10.1.31),
\[ J_\sigma^{(n)} = \frac{1}{\beta V} \frac{\partial F^{(n)}}{\partial \phi_\sigma}. \] (10.1.32)

Thus integrating both sides we have
\[ F^{(0)} = \beta V \sum_\sigma \int J_\sigma^{(0)} \frac{\partial \phi_\sigma}{\partial J_\sigma^{(0)}} dJ_\sigma^{(0)} = \beta V \sum_\sigma J_\sigma^{(0)} \phi_\sigma - \sum_\sigma (\ln [G_\sigma^{(0)}]^{-1})_{xx}. \] (10.1.33)

We have integrated the second expression by part and have also used
\[ -\beta V \phi_\sigma = \frac{\delta \Omega^{(0)}[J^{(0)}]}{\delta J_\sigma^{(0)}} \] (10.1.34)
and
\[ \Omega^{(0)} = -\sum_\sigma (\ln [G_\sigma^{(0)}]^{-1})_{xx} \] (10.1.35)

to obtain the last expression. The quantity \( F^{(1)} \) is readily obtained by integrating (10.1.27) with respect to \( \phi_\sigma \),
\[ \frac{1}{\beta V} F^{(1)} = U \phi, \phi = U(N^2/4-M^2)/V^2. \] (10.1.36)

It is easy to see that \( F^{(0)} + F^{(1)} \) is the free energy of the Stoner theory. Thus the inversion method up to the first order coincides with the mean-field result.

Next, \( F^{(2)} \) can also be obtained if we notice that
\[ J^{(1)}_\sigma = \frac{1}{\beta V} \frac{\partial F^{(2)}}{\partial \phi_\sigma} = \frac{1}{\beta V} \frac{\partial J^{(0)}_\sigma}{\partial \phi_\sigma} \frac{\partial F^{(2)}}{\partial J^{(0)}_\sigma}, \] (10.1.37)

and also that the left-hand side of (10.1.29) can be written as \( \beta V \partial \phi_\sigma \mid \partial J^{(0)}_\sigma \cdot J^{(2)}_\sigma \). Namely, the right-hand side of (10.1.29) is just \( \partial F^{(2)}/\partial J^{(0)}_\sigma \). Thereby we get
\[ F^{(2)} = \circlearrowleft. \] (10.1.38)

Now we introduce the frequency-momentum representation where \( p \) or \( p' \) represents a set \((n, k)\) or \((n', k')\) respectively,
\[ [G_\sigma]_{pp'} = \frac{1}{\beta V} \int_0^\beta dt \int_0^\beta d\tau \sum_k \sum_{e} e^{i\xi_n t - ik \cdot r} [G_\sigma]_{xx} e^{-i\xi_n t' + ik' \cdot r'} \] (10.1.39)
\[ = (-i\delta_n + t_\sigma - J_\sigma) \delta_{pp'} \equiv G_\sigma \delta_{pp'}, \] (10.1.40)

where the odd frequency \( \xi_n \) and \( t_\sigma \) are given by
\[ \xi_n = (2n+1)\pi T, \] (10.1.41)
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\[ t_{h}\delta_{h'h'} = \frac{1}{V} \sum_{r,r'} e^{-ik\cdot r} t_{rr'} e^{i k\cdot r'} . \] (10.1.42)

Here we have assumed that \( t_{rr'} \) is a function of \( r-r' \). In this way we have from (10.1.20)

\[ \phi_{0}(a) = -\frac{1}{\beta V} \sum_{n,h} \frac{1}{-i\xi_{n} + t_{h} - a} = \frac{1}{V} \sum_{k} f_{\beta}(t_{h} - a) , \] (10.1.43)

where

\[ f_{\beta}(x) = \frac{1}{e^{x\beta} + 1} . \] (10.1.44)

Thus we have

\[ \phi_{\sigma} = \phi_{0}(J_{\sigma}^{(0)}) = \frac{1}{V} \sum_{k} f_{\beta}(t_{h} - J_{\sigma}^{(0)}) . \] (10.1.45)

Let us examine the physical meaning of \( J_{\sigma}^{(0)} \). When \( T > T_{c} \) and \( H = 0 \), one gets \( \phi_{\downarrow} = \phi_{\uparrow} = n/2 \) because \( m = 0 \), and thus we have \( J_{\uparrow}^{(0)} = J_{\downarrow}^{(0)} = \mu_{0} \). The physical meaning of \( \mu_{0} \) is the chemical potential for the system with \( m = 0 \) (\( T > T_{c}, H = 0 \)) and \( U = 0 \) (non-interacting) at finite temperature. This is understood from (10.1.45) for the case \( \phi_{\sigma} = \phi_{\uparrow} = n/2 \) or

\[ \frac{N}{2} = \sum_{k} f_{\beta}(t_{h} - \mu_{0}) . \] (10.1.46)

Thus \( J_{\sigma}^{(0)} \) is the usual chemical potential in this case.

The algebraic expression of \( F^{(2)} \) is given by

\[ F^{(2)} = -\frac{U^{2}}{2} \sum_{xy} G_{xy}^{(0)} G_{yx}^{(0)} G_{xx}^{(0)} G_{xx}^{(0)} \]

\[ = -\frac{U^{2}}{2 V^{2}} \frac{1}{\sum_{p} G_{p}^{(0)} G_{p+\cdot}^{(0)}} \left( \sum_{p} G_{p}^{(0)} G_{p}^{(0)} \right) \left( \sum_{p} G_{p}^{(0)} G_{p}^{(0)} \right) , \] (10.1.47)

where \( G_{xy}^{(0)} = (-i\xi_{n} + t_{h} - J_{\sigma}^{(0)})^{-1} \) with \( p = (n, h) \). For later convenience we introduce \( F^{(2)}(J_{1}, J_{2}) \) as follows,

\[ F^{(2)}(J_{1}, J_{2}) = -\frac{U^{2}}{2} \sum_{k} \chi_{k}^{0}(J_{1}) \chi_{k}^{0}(J_{2}) , \] (10.1.48)

where

\[ \chi_{k}^{0}(J) = -\frac{1}{\beta V} \sum_{p} G_{p}^{J} G_{p+\cdot}^{J} \] (10.1.49)

and \( G_{p}^{J} = (-i\xi_{n} + t_{h} - J)^{-1} \) with \( p = (n, h) \). Then \( F^{(2)} \) is given by

\[ F^{(2)} = F^{(2)}(J_{1}, J_{2})|_{J_{1}=J_{2}^{(0)}, J_{2}=J_{2}^{(0)}} . \] (10.1.50)

The quantity \( \chi_{p}^{0}(J) \) reduces to the dynamical susceptibility of the free electron system \( (U = 0) \) in zero magnetic field if we set \( J = \mu_{0} \) and further reduces to the Pauli (static) susceptibility when \( p = (n, h) = 0 \). This is because \( \chi_{p}^{0}(J) \) can be rewritten as
\[
\chi^{\theta}(f) = -\frac{1}{\beta V} \sum_{k} i\omega_{n} + t_{k} - t_{k + h} \sum_{n} \left( \frac{1}{i\xi_{n} - t_{k} + f} - \frac{1}{i\xi_{n} - t_{k + h} + f} \right)
\]
\[
= \frac{1}{V} \sum_{k} \frac{f_{\sigma}(t_{k + h} - f) - f_{\sigma}(t_{k} - f)}{i\omega_{n} + t_{k} - t_{k + h}},
\]
where \(\omega_{n}\) is the even frequency,
\[
\omega_{n} = 2n\pi T.
\]

STEP 4—Turning off the source

In order to go back to the starting theory we set \(H = 0\) at this stage. This is done by the following replacement,
\[
\frac{1}{\beta V} \frac{\partial F}{\partial \phi_{\sigma}} = J_{\sigma} = \frac{\sigma}{2} H + \mu \Rightarrow \mu.
\]

Specifically this equation is written, by using (10.1.33), (10.1.36), and (10.1.48), as
\[
\mu = f_{\sigma}^{(0)} + U\phi_{-\sigma} - \frac{U^{2}}{2} \frac{1}{\beta V} \frac{\partial J_{1}}{\partial \phi_{\sigma}} \sum_{k} \left. \frac{\partial \chi^{\theta}(f_{1})}{\partial f_{1}} \chi^{\theta}(f_{2}) \right|_{f_{1} = f_{\sigma}^{(0)}, f_{2} = f}.
\]

Two equations (10.1.54) for \(\sigma = \uparrow\) and \(\downarrow\) can be looked upon as relations determining the magnetization \(M\) and the chemical potential \(\mu\) as functions of the total number of electrons \(N\).

10.1.2. First order of inversion method — Stoner theory —

The result of the inversion series up to the first order corresponds to neglecting the last term in (10.1.54),
\[
J_{\sigma}^{(0)} = \mu - U\phi_{-\sigma}.
\]

By operating \(\phi_{0}\) from the left on both sides of the above equation we get from (10.1.23)
\[
\phi_{\sigma} = \phi_{0}(\mu - U\phi_{-\sigma}) = \frac{1}{V} \sum_{k} f_{\sigma}(t_{k} + U\phi_{-\sigma} - \mu).
\]

Hence we arrive at
\[
N = \sum_{k} \left( f_{\sigma}(t_{k} - Um - \bar{\mu}) + f_{\sigma}(t_{k} + Um - \bar{\mu}) \right),
\]
\[
m = \frac{1}{2V} \sum_{k} \left( f_{\sigma}(t_{k} - Um - \bar{\mu}) - f_{\sigma}(t_{k} + Um - \bar{\mu}) \right),
\]
where \(\bar{\mu} = \mu - Un/2\). These two equations are the self-consistent equations of \(m\) and \(\mu\) for a given \(N\) in the Stoner theory. Thus we see that the inversion method up to the first order reproduces the mean-field result. (Note that in obtaining the above equation the explicit form of the inverse function \(\phi_{0}^{-1}(\phi_{\sigma})\) is not necessary.)

For example, keeping only the first order of the Sommerfeld expansion (see the standard textbook such as Ref. 4), the Stoner criterion for the presence of the ferromagnetic phase is obtained,
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\[ UD(\varepsilon_f) > 1, \quad N = 2 \int_{\varepsilon_0}^{\varepsilon_f} d\varepsilon D(\varepsilon), \quad (10\cdot1\cdot59) \]

where \( D(\varepsilon) \) is the density of state per volume of the unperturbed system, \( \varepsilon_0 \) corresponds to the energy of the bottom of the band, and the Fermi energy of the free electron \( \varepsilon_f \) is \( \mu_0 \) evaluated at \( T=0 \).

10.1.3. **Second order of inversion method — spin fluctuation**

Let us study the static susceptibility above the critical temperature using the results up to the second order of inversion series. The inverse of the static susceptibility is given by the second derivative of the free energy with respect to \( M \). The susceptibility \( \chi \) for \( T > T_c \) and \( H = 0 \) is given by

\[
\chi^{-1} = \frac{1}{\beta V} \left. \frac{\partial^2 F}{\partial m^2} \right|_{J^{(0)} = \mu_0} = \frac{1}{\beta V} \left( F_{\uparrow\uparrow} + F_{\downarrow\downarrow} - 2F_{\uparrow\downarrow} \right)_{J^{(0)} = \mu_0}, \quad (10\cdot1\cdot60)
\]

where \( F_{\sigma\sigma} = (\partial^2 F/\partial \phi_\sigma \partial \phi_\sigma) \). (Note that in the above equation the subscript \( J^{(0)} = J^{(0)} = \mu_0 \) does not imply that the derivative with respect to \( m \) is taken by fixing \( J^{(0)} \) but implies merely that \( J^{(0)} \) is set to \( \mu_0 \) after the derivative, see the arguments just below (10\cdot1\cdot45)). Hence the 0-th order of the inverse of the susceptibility is obtained as

\[
[\chi^{-1}]^{(0)} = \sum_{\sigma} \left. \frac{\partial f^{(0)}_{\sigma}}{\partial \phi_\sigma} \right|_{J^{(0)} = \mu_0}.
\]

(10\cdot1\cdot61)

By noting (10\cdot1\cdot45) we get

\[
[\chi^{-1}]^{(0)} = 2[\phi_\sigma(\mu_0)]^{-1},
\]

(10\cdot1\cdot62)

where \( \phi_\sigma(J) = \partial \phi_\sigma(J)/\partial J \) and \( \phi_\sigma(J) = -\sum_\omega G_{\omega\sigma}/\beta V \). The first order is easily given from (10\cdot1\cdot36),

\[
[\chi^{-1}]^{(1)} = -2U.
\]

(10\cdot1\cdot63)

Therefore we have

\[
\chi = [\chi^{-1}]^{(0)} + [\chi^{-1}]^{(1)} = 2[\phi_\sigma(\mu_0)]^{-1} - U,
\]

(10\cdot1\cdot64)

which corresponds to the mean-field result. If we denote \( \phi_\sigma(\mu_0) \) by the graph in (10\cdot1\cdot24), the graphs of \( \chi_{MF} \) are represented by so-called ring diagrams. Thus we again see that as the result of the inversion an infinite number of graphs has been summed up.

In order to derive the second order of the inverse of the susceptibility we first note

\[
F_{\uparrow\downarrow}^{(2)} = \left. \frac{\partial^2 f_{\uparrow\downarrow}}{\partial \phi_\uparrow \partial \phi_\downarrow} \right|_{J^{(0)} = \mu_0} = \left. \frac{\partial^2 f_{\uparrow\downarrow}}{\partial \phi_\downarrow \partial \phi_\uparrow} \right|_{J^{(0)} = \mu_0},
\]

(10\cdot1\cdot65)

\[
F_{\uparrow\downarrow}^{(2)} = \left. \left( \frac{\partial^2 f_{\downarrow\uparrow}}{\partial \phi_\uparrow \partial \phi_\downarrow} + \left( \frac{\partial f_{\downarrow\uparrow}}{\partial \phi_\uparrow} \right)^2 \right) \frac{\partial^2 f_{\downarrow\uparrow}}{\partial \phi_\downarrow \partial \phi_\uparrow} \right|_{J^{(0)} = \mu_0}.
\]

(10\cdot1\cdot66)

Since the susceptibility for \( T > T_c \) and \( H = 0 \) is evaluated at \( J^{(0)} = J^{(0)} = \mu_0 \), in the above equations, \( \partial f/\partial \phi_\sigma \) reduces to \([\phi_\sigma(\mu_0)]^{-1}\) as before and the quantity
\[
\frac{\partial^2 f_i}{\partial \phi_i^2} = -\frac{\partial}{\partial \phi_i} \left( \frac{\partial f_i}{\partial \phi_i} \right)^{-1} = -\left( \frac{\partial f_i}{\partial \phi_i} \right)^{-3} \frac{\partial^2 f_i}{\partial \phi_i^2}
\]

(10.1.67)

reduces to \(- [\phi_0'(\mu_0)]^{-3} \phi_0''(\mu_0)\). Thus from (10.1.60) and (10.1.48) the second order of \(\chi^{-1}\) is given by

\[
\Delta \chi^{-1} = [\chi^{-1}]^{[2]} = \left( \frac{U}{\phi_0'(\mu_0)} \right)^2 \left( \frac{\phi_0''(\mu_0)}{\phi_0'(\mu_0)} \right) \frac{\partial}{\partial f_1} \left[ \frac{\partial}{\partial f_1} + \frac{\partial}{\partial f_2} \right] \frac{1}{\beta V} \sum_k \chi_k \phi'(f_1) \chi_k \phi'(f_2) \bigg|_{f_1 = f_2 = \mu_0}
\]

(10.1.68)

We now obtain the inverse of the susceptibility for \(T > T_c\) and \(H=0\) up to the second order of the inversion method, which is given by

\[
\chi^{-1} = \chi_0^{-1} + \Delta \chi^{-1}
\]

(10.1.69)

with (10.1.64) and (10.1.68). This expression is exact except for the approximation by the inversion method so that we expect that it approaches the correct value if the coupling constant \(U\) becomes small. We note here that without further approximation the even-frequency summation in (10.1.68) (see \(\omega_n\) appearing in (10.1.51)) can be performed,

\[
\frac{1}{\beta V} \sum_k \chi_k \phi'(f_1) \chi_k \phi'(f_2)
\]

\[
= \frac{1}{2 \sqrt{V}} \sum_{k_1, k_2} \{f_0(\bar{\mu}_1) - f_0(\mu_1)\} \{f_0(\bar{\mu}_2) - f_0(\mu_2)\} \frac{\coth \frac{\beta \varepsilon_2}{2}}{\varepsilon_1 - \varepsilon_2} - \frac{\coth \frac{\beta \varepsilon_1}{2}}{\varepsilon_1 - \varepsilon_2},
\]

(10.1.70)

where \(\bar{\mu}_i = t_{k_1 + k_2} - f_i, \mu_i = t_{k_1 - f_i}, \varepsilon_i = t_{k_1 + k_2} - t_{k_1}\).

For the numerical estimation of (10.1.69), see Refs. 5) and 6) where the parabolic band with the momentum cut off \(k_c\) was assumed. Although the result depends on \(k_c\), it was found that for \(k_c\) slightly less than twice the Fermi momentum \(\chi^{-1}\) shows the linear behavior in \(T\) in the physically interesting region of the temperature and the magnitude of the critical temperature is substantially reduced at the same time. The comparison with the SCR (self-consistent renormalization) theory by Moriya and Kawabata\(^{5,6}\) has also been given there.

What we want to stress again here is that the inversion method provides a systematic way of calculating the higher-order expressions in a mathematically well defined manner. In Chapter XI, an analysis will be given as to the higher orders in a diagrammatic language.

The application of the inversion method up to second order of the weak coupling expansion to the antiferromagnetic case has been done in Ref. 8).

10.1.4. \(SU(2)\) symmetric Stoner theory

As is well known, the Hubbard Hamiltonian (10.1.1) has the \(SU(2)\) symmetry which is larger than the symmetry group \(\mathbb{Z}_2\). Inversion method can straightforwardly be extended to keep the \(SU(2)\) symmetry. For example, the free energy in this case is obtained by simply replacing \(m_z\) of the previous section by \(\sqrt{m_x^2 + m_y^2} = m_z\). In
order to discuss the problem, the source term is introduced in the $SU(2)$ symmetric manner, that is, $\mathcal{H}_J$ is given as (instead of (10.1.6)),

$$\mathcal{H}_J = \mathcal{H} - \mu \tilde{N} - \sum_r \mathbf{H}(x) \cdot \tilde{S}(r)$$

$$= \mathcal{H} - \sum_r \sum_{\sigma, \sigma'} J_{\sigma, \sigma'} x a^{\dagger}_{\sigma} a_{\sigma' r, \sigma'} ,$$  \hspace{1cm} (10.1.71)

where $\mathbf{H}(x) = \mathbf{H}(\tau, r)$ and $\tilde{S}(r)$ is the local spin operator given in (10.1.5). We made the source $\mathbf{H}$ to be $\mathbf{r}$-dependent for the calculational convenience while the $\tau$-dependence is introduced so that we can investigate the excitation mode in the following section. The $2 \times 2$ matrix of the source $J$ has been introduced as

$$J_{\sigma, \sigma'} = \frac{1}{2} \begin{pmatrix} H_3 + 2 \mu & H_1 - i H_2 \\ H_1 + i H_2 & -H_3 + 2 \mu \end{pmatrix} .$$  \hspace{1cm} (10.1.72)

Then the generalized thermodynamic potential $\Omega[J]$ is defined by

$$e^{-\Omega[J]} = \text{Tr} e^{-\beta \mathcal{H}_J} .$$  \hspace{1cm} (10.1.73)

Owing to the $SU(2)$ invariance of $\mathcal{H}$, $\Omega$ is invariant under the rotation of $\mathbf{H}$:

$$\Omega[\mathbf{H}] = \Omega[R \mathbf{H}] ,$$  \hspace{1cm} (10.1.74)

where $R$ is an arbitrary $3 \times 3$ $x$-independent orthogonal matrix corresponding to the rotation in $\mathbf{H}$ space.

Now the path-integral representation of $\Omega[J]$ is written as (see Appendix H)

$$e^{-\Omega} = \int_{z_0 = -z_s} z^* Dz \exp \left\{ -z^* \left[ G' \right]_{\sigma' \sigma} z - U z^* z, z^* z \right\} ,$$  \hspace{1cm} (10.1.75)

where

$$[G']^{-1} = G_{\sigma' \sigma, xx'} - \delta_{xx'} J_{\sigma', x} ,$$  \hspace{1cm} (10.1.76)

$$G_{\sigma' \sigma, xx'} = \delta_{\sigma' \sigma} \delta_{xx'} \left( \frac{\partial}{\partial \tau'} + t_{rr'} \right) .$$  \hspace{1cm} (10.1.77)

Here we have used the simple notation $x = (\tau, \mathbf{r})$ and summation over $\sigma$ and $x$ are suppressed. Then by the Feynman rule we obtain

$$\Omega = \Omega^{(0)} + \Omega^{(1)} + \cdots$$  \hspace{1cm} (10.1.78)

with

$$\Omega^{(0)} = - \text{Tr} \ln [G']^{-1} ,$$  \hspace{1cm} (10.1.79)

$$\Omega^{(1)} = U \sum_x (G^\dagger_{1, xx} G^\dagger_{1, xx} - G^\dagger_{1, xx} G^\dagger_{1, xx}) .$$  \hspace{1cm} (10.1.80)

In the present case the variable of interest is given by the matrix

$$\phi_{\sigma, \sigma'} = - \frac{\delta \Omega}{\delta J_{\sigma, \sigma'}} = (\phi^{(0)}[J] + \phi^{(1)}[J] + \cdots)_{\sigma, \sigma'} .$$  \hspace{1cm} (10.1.81)
Then $\phi^{(0)}$ is given by

$$
\phi^{(0)}(x) = -\begin{pmatrix} G_1^t & G_1^t \\ G_1^t & G_1^t \end{pmatrix} x,
$$

(10.1.82)

and $Q^{(1)}$ is rewritten as

$$
Q^{(1)} = U \sum_y (\phi^{(0)}_1, \phi^{(0)}_1 - \phi^{(0)}_1, \phi^{(0)}_1)_y.
$$

(10.1.83)

By using the inversion formulas of many variables of Appendix I, (I.5), (I.6),

$$
\phi_{\sigma\sigma',x} = \phi^{(0)}_{\sigma\sigma',x}[J^{(0)}],
$$

(10.1.84)

$$
\frac{\delta \phi^{(0)}_{\sigma\sigma',x}[J]}{\delta J_{\sigma\sigma',y}} \bigg|_{J^{(0)}} \cdot J^{(1)}_{\sigma\sigma',y} + \phi^{(0)}_{\sigma\sigma',x}[J^{(0)}] = 0,
$$

(10.1.85)

we arrive at the following result after some calculation,

$$
J^{(1)} = U \begin{pmatrix} \phi_1^t & -\phi_1^t \\ -\phi_1^t & \phi_1^t \end{pmatrix}.
$$

(10.1.86)

Actually this result can be easily obtained in the following manner. The generalized free energy $F[\phi]$ is defined by

$$
F[\phi] = Q[J] + \sum_x \sum_{\sigma\sigma'} J_{\sigma\sigma',x} \phi_{\sigma\sigma',x} = F^{(0)} + F^{(1)} + \cdots.
$$

(10.1.87)

By using the formulas for $F$, (7.2.14, 15) or (I.13, 14),

$$
F^{(0)} = Q^{(0)}[J^{(0)}] + J^{(0)}[\phi] \cdot \phi,
$$

(10.1.88)

$$
F^{(1)} = Q^{(0)}[J^{(0)}] \cdot J^{(1)}[\phi] + Q^{(1)}[J^{(0)}] + J^{(1)}[\phi] \cdot \phi,
$$

(10.1.89)

where

$$
J^{(0)}[\phi] \cdot \phi = \sum_{\sigma\sigma'} J_{\sigma\sigma'}^{(0)}[\phi] \cdot \phi_{\sigma\sigma'}, \quad Q^{(0)}[J^{(0)}] \cdot J^{(1)}[\phi] = \sum_{\sigma\sigma'} \frac{\partial Q^{(0)}[J^{(0)}]}{\partial J_{\sigma\sigma'}^{(0)}} J_{\sigma\sigma'}^{(1)}[\phi].
$$

Note here that $Q^{(1)}$ is a scalar quantity which is a functional of $2 \times 2$ matrices $J_{\sigma\sigma'}^{(0)}[\phi]$'s and $F^{(1)}$ is a scalar quantity which is a functional of matrices $J_{\sigma\sigma'}^{(0)}[\phi]$'s. From (10.1.81) and (10.1.84), we have $\phi = -Q^{(0)}[J^{(0)}]$, or explicitly,

$$
\phi_{\sigma\sigma'} = -\frac{\partial Q^{(0)}[J^{(0)}]}{\partial J_{\sigma\sigma'}^{(0)}},
$$

to get (see (7.2.15) or (I.14)),

$$
F^{(1)} = Q^{(1)}[J^{(0)}] = U \sum_y (\phi_1^t, \phi_1^t - \phi_1^t, \phi_1^t)_y.
$$

(10.1.90)

Here we have used (10.1.83) and (10.1.84). Then by using the relation $J^{(1)} = (\delta F^{(1)}/\delta \phi)$ we arrive at (10.1.86).

Since the series

$$
J = J^{(0)} + J^{(1)} + \cdots
$$

(10.1.91)
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is given up to the first order in $U$ by (10·1·84) and (10·1·86), we can write, neglecting higher orders,

$$J^{(0)} = J - J^{(1)}.$$  \hfill (10·1·92)

Operating $\phi^{(0)}_{\sigma \tau}$ on the above equation and returning to the original theory by setting $J_{\sigma \tau} = \mu \delta_{\sigma \tau}$, we get

$$\phi_{\sigma \tau} = \phi^{(0)}_{\sigma \tau} [\mu - J^{(1)}] = \begin{pmatrix} G_{\uparrow \downarrow}^{\tau} & G_{\downarrow \uparrow}^{\tau} \\ G_{\downarrow \uparrow}^{\tau} & G_{\uparrow \downarrow}^{\tau} \end{pmatrix} \begin{pmatrix} J_{\sigma \tau} \end{pmatrix} \begin{pmatrix} \mu - J^{(1)} \end{pmatrix},$$  \hfill (10·1·93)

since we have the lowest inversion formula $\phi = \phi^{(0)}_{\sigma \tau} [J^{(0)} [\phi]]$. The subscript implies that the matrix $J$ is replaced as

$$J \rightarrow \begin{pmatrix} \mu - U\phi_{\uparrow \downarrow} & U\phi_{\downarrow \uparrow} \\ U\phi_{\downarrow \uparrow} & \mu - U\phi_{\uparrow \downarrow} \end{pmatrix}.$$  \hfill (10·1·94)

This replacement is equivalent to the following prescription,

$$H_1 = J_{12} + J_{21} \quad \Longrightarrow \quad U(\phi_{\uparrow \downarrow} + \phi_{\downarrow \uparrow}) = -2Um_1,$$

$$H_2 = i (J_{12} - J_{21}) \quad \Longrightarrow \quad Ui(\phi_{\uparrow \downarrow} - \phi_{\downarrow \uparrow}) = -2Um_2,$$

$$H_3 = J_{11} - J_{22} \quad \Longrightarrow \quad U(\phi_{\uparrow \downarrow} - \phi_{\downarrow \uparrow}) = -2Um_3,$$

$$\mu = (J_{11} + J_{22})/2 \quad \Longrightarrow \quad \mu - U(\phi_{\uparrow \downarrow} + \phi_{\downarrow \uparrow})/2 = \mu - Un/2 = \bar{\mu}. \quad (10·1·95)$$

Here $m_\sigma$ is the expectation value of the magnetization operator $\hat{m}_\sigma = -\hat{S}_\sigma/V$ where $\hat{S}_\sigma$ is given by (10·1·5). We have assumed $\phi$ to be $x$-independent since we are interested in the homogeneous ferromagnetic phase. $\phi$ is assumed to be $x$-independent at this point.

Now we rewrite (10·1·93). First, we observe that, for $x$-independent $J$, $G'$ can be expressed as

$$G' = [(G^{-1} - \mu - \tau \cdot H/2)^{-1}$$

$$= \frac{1}{2} (I + \tau \cdot H/H) G^{\mu + H/2} + \frac{1}{2} (I - \tau \cdot H/H) G^{\mu - H/2}, \quad (10·1·96)$$

where $H = \sqrt{H_1^2 + H_2^2 + H_3^2}$, $G^A = (G^{-1} - A)^{-1}$, and $I$ is the $2 \times 2$ unit matrix. Then by the replacement of (10·1·94) or (10·1·95), $G'$ becomes

$$G' \rightarrow (I/2 - \tau \cdot m/m) G^{\bar{\mu} + Um} + (I/2 + \tau \cdot m/m) G^{\bar{\mu} - Um}, \quad (10·1·97)$$

where $m = \sqrt{m_1^2 + m_2^2 + m_3^2}$. Then by (10·1·93), we get

$$m_3 = -\frac{1}{2\beta V} \sum_x (\phi_{\uparrow \downarrow} - \phi_{\downarrow \uparrow})$$

$$= \frac{m_3}{2\beta V} \sum_x (G^{\bar{\mu} + Um} - G^{\bar{\mu} - Um}). \quad (10·1·98)$$

By using (10·1·20) and (10·1·43), we obtain
\[ m_3 = \frac{m_3}{m} \left( \frac{1}{2V} \sum_k \left( f_\beta(t_k + Um - \bar{\mu}) - f_\beta(t_k - Um - \bar{\mu}) \right) \right). \quad (10 \cdot 1 \cdot 99) \]

In the same way we arrive at
\[ m_3 = \frac{m_3}{m} \left( \frac{1}{2V} \sum_k \left( f_\beta(t_k + Um - \bar{\mu}) - f_\beta(t_k - Um - \bar{\mu}) \right) \right) \quad (10 \cdot 1 \cdot 100) \]

in addition to (10 \cdot 1 \cdot 57). Clearly three equations of (10 \cdot 1 \cdot 100) can be replaced with a single equation (10 \cdot 1 \cdot 58) if we interpret \( m = \sqrt{m_1^2 + m_2^2 + m_3^2} \) in (10 \cdot 1 \cdot 58). (Originally \( m \) is the expectation value of \( \bar{m}_3 \) in (10 \cdot 1 \cdot 58).)

What we have done can be generalized to full order by looking at the problem in a formal way. Since we know that \( Q[RH] = Q[H] \), \( F[\phi] = F[m, N] \) has the same property,
\[ F[Rm, N] = F[m, N]. \quad (10 \cdot 1 \cdot 101) \]

If we assume that \( m \) is \( x \)-independent, \( F \) depends on \( m \) only through \( m = \sqrt{m_1^2 + m_2^2 + m_3^2} \). It follows that \( F \) as a function of \( m \) is easily obtained first by calculating \( F \) with \( m_1 = m_2 = 0 \) to know \( F \) as a function of \( m_3 \) and then by replacing \( m_3 \) with \( m \) in the expression of \( F \) thus obtained. Keeping this fact in mind we notice that the result of (10 \cdot 1 \cdot 100) is only the lowest order example of the full order theorem.

10.1.5. Excitation modes —— on-shell equation ——

The excitation modes are studied by the on-shell equation (2 \cdot 1 \cdot 4a) for zero temperature case. It is the equation which determines the poles of the causal (i.e., time ordered) Green’s function. On-shell equation in the case of non-zero temperature will be discussed in Chapter XII in real time formalism where it is shown that the retarded Green’s function appears in the mode determining equation. But here we look into the excitation modes in non-zero temperature starting from the imaginary time formalism since we know that the retarded and the \( \tau \)-ordered Green’s function is the analytic continuation of each other in complex \( \omega \) space. Namely the excitation modes are given by solving (2 \cdot 1 \cdot 4a) using the second derivative of \( F[m_\nu] \) in place of \( \Gamma^{\mu \nu} \) there:

\[ \Sigma \int d\tau' \int d^3y \left( \frac{\partial^2 F}{\partial m_\mu(x) \partial m_\nu(y)} \right)_0 \Delta m_\nu(y) = 0, \quad (10 \cdot 1 \cdot 102) \]

where \( x = (\tau, \mathbf{x}), y = (\tau', \mathbf{y}) \). We have also defined \( m_\nu = (m_1, m_2, m_3, m_4) \) with \( m_4 = n/2 \). The quantities \( m_1, m_2, m_3 \) are defined in (10 \cdot 1 \cdot 95). For the relation between the on-shell expansion in real and imaginary time formalism, see §12.3.3.

10.1.6. Second derivative of effective action

We need the second derivative of the imaginary time effective action (free energy) which is evaluated at the stationary point determined by (see (10 \cdot 1 \cdot 86))
\[ J - \mu = \frac{\partial F}{\partial \phi} - \mu = 0 \quad \text{or} \quad J^{(0)} + U \begin{pmatrix} \phi_{1 \downarrow} & -\phi_{1 \uparrow} \\ -\phi_{1 \uparrow} & \phi_{1 \downarrow} \end{pmatrix} + \cdots = \mu. \quad (10 \cdot 1 \cdot 103) \]
As the stationary solution to the above equation we take a ferromagnetic one in which the magnetization points in \(z\)-direction without loss of generality (see the discussion following (10\,1\,101)),

\[
\phi = \begin{pmatrix} -m + n/2 & 0 \\ 0 & m + n/2 \end{pmatrix},
\]

(10\,1\,104)

where \(m\) and \(n\) are \((\tau, r)\)-independent (see (10\,1\,95), or (10\,1\,115) below). Hereafter we use the result of the first order of the inversion method, higher-order contributions being neglected in what follows. Then at the stationary point \(J^{(0)}\) is given by

\[
J^{(0)}_{\sigma\sigma'} = \begin{pmatrix} \mu - U(n/2 + m) & 0 \\ 0 & \mu - U(n/2 - m) \end{pmatrix} = (\bar{\mu} - \sigma Um) \delta_{\sigma\sigma'} = J^{(0)}_\sigma \delta_{\sigma\sigma'},
\]

(10\,1\,105)

where \(\bar{\mu} = \mu - U n/2\). The second derivative of the effective action is given by taking the derivative of the following expression,

\[
\frac{\partial F}{\partial \phi_{\sigma\sigma'}} = J^{(0)}_{\sigma\sigma'}[\phi] + U \begin{pmatrix} \phi_{\uparrow\uparrow} & -\phi_{\downarrow\downarrow} \\ -\phi_{\uparrow\downarrow} & \phi_{\downarrow\uparrow} \end{pmatrix}.
\]

(10\,1\,106)

Let us first consider the derivative of the first term, that is, \(\partial J^{(0)}_{\sigma\sigma'}/\partial \phi_{\sigma\sigma'}\). This is the inverse of

\[
\frac{\partial \phi_{\uparrow\downarrow',x}}{\partial J^{(0)}_{\sigma\sigma'}}, x = \frac{\partial \phi_{\uparrow\uparrow}, x}{\partial J^{(0)}_{\sigma\sigma'}}, x = -\frac{\partial^2 G^{(0)}[J^{(0)}]}{\partial J^{(0)}_{\sigma\sigma'}, x}, y = -G^{(0)}_{\sigma\sigma'(yx)}G^{(0)}_{\sigma\tau}(xy),
\]

(10\,1\,107)

where we have used (10\,1\,84) and (10\,1\,79). Here the inverse is defined by

\[
\sum_{\sigma\tau, y} \frac{\partial \phi_{\sigma\sigma'r, x}}{\partial J^{(0)}_{\sigma\sigma'}, x} \frac{\partial J^{(0)}_{\sigma\sigma', y}}{\partial \phi_{\sigma\tau, x}} = \delta_{\sigma\tau} \delta_{\sigma'\tau} \delta_{xx},
\]

(10\,1\,108)

which is obtained by taking the derivative of \(\phi_{\sigma\sigma'}\) with respect to \(\phi_{\sigma\tau}\) and by using the chain rule. Note here that \(\phi\) can be regarded as a functional of \(J^{(0)}\) (see (10\,1\,84)). If we evaluate the quantity in (10\,1\,107) at the stationary point where \(J^{(0)}_{\sigma\sigma'}\) becomes diagonal as in (10\,1\,104), then the Fourier transform of it takes the form

\[
\left( \frac{\partial \phi_{\sigma\tau}}{\partial J^{(0)}_{\sigma\sigma'}} \right)_{\rho q} = -\delta_{\tau', \sigma} \delta_{\sigma', \rho} \delta_{pq} \frac{1}{V} \sum_k G^{(0)}_{\sigma, k} G^{(0)}_{\sigma', \rho + k},
\]

(10\,1\,109)

where \(G^{(0)}_{\sigma, k}\) is given by

\[
G^{(0)}_{\sigma, k} = \frac{1}{-i\xi_n + t_k - J^{(0)}_\sigma} = \frac{1}{-i\xi_n + t_k - \bar{\mu} + \sigma Um}
\]

(10\,1\,110)

with \(k = (n, k)\). The overline in (10\,1\,109) implies that the quantity is evaluated at the stationary point. Thereby we get the leading order (of the inversion series) of the second derivative of the effective action evaluated at the ferromagnetic stationary point,
\[
\frac{\partial^2 F^{(0)}}{\partial \phi_{\sigma \sigma'} \partial \phi_{\tau \tau'}}_{pq} = \delta_{\sigma \tau} \delta_{\sigma' \tau'} \delta_{pq} F_{2, \sigma \sigma'}, 
\]
(10.1.111)

\[
F_{2, \sigma \sigma'} = -\left[ \frac{1}{\beta V} \sum_k G^{(0)}_{\sigma,k} G^{(0)}_{\sigma', k+p} \right]^{-1}.
\]
(10.1.112)

From (10.1.106) and (10.1.111) we obtain the second derivative at the stationary point up to the desired order,

\[
\frac{\partial^2 F}{\partial \phi_{\sigma \sigma'} \partial \phi_{\tau \tau'}}_{pq} = \delta_{pq} (\delta_{\sigma \tau} \delta_{\sigma' \tau'} F_{2, \sigma \sigma'} + \eta_{\sigma \sigma' \tau \tau'} U),
\]
(10.1.113)

where \( \eta_{\sigma \sigma' \tau \tau'} \) is defined as follows,

\[
\eta_{\sigma \sigma' \tau \tau'} = \begin{cases} 
1 & (\sigma' \tau' = (\uparrow \downarrow \downarrow \uparrow), (\downarrow \downarrow \uparrow \downarrow)) \\
-1 & (\sigma' \tau' = (\uparrow \downarrow \uparrow \downarrow), (\downarrow \uparrow \uparrow \downarrow)) \\
0 & (\sigma' \tau' = \text{others})
\end{cases}.
\]
(10.1.114)

Up to now we have considered \( \phi_{\sigma \sigma'} \) as our variable, but it is convenient to regard \( m \) and \( n \) as independent variables instead. Both variables are connected by

\[
\phi_{\sigma \sigma'} = \begin{pmatrix} m/2 - m_3 & -m_1 - im_2 \\ -m_1 + im_2 & n/2 + m_3 \end{pmatrix}.
\]
(10.1.115)

For convenience we employ the notation \( m_\mu \) as in (10.1.102). Now we derive the second derivative of \( F \) in terms of \( m_\mu \) from (10.1.113). After some simple calculation by using

\[
\frac{\partial}{\partial m_1} = -\left( \frac{\partial}{\partial \phi_{\uparrow \downarrow}} + \frac{\partial}{\partial \phi_{\downarrow \uparrow}} \right), \quad \frac{\partial}{\partial m_2} = -i \left( \frac{\partial}{\partial \phi_{\uparrow \downarrow}} - \frac{\partial}{\partial \phi_{\downarrow \uparrow}} \right),
\]

\[
\frac{\partial}{\partial m_3} = -\left( \frac{\partial}{\partial \phi_{\uparrow \uparrow}} - \frac{\partial}{\partial \phi_{\downarrow \downarrow}} \right), \quad \frac{\partial}{\partial m_4} = 2 \frac{\partial}{\partial n} = \left( \frac{\partial}{\partial \phi_{\uparrow \uparrow}} + \frac{\partial}{\partial \phi_{\downarrow \downarrow}} \right),
\]
(10.1.116)

we arrive at

\[
\frac{\partial^2 F}{\partial m_\mu \partial m_\nu} = \delta_{pq} \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = \delta_{pq}.
\]

\[
\times \begin{pmatrix} F_{2, \uparrow \downarrow} + F_{2, \downarrow \uparrow} - 2U & -i(F_{2, \uparrow \downarrow} - F_{2, \downarrow \uparrow}) & 0 & 0 \\ -i(F_{2, \downarrow \uparrow} - F_{2, \uparrow \downarrow}) & F_{2, \uparrow \downarrow} + F_{2, \downarrow \uparrow} - 2U & 0 & 0 \\ 0 & 0 & F_{2, \uparrow \uparrow} + F_{2, \downarrow \downarrow} - 2U & F_{2, \uparrow \uparrow} - F_{2, \downarrow \downarrow} \\ 0 & 0 & F_{2, \downarrow \uparrow} - F_{2, \uparrow \downarrow} & F_{2, \downarrow \uparrow} + F_{2, \uparrow \downarrow} + 2U \end{pmatrix}.
\]
(10.1.117)

For later use we show the explicit expression of \( F_{2, \sigma \sigma'} \),

\[
(1/F_{2, \sigma \sigma'})_k = \frac{1}{V^2} \sum_{k'} f_k (t_{k, k'} - J_{\sigma}^{(0)}) - f_k (t_{k'} - J_{\sigma'}^{(0)})
\]
(10.1.118)

where \( k = (n, k) \),
\( J^{\sigma \sigma'}_{\beta} = \tilde{\mu} - \sigma U m \) and \( J^{\sigma \sigma'}_{\beta} = -U m (\sigma - \sigma') \).

This expression is obtained by the way similar to that used to derive the final form in (10.1.51).

10.1.7. Study of excitation modes

Now we analytically continue \( \frac{\partial^2 F}{\partial m_\mu \partial m_\nu} \) given in (10.1.117) so that the inverse of it becomes an analytic function in the upper half-plane of complex \( \omega \). All we have to do is to change \( i\omega_n \) in (10.1.117) to \( \omega + i\eta \). This fact will be confirmed later by showing that the zeros of the analytically continued \( \frac{\partial^2 F}{\partial m_\mu \partial m_\nu} \) never appear in the upper half-plane.

Since the excitation mode is given by the zero of the matrix (10.1.117) but \( i\omega_n \) in \( F_{\omega \sigma \sigma'} \) is replaced by \( \omega + i\eta \). The modes are thus determined by

\[
\det \left[ \left( \frac{\partial^2 F}{\partial m_\mu \partial m_\nu} \right)_{\mu \nu} \right]_{\omega = \omega + i\eta} = 0.
\]

This condition is equivalent to

\[
(F_{\uparrow \uparrow} + F_{\downarrow \downarrow} - 2U)^2 - (F_{\uparrow \downarrow} - F_{\downarrow \uparrow})^2 = 0
\]

and

\[
(F_{\uparrow \uparrow} + F_{\downarrow \downarrow} - 2U)(F_{\uparrow \downarrow} + F_{\downarrow \uparrow} + 2U) - (F_{\uparrow \downarrow} - F_{\downarrow \uparrow})^2 = 4(F_{\uparrow \downarrow} F_{\downarrow \uparrow} - U^2) = 0,
\]

where \( F_{\sigma \sigma'} \) is given by

\[
\frac{1}{F_{\sigma \sigma'}} = \frac{1}{V} \sum_{\kappa} \frac{f_\beta(t_{\kappa + \kappa'} - \tilde{\mu} + \sigma U m) - f_\beta(t_{\kappa' - \tilde{\mu}} + \sigma' U m)}{\omega + i\eta - t_{\kappa + \kappa'} + t_{\kappa'} + (\sigma - \sigma') U m},
\]

where \( \tilde{\mu} = \mu - Un/2 \). Here we see, as mentioned before, that the zero of \( \left( \frac{\partial^2 F}{\partial m_\mu \partial m_\nu} \right)_{\mu \nu} \) never appear in the upper half-plane, since in (10.1.120) and (10.1.121) no imaginary quantities come out other than in the form \( \omega + i\eta \) so that the zeros are expected to emerge in the form \( \omega + i\eta = \text{real} \).

Let us examine the mode determining equation (10.1.120). We can show the following property of \( F_{\sigma \sigma'} \) easily from the definition (10.1.122). (We do not write \( i\eta \) explicitly in what follows.)

\[
F_{\sigma \sigma'}(\omega) = F_{\sigma' \sigma}(-\omega),
\]

where we have written \( \omega \) dependence explicitly. Thus if we denote \( F_{\uparrow \downarrow} = F(\omega) \) and \( F_{\downarrow \uparrow} = F(-\omega) \), we have from (10.1.120)

\[
F(\omega) + F(-\omega) - 2U = \pm (F(\omega) - F(-\omega))
\]

or

\[
F(\pm \omega) = U.
\]

The last equation can be written as
\[ \frac{1}{V} \sum_{k} \frac{f_{\lambda}(\epsilon_{k} - \Delta) - f_{\lambda}(\epsilon_{k + \mathbf{k}} + \Delta)}{\epsilon_{k + \mathbf{k}} - \epsilon_{k} + 2\Delta + \omega} = \frac{1}{U}, \]  
(10.1.126)

where \( \epsilon_{k} = t_{k} - \mu \) and \( \Delta = Um. \) This coincides with the equation obtained by RPA approximation\(^{(3,6)}\) and the following dispersion relation of the spin wave can be obtained by the well-known procedure,

\[ \omega = \pm \frac{n}{4Mm} k^2, \]  
(10.1.127)

where \( M \) is the electron mass.

The above result can be interpreted in the language of the Goldstone mode presented in § 3.5, where in (3.5.7) the wave function of the Goldstone mode is given by \( a_{j,k} \phi_{k}^{(o)}. \) For the problem here it takes the form \( a_{\mu,\nu}m_{\nu}. \) Here the matrix \( a_{\mu,\nu} \) corresponds to the infinitesimal space rotation so that its non-zero components are \( a_{j,k} \) for \( j, k = 1, 2, 3 \) and others are zero. Since we have taken \( m \) in \( z \)-axis, only \( k = 3 \) contributes. Thus we expect two kinds of Goldstone modes, one for \( i = 1 \) and the other for \( i = 2 \) and the wave functions \( \Delta m_{\nu} \) of the Goldstone modes at \( \omega = k = 0 \) are proportional to \((1, 0, 0, 0)\) and \((0, 1, 0, 0)\). The fact that this is indeed the case can be seen by noting that both \( F_{2,1,i} + F_{2,1,i} - 2U \) and \( -i(F_{2,1,i} - F_{2,1,i}) \) vanish at \( \omega = k = 0 \) if they are evaluated by the stationary solution. These properties are easily seen from (10.1.122).

\section{10.2. Strong coupling inversion}

The strong coupling region (large \( U \)) of the Hubbard model cannot be examined appropriately by using the weak coupling expansion unless the infinite number of the expansion terms are taken into account. In this section, the method of inversion is applied to the problem taking \( 1/U \), instead of \( U \), as an expansion parameter of the inversion series. Here the problem is that we cannot calculate the original series (7.2.2) exactly (otherwise the strong coupling problems are exactly solvable). We take the following strategy; each term \( f_{n}[J] \) is expanded in powers of the hopping parameter \( t \) and the terms up to \( t^2 \) are kept. (The terms linear in \( t \) vanish.) Since \( f_{n}[J] \) is a function of \( t^2 \), (7.2.2) has the form (here \( J \) is the magnetic field and \( \phi \) the magnetization),

\[ \phi = f_{0}[J, t^2] + \frac{1}{U} f_{1}[J, t^2] + \cdots \]

\[ = f_{0}[J, 0] + f_{0}[J, 0] t^2 + \frac{1}{U} \left( f_{1}[J, 0] + f_{1}[J, 0] t^2 \right) + \cdots. \]  
(10.2.1)

The inversion is performed up to the order \( 1/U \) and the coefficients are again expanded in \( t \) up to \( t^2 \). Thus we get the inverted series,

\[ J = g_{0}[\phi, t^2] + \frac{1}{U} g_{1}[\phi, t^2] + \cdots. \]
\[
= g_0[\phi, 0] + g_0[\phi, 0] t^2 + \frac{1}{U} \left( g_1[\phi, 0] + g_1[\phi, 0] t^2 \right) + \cdots \\
= \left( g_0[\phi, 0] + \frac{1}{U} g_0[\phi, 0] \right) t^2 + \frac{1}{U} \left( g_0[\phi, 0] + \frac{1}{U} g_0[\phi, 0] \right) + \cdots .
\] (10.2.2)

The above approach can be said to be a kind of strong coupling mean-field theory. Alternatively, as the process indicates, the same formula as (10.2.2) is obtainable taking \( t^2 \) as the inversion parameter and after the inversion we expand in powers of \( 1/U \). Since this route is more transparent, we adopt the latter way in the following.

Recall that the filling factor is arbitrary in the following discussions. Starting from the exact result due to Nagaoka,\(^{10}\) the theory of strong coupling was extended to the case where the electron number differs from that of half filling by a finite limited number.\(^{11,12}\) The physically interesting case is of course where the electron number deviates macroscopically from the half filling. Our approach below is one of the examples to attack the problem but, like most of the mean-field treatments, the results do not have strong dependence on the dimension and it is expected that the conclusion cannot be valid for small dimension. Our method is equivalent to the high temperature expansion in the Legendre transformed world and the results below are due to Hondou.\(^{13}\)

10.2.1. Ferromagnetic state

The Hamiltonian of the standard Hubbard model in the homogeneous magnetic field is shown here using the discrete indices \( i \) to denote the lattice points,

\[
\mathcal{H} = - t \sum_{\langle \ell, \sigma \rangle} a^\dagger_{\ell \sigma} a_{\ell \sigma} + \sum_i \left[ U n_{i \uparrow} n_{i \downarrow} + H (n_{i \uparrow} - n_{i \downarrow}) - \mu (n_{i \uparrow} + n_{i \downarrow}) \right].
\] (10.2.3)

\[
\mathcal{H}_1 = \mathcal{H}_0
\]

Here we have indicated that the hopping term is treated as a perturbation. Let us assume that the system has \( N_0 \) sites and each site has \( z \) nearest neighbors.

(i) Zeroth order

In zeroth order of \( t \), we get the partition function in the form

\[
Z = e^{-\beta W} = \text{Tr} e^{-\beta \mathcal{H}} = (X^2 e^{-\beta H} + 2X \cosh \beta H + 1)^{N_0},
\] (10.2.4)

where \( \beta = 1/k_B T \), and

\[
X = e^{\beta \mu}.
\] (10.2.5)

Thus the number density of electrons for \( H = 0 \) is given by

\[
n = \frac{N}{N_0} = \frac{1}{N_0} \frac{\partial W}{\partial \mu} = \frac{2X^2 e^{-\beta H} + 2X}{X^2 e^{-\beta H} + 2X + 1},
\] (10.2.6)

where \( 0 \leq n \leq 2 \), and we can solve this equation with respect to \( X \) as

\[
X = \frac{1 \pm \sqrt{(1-n)^2 + e^{-\beta H} (2-n)n}}{e^{-\beta H} (n-2)}.
\] (10.2.7)
If we consider the case where \( U \to \infty \), \( X \) is found to have the form

\[
X = \begin{cases} 
\frac{n}{2(1-n)}, & (n<1) \\
e^{\beta U/2}, & (n=1) \\
\frac{2(n-1)}{2-n} e^{\beta U}. & (n>1)
\end{cases}
\tag{10.2.8}
\]

Then the magnetization for fixed \( \mu \) is written by

\[
m = \frac{M}{N_0} = -\frac{1}{N_0} \frac{\partial W}{\partial H} = \frac{2X \sinh \beta H}{X^2 e^{-\beta U} + 2X \cosh \beta H + 1} \quad (\mu \to 0),
\tag{10.2.9}
\]

and the susceptibility for fixed \( \mu \) has the form

\[
\chi = \frac{\partial m}{\partial H} = 2\beta \frac{X}{X^2 e^{-\beta U} + 2X + 1} \to \beta(1-|n-1|).
\tag{10.2.10}
\]

These results show the feature of the paramagnetism.

(ii) **Next order**

We perform the perturbation expansion for \( e^{-\beta(\mathfrak{H}_0 + \mathfrak{H}_1)} \) using the formula

\[
e^{-\beta(\mathfrak{H}_0 + \mathfrak{H}_1)} = e^{-\beta \mathfrak{H}_0} \text{Tr} \exp \left( -\int_0^\beta d\tau e^{\mathfrak{H}_0(\mathfrak{H}_1 - e^{-\tau \mathfrak{H}_0})} \right).
\tag{10.2.11}
\]

The partition function up to second order of \( \mathfrak{H}_1 \) is written as

\[
Z = e^{-\beta W} = \text{Tr} e^{-\beta \mathfrak{H}} = \sum_{\mathfrak{H}_0} e^{-\beta \mathfrak{H}_0} \sum_{\{n_{10}\}} \int_0^\beta dt e^{-\beta \mathfrak{H}_0 t} e^{(\mathfrak{H}_1 - \mathfrak{H}_0 - \mathfrak{H}_0 \mathfrak{H}_1 - \mathfrak{H}_1 \mathfrak{H}_0)} \langle n_{10} | \mathfrak{H}_1 | n_{10} \rangle^2,
\tag{10.2.12}
\]

where

\[
\mathfrak{H}_0 | n_{10} \rangle = \mathfrak{H}_0 | n_{10} \rangle | n_{10} \rangle.
\tag{10.2.13}
\]

Configurations of \( \{n_{10}\}, \{n'_{10}\} \) for which \( \langle n'_{10} | \mathfrak{H}_1 | n_{10} \rangle \) does not vanish are given in Table 10.1. Then Eq. (10.2.14) becomes

\[
Z = e^{-\beta N_0 \bar{w}} = e^{-\beta \omega}
\]

<table>
<thead>
<tr>
<th>( n_{10} )</th>
<th>( n_{1-0} )</th>
<th>( n_{0-0} )</th>
<th>( n_{10} )</th>
<th>( n_{10} )</th>
<th>( n_{10} )</th>
<th>( n_{10} )</th>
<th>( n_{10} )</th>
<th>( \mathfrak{H}_{10} )</th>
<th>( \mathfrak{H}_{01} )</th>
<th>( \mathfrak{H}<em>0[n</em>{10}] - \mathfrak{H}<em>0[n'</em>{10}] )</th>
</tr>
</thead>
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<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>( H_{10} - \mu )</td>
<td>( (H_1 - H_0) \sigma )</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>( U - 2\mu )</td>
<td>( (H_1 - H_0) \sigma + U )</td>
<td></td>
</tr>
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<td>0</td>
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<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>( -(H_1 + H_0) - 2\mu )</td>
<td>( (H_1 - H_0) \sigma - U )</td>
<td></td>
</tr>
<tr>
<td>0</td>
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<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>( U - H_0 \sigma - 3\mu )</td>
<td>( (H_1 - H_0) \sigma )</td>
<td></td>
</tr>
</tbody>
</table>
\[= [1 + e^{-\beta(H - \mu)} + e^{-\beta(-H - \mu)} + e^{-\beta(U - 2\mu)}]N_0 \]
\[+ zN_0 \tau [1 + e^{-\beta(H - \mu)} + e^{-\beta(-H - \mu)} + e^{-\beta(U - 2\mu)}]N_0^{-2} \]
\[\times \sum_{\sigma=\pm 1} \int_0^\beta dt \int_0^\tau d\tau' \left[ e^{-\beta(H\sigma - \mu)} + e^{-\beta(U - 2\mu)} + (\tau - \tau') \right. \]
\[+ e^{-\beta(2\mu)} + (\tau - \tau')(\tau') + e^{-\beta(UH\sigma - 3\mu)} \]
\[= [X^2 e^{-\tilde{\beta}} + 2X \cosh \tilde{H} + 1]N_0 \]
\[\times \left[ 1 + zN_0 \tilde{t}^2 \frac{(X + X^3 e^{-\tilde{\beta}}) \cosh \tilde{H} + 2 \tilde{U}^{-1} X^2(1 - e^{-\tilde{\beta}})}{(X^2 e^{-\tilde{\beta}} + 2X \cosh \tilde{H} + 1)^2} \right] \]
\[\approx [X^2 e^{-\tilde{\beta}} + 2X \cosh \tilde{H} + 1]N_0 \]
\[\times \exp \left[ zN_0 \tilde{t}^2 \frac{(X + X^3 e^{-\tilde{\beta}}) \cosh \tilde{H} + 2 \tilde{U}^{-1} X^2(1 - e^{-\tilde{\beta}})}{(X^2 e^{-\tilde{\beta}} + 2X \cosh \tilde{H} + 1)^2} \right], \quad (10.2.16) \]

where we have introduced scaled variables,

\[w = \frac{W}{N_0}, \quad \tilde{w} = \beta w, \quad \tilde{U} = \beta U, \quad \tilde{t} = \beta t, \quad \tilde{H} = \beta H, \quad \tilde{\mu} = \beta \mu, \quad X = e^{\tilde{\beta}}. \quad (10.2.17)\]

The fact that the order of free energy density \(w\) must be unity as \(N_0 \to \infty\), i.e., \(W\) is of the order \(N_0\), justifies the approximation made in (10.2.16). Then the free energy density \(w\) is written by

\[\tilde{w} = \beta w = -\log[X^2 e^{-\tilde{\beta}} + 2X \cosh \tilde{H} + 1] \]
\[- z \tilde{t}^2 \frac{(X + X^3 e^{-\tilde{\beta}}) \cosh \tilde{H} + 2 \tilde{U}^{-1} X^2(1 - e^{-\tilde{\beta}})}{(X^2 e^{-\tilde{\beta}} + 2X \cosh \tilde{H} + 1)^2} \]
\[= \tilde{w}_0(\tilde{H}) + z \tilde{t}^2 \tilde{w}_1(\tilde{H}). \quad (10.2.18)\]

Thus the number density of electrons for \(H = 0\) becomes

\[n = \frac{N}{N_0} = -\frac{\partial \tilde{w}}{\partial \tilde{\mu}} \]
\[= \frac{2X^2 e^{-\tilde{\beta}} + 2X}{X^2 e^{-\tilde{\beta}} + 2X + 1} \]
\[+ z \tilde{t}^2 \frac{(-X^3 e^{-2\tilde{\beta}} - 2X^2 + 2X^4 e^{-\tilde{\beta}} + X) + \tilde{U}^{-1}(1 - e^{-\tilde{\beta}})(-4X^4 e^{-\tilde{\beta}} + 4X^2)}{(X^2 e^{-\tilde{\beta}} + 2X + 1)^3}. \quad (10.2.19)\]

Thus for \(n < 1\) we have the following expression for the deviation from the half-filling \(\nu\),

\[\nu = |n - 1| = -\frac{1 - X^2 e^{-\tilde{\beta}}}{X^2 e^{-\tilde{\beta}} + 2X + 1} \]
\[+ z \tilde{t}^2 \frac{(X^3 e^{-2\tilde{\beta}} + 2X^2 - 2X^4 e^{-\tilde{\beta}} - X) + \tilde{U}^{-1}(1 - e^{-\tilde{\beta}})(4X^4 e^{-\tilde{\beta}} - 4X^2)}{(X^2 e^{-\tilde{\beta}} + 2X + 1)^3}. \quad (10.2.20)\]
For \( n > 1 \), the above expression holds if one replaces \( X \) by \( X' \) defined by

\[
X' = \frac{e^\tilde{\phi}}{X}.
\]  

(10.2.21)

Since \( |n - 1| \) has the same form for \( X \) and \( X' \), we can invert the relation and write them, using single function \( \xi(\nu, T) \), as

\[
X = \xi(\nu, T), \quad (n < 1) \quad X' = \xi(\nu, T), \quad (n > 1)
\]  

(10.2.22)

As is well-known, the symmetry property for \( n < 1 \) and \( n > 1 \) is a consequence of particle hole symmetry of the Hubbard Hamiltonian.

At this point we take the limit \( U \to \infty \). We expect that in this limit the order (in \( 1/U \)) of \( X \) in second order of \( t \) is equal to that in zeroth order. Thus the order of \( \xi \) is given from (10.2.8) and (10.2.22) as

\[
\xi(\nu, T) \sim 1. \quad (\nu > 0)
\]  

(10.2.23)

Now, considering up to the order \( 1/U \) and neglecting \( \exp(-\tilde{U}) \) in (10.2.20), we get the equation for \( \xi \) as

\[
\nu = \frac{1}{2\xi(\nu, T) + 1} + z \tilde{t} \frac{2\xi(\nu, T)^2 - \xi(\nu, T) - 4\tilde{U}^{-1}\xi(\nu, T)}{(2\xi(\nu, T) + 1)^3}.
\]  

(10.2.24)

Let us rewrite \( \tilde{w} \) using \( \xi \) as

\[
\tilde{w} = -\log[X^2e^{-\tilde{\phi}} + 2X\cosh\tilde{H} + 1] - z \tilde{t} \frac{[X + X^2e^{-\tilde{\phi}}] \cosh\tilde{H} + 2\tilde{U}^{-1}X^2(1 - e^{-\tilde{\phi}})}{(X^2e^{-\tilde{\phi}} + 2X\cosh\tilde{H} + 1)^2}
\]

\[
= -\log[X^2e^{-\tilde{\phi}} + 2X\cosh\tilde{H} + 1] + \log[X^2e^{-\tilde{\phi}}]
\]

\[
-z \tilde{t} \frac{[X' + X^2e^{-\tilde{\phi}}] \cosh\tilde{H} + 2\tilde{U}^{-1}X^2(1 - e^{-\tilde{\phi}})}{(X^2e^{-\tilde{\phi}} + 2X\cosh\tilde{H} + 1)^2}
\]

\[
= -\log[\xi^2e^{-\tilde{\phi}} + 2\xi\cosh\tilde{H} + 1] + \theta(n - 1)\log[\xi^2e^{-\tilde{\phi}}]
\]

\[
-z \tilde{t} \frac{[\xi + \xi^2e^{-\tilde{\phi}}] \cosh\tilde{H} + 2\tilde{U}^{-1}\xi^2(1 - e^{-\tilde{\phi}})}{(\xi^2e^{-\tilde{\phi}} + 2\xi\cosh\tilde{H} + 1)^2}
\]  

(10.2.25)

\[
\approx -\log[2\xi\cosh\tilde{H} + 1] + \theta(n - 1)\log[\xi^2e^{-\tilde{\phi}}] - z \tilde{t} \frac{\xi\cosh\tilde{H} + 2\tilde{U}^{-1}\xi^2}{(2\xi\cosh\tilde{H} + 1)^2}.
\]  

(10.2.26)

The magnetization is then written by

\[
m = \frac{M}{N_0} = -\frac{\partial \tilde{w}}{\partial \tilde{H}} = \frac{2\xi\sinh\tilde{H}}{2\xi\cosh\tilde{H} + 1} + z \tilde{t} \frac{[1 - 2\xi\cosh\tilde{H} - 8\tilde{U}^{-1}\xi^2] \xi\sinh\tilde{H}}{(2\xi\cosh\tilde{H} + 1)^3}.
\]  

(10.2.27)

If we set \( \tilde{H} = 0 \) in (10.2.27), the magnetization vanishes. Actually it vanishes for all orders of perturbation. In order to get the non-vanishing magnetization we rely on the inversion method.
(iii) Inversion—magnetization and susceptibility—

In the inversion formulae presented in § 7.2, we take \( J, \phi \) as \( J = - \tilde{H}, \phi = m \) and use the result of the inversion formulas up to first order: \( h_0 \) and \( h_1 \) of (7.2.3). The expansion parameter in this case is \( z i \tilde{\tau}^2 \) which plays the role of \( g \) in these formulas.

The Gibbs free energy density \( \gamma \) is given, up to the order \( z i \tilde{\tau}^2 \), by the sum of (7.2.14) and (7.2.15),

\[
\gamma = \beta \gamma = \tilde{\omega} + \tilde{H}m \\
\approx \tilde{\omega}^{(0)}(\tilde{H}_0(m)) + z \tilde{\tau}^2 \tilde{\omega}^{(1)}(\tilde{H}_0(m)) + \tilde{H}_0(m)m \\
\approx \tilde{\omega}(\tilde{H}_0(m)) + \tilde{H}_0(m)m, \tag{10.2.28}
\]

where \( \tilde{H}_0(m) \) is the function which is defined by the lowest relation of the inversion

\[
m = - \tilde{\omega}_0^{(1)}(\tilde{H}_0(m)) = \frac{-2\xi \sinh \tilde{H}_0(m)}{2\xi \cosh \tilde{H}_0(m) + 1}. \tag{10.2.29}
\]

Here the superscript (1) implies that we have differentiated once with respect to the argument. Therefore we can write \( \tilde{H}_0(m) \) as

\[
\tilde{H}_0(m) = \log \left[ \frac{-m + \sqrt{m^2 - 4\xi^2 (m^2 - 1)}}{2\xi (m - 1)} \right]. \tag{10.2.30}
\]

It is convenient to regard \( \tilde{H}_0(m) \) as the order parameter instead of \( m \),

\[
m \to \tilde{H}_0(m) = \varphi, \tag{10.2.31}
\]

because \( \varphi = 0 \) when \( m = 0 \). Then \( \tilde{\gamma} \) is written as a function of \( \phi \):

\[
\tilde{\gamma} = \tilde{\omega}(\varphi) - \tilde{\omega}_0^{(1)}(\varphi) \varphi, \tag{10.2.32}
\]

where

\[
\tilde{\omega}(\varphi) = \tilde{\omega}_0(\varphi) + z \tilde{\tau}^2 \tilde{\omega}_1(\varphi). \tag{10.2.33}
\]

From (10.2.32), the non-vanishing order parameter for \( H = 0 \) is obtained by solving the equation

\[
0 = H = \frac{\partial \tilde{\gamma}}{\partial m} = \frac{\partial \varphi}{\partial m} \frac{\partial \tilde{\gamma}}{\partial \varphi}. \tag{10.2.34}
\]

Since \( \partial \varphi / \partial m \neq 0 \), we have only to solve

\[
0 = \frac{\partial \tilde{\gamma}}{\partial \varphi} = - \tilde{\omega}_0^{(2)}(\varphi) \varphi + z \tilde{\tau}^2 \tilde{\omega}_1^{(1)}(\varphi)

= \frac{2\xi(\nu, T)(2\xi(\nu, T) + \cosh \varphi)}{(2\xi(\nu, T) \cosh \varphi + 1)^2} \varphi

- z \tilde{\tau}^2 \left[ 1 - 2\xi(\nu, T) \cosh \varphi - 8 U^{-1} \xi(\nu, T)^2 \xi(\nu, T) \sinh \varphi \right]. \tag{10.2.35}
\]

This is the inverted series (10.2.2). From (10.2.35), we write the solution of the order parameter as
\[ \varphi = \varphi(\nu, T). \] (10.2.36)

Then, using this solution, the magnetization is written by
\[ m(\nu, T) = -\tilde{w}_0(1)(\varphi(\nu, T)) = \frac{2\tilde{\xi}(\nu, T) \sinh \varphi(\nu, T)}{2\tilde{\xi}(\nu, T) \cosh \varphi(\nu, T) + 1}. \] (10.2.37)

In the same way, the susceptibility \( \chi \) for \( H=0 \) is calculated from Eq. (10.2.32) as
\[ \chi^{-1} = \frac{\partial H}{\partial m} \bigg|_{H=0} = \frac{1}{\beta} \left( \frac{\partial^2 \tilde{\eta}}{\partial \varphi^2} \right) \bigg|_{\tilde{H}(m)=\varphi} = \frac{1}{\beta} \left( \frac{\partial \varphi}{\partial \varphi} \right) \left[ \frac{\partial \varphi}{\partial m} \frac{\partial \varphi}{\partial \varphi} \right] \] (10.2.38)
\[ = \frac{1}{\beta} \left[ -\frac{1}{\tilde{w}_0(2)(\varphi)} \right] \frac{\partial \varphi}{\partial \varphi} \left[ -\frac{1}{\tilde{w}_0(3)(\varphi)} \frac{\partial \varphi}{\partial \varphi} \right] \] (10.2.39)
\[ = \left[ 1 + z \tilde{t}^2(4\tilde{\xi}^2 + 4\tilde{\xi} \cosh \varphi + 1)(-2\tilde{\xi} \cosh \varphi + 1 - 8\tilde{U}^{-1} \tilde{\xi}^2) \sinh^2 \varphi \right. \] (10.2.40)
\[ \left. \frac{2(2\tilde{\xi} + \cosh \varphi)(2\tilde{\xi} \cosh \varphi + 1)^2}{2(2\tilde{\xi} + \cosh \varphi)(2\tilde{\xi} \cosh \varphi + 1)^2} \right] \frac{1}{\beta} \frac{(2\tilde{\xi} \cosh \varphi + 1)^2}{2(2\tilde{\xi} + \cosh \varphi)(2\tilde{\xi} \cosh \varphi + 1).} \]

Let us consider the case above the transition temperature where the magnetization vanishes. The susceptibility is then given by
\[ \chi^{-1} = \frac{1}{\beta} \left( \frac{\partial^2 \tilde{\eta}}{\partial \varphi^2} \right) \bigg|_{m=0} = \frac{1}{\beta} \left[ -\frac{1}{\tilde{w}_0(2)(0)} \right]^{\frac{\partial^2 \tilde{\eta}}{\partial \varphi^2}} \bigg|_{\varphi=0} = \frac{1}{\beta} \left[ -\frac{1}{\tilde{w}_0(3)(0)} \right] \left[ 1 - z \tilde{t}^2 \tilde{w}_0(2)(0) \tilde{w}_0(3)(0) \right] \] (10.2.41)
\[ = \frac{1}{\beta} \left[ 1 + \frac{2\tilde{\xi}(\nu, T)}{2 \tilde{\xi}(\nu, T)} \right] \left[ 1 - z \tilde{t}^2 \frac{1 - 2\tilde{\xi}(\nu, T) - 8\tilde{U}^{-1} \tilde{\xi}(\nu, T)^2}{2(1 + 2\tilde{\xi}(\nu, T)^2)} \right]. \]

From Eq. (10.2.41), the equation \( \chi^{-1} = 0 \) which determines the transition temperature \( T_c \) turns out to be
\[ 1 = z \tilde{t}_c \frac{2(1 - 2\tilde{\xi}(\nu, T_c) - 8\tilde{U}_c \tilde{\xi}(\nu, T_c)^2)}{2(1 + 2\tilde{\xi}(\nu, T_c)^2)}, \] (10.2.42)
where
\[ \beta_c = \frac{1}{k_b T_c}, \quad \tilde{t}_c = \beta_c t, \quad \tilde{U}_c = \beta_c U. \] (10.2.43)

Rewriting (10.2.41) with the solution \( T_c \) of (10.2.42), it becomes the form
\[ \chi^{-1} = \frac{1}{\beta} \left[ 1 + \frac{2\tilde{\xi}(\nu, T_c)}{2 \tilde{\xi}(\nu, T_c)} \right] \left[ z \tilde{t}^2 \frac{1 - 2\tilde{\xi}(\nu, T) - 8\tilde{U}^{-1} \tilde{\xi}(\nu, T)^2}{2(1 + 2\tilde{\xi}(\nu, T)^2)} \right] \] (10.2.44)
\[ \approx \frac{1}{\beta} \left[ 1 + \frac{2\tilde{\xi}(\nu, T_c)}{2 \tilde{\xi}(\nu, T_c)} \right] \frac{\partial}{\partial T} \left[ z \tilde{t}^2 \frac{1 - 2\tilde{\xi}(\nu, T) - 8\tilde{U}^{-1} \tilde{\xi}(\nu, T)^2}{2(1 + 2\tilde{\xi}(\nu, T)^2)} \right] \bigg|_{T=T_c} (T - T_c). \] (10.2.45)

Although Eq. (10.2.45) shows the Curie-Weiss law for the susceptibility near \( T_c \), for \( T \) away from \( T_c \), the numerical work is required, see § 10.2.3 and Fig. 10.4.

Now, we have obtained equations for getting the non-vanishing magnetization, the susceptibility and the transition temperature. But there is some parameter region
where these quantities show unphysical values indicating that our equation cannot be used in such a region. First, since we expand the partition function considering $\tilde{t} = \beta t$ as the perturbation parameter, our theory is not expected to be reliable for large $\beta$. Next, the susceptibility becomes unphysical for small $\nu$. In order to look at this fact simply, consider the case where $U \to \infty$. Then, from (10.2.24) and (10.2.42), we can calculate the transition temperature exactly as

$$ g_e = \frac{4}{\nu(\nu+1)}, \quad (10.2.46) $$

where $g = z \tilde{t}^2$, $g_e = z \tilde{t}_e^2$. From (10.2.46), if we expand $\chi^{-1}$ above $T_c$ to first order considering $\Delta g = g - g_e < 0$ as the expansion parameter, it is written by

$$ \chi^{-1} = \Delta g \frac{1}{\beta_c} \frac{2}{1 - \nu} \frac{\nu^2(\nu+1)^2}{2(-4\nu^2 - \nu + 1)}. \quad (10.2.47) $$

Thus, we see that if $-4\nu^2 - \nu + 1 > 0$, or $\nu < (\sqrt{17} - 1)/8 \equiv \nu_c$ ($= 0.39038\cdots$), the Curie-Weiss coefficient becomes negative. From this result, our susceptibility is not reliable for small $\nu$. This is in accord with (10.2.46) which states that for small $\nu$, $g_e$ becomes large and for large $g$ our expansion scheme cannot be used. In the following we assume $\nu > \nu_c$. Numerical estimates of various quantities are given in §10.2.3 below.

10.2.2. Antiferromagnetic state

In order to study the antiferromagnetic state together with the ferromagnetic state, we put the magnetic field into the Hamiltonian as

$$ \mathcal{H} = -t \sum_{\sigma \leq \sigma'} a^\dagger_{\sigma \sigma} a_{\sigma'} + \sum_{i} \left[ H_i (n_{i_1} - n_{i_1'} - \mu (n_{i_1} + n_{i_1'})) \right], \quad (10.2.48) $$

where

$$ H_i = \begin{cases} H_A, & (i \in A) \\ H_B, & (i \in B) \end{cases} \quad (10.2.49) $$

Here, A and B imply two sublattices such that all the nearest neighbors of each point on one sublattice belong to another sublattice as in Fig. 10.1. We are assuming that the system is the $d$-dimensional analog of the square lattice ($z = 2d$).

(i) **Gibbs free energy**

Let us consider the perturbation to second order of $\mathcal{H}$, as before. The partition function is then written by

$$ Z = e^{-\beta \mathcal{W}} = e^{-\beta N_0 \mathcal{W}} = e^{-\beta \mathcal{W}} = \text{Tr} e^{-\beta \mathcal{H}} \quad (10.2.50) $$

Fig. 10.1. Sublattices A and B.
\[
\prod_{a=A,B} \left[ 1 + e^{-\beta (H_a - \mu)} + e^{-\beta (H_a - \mu^{-} + e^{-\beta (U - 2\mu)})} \right]^{N_0/2} \\
+ z \frac{N_0}{2} e^{\beta \mu} \prod_{a=A,B} \left[ 1 + e^{-\beta (H_a - \mu)} + e^{-\beta (H_a - \mu^{-} + e^{-\beta (U - 2\mu)})} \right]^{N_0/2-1} \\
\times \sum_{a=A,B} \sum_{\sigma=\mp 1} \int_0^\beta \int_0^{\beta'} d\tau' \int d\tau \left[ e^{-\beta ((H_a \sigma - \mu) + (\tau - \tau')((H_a \sigma - \mu) + (\tau - \tau'))((H_a \sigma - \mu) + (\tau - \tau'))} + e^{-\beta (U - 2\mu) + (\tau - \tau')((H_a \sigma - \mu) + (\tau - \tau'))} \right].
\]
\[ (10 \cdot 2.51) \]

Here \( H_a \) is the magnetic field at the lattice site \( a \), which has the non-zero matrix element of \( \mathcal{H}_1 \) with the site \( a \). See (10 \cdot 2.14). The \( Z \) can be calculated as

\[
Z = [(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\Delta H + cosh2\bar{H})]^{N_0/2}
\]

\[
\times \left[ 1 + zN_0 \bar{\eta}^2 \right]
\]

\[
\frac{X(X^2 e^{-\bar{\eta}} + 1)cosh\bar{H} sinh\Delta H}{\Delta H} \frac{\bar{U}^{-1}(e^{-\bar{\eta}} - e^{-2\Delta H})X^2}{1 - 2U^{-1}\Delta H} \frac{\bar{U}^{-1}(e^{-\bar{\eta}} - e^{2\Delta H})X^2}{1 + 2U^{-1}\Delta H}
\]

\[
\times \frac{(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)}{(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)}
\]

\[ (10 \cdot 2.52) \]

\[
\approx [(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)]^{N_0/2}
\]

\[
\times \exp \left[ zN_0 \bar{\eta}^2 \right]
\]

\[
\frac{X(X^2 e^{-\bar{\eta}} + 1)cosh\bar{H} sinh\Delta H}{\Delta H} \frac{\bar{U}^{-1}(e^{-\bar{\eta}} - e^{-2\Delta H})X^2}{1 - 2U^{-1}\Delta H} \frac{\bar{U}^{-1}(e^{-\bar{\eta}} - e^{2\Delta H})X^2}{1 + 2U^{-1}\Delta H}
\]

\[
\times \frac{(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)}{(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)}
\]

\[ (10 \cdot 2.53) \]

where we have defined

\[
H = \frac{H_A + H_B}{2}, \quad \Delta H = \frac{H_A - H_B}{2}, \quad \bar{H} = \beta H, \quad \Delta \bar{H} = \beta \Delta H.
\]

\[ (10 \cdot 2.54) \]

Thus the free energy density \( w \) is obtained as

\[
\bar{w} = \beta w = -\frac{1}{2} \log[(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)]
\]

\[
\times \frac{X(X^2 e^{-\bar{\eta}} + 1)cosh\bar{H} sinh\Delta H}{\Delta H} \frac{\bar{U}^{-1}(e^{-\bar{\eta}} - e^{-2\Delta H})X^2}{1 - 2U^{-1}\Delta H} \frac{\bar{U}^{-1}(e^{-\bar{\eta}} - e^{2\Delta H})X^2}{1 + 2U^{-1}\Delta H}
\]

\[
\times \frac{(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)}{(e^{-\bar{\eta}} X^2 + 1)^2 + 4X(e^{-\bar{\eta}} X^2 + 1)cosh\Delta H cosh\bar{H} + 2X^2(cosh2\bar{H} + cosh2\Delta H)}
\]
\[ = \frac{1}{2} \log[(e^{-\tilde{\gamma}} X^2 + 1)^2 + 4X^2(e^{-\tilde{\gamma}} X^2 + 1) \cosh \Delta \tilde{H} \cosh \tilde{H} + 2X^2(\cosh 2\tilde{H} + \cosh 2\Delta \tilde{H})] \]

\[ \frac{X'(X^2 e^{-\tilde{\gamma}} + 1) \cosh \tilde{H} \sinh \Delta \tilde{H}}{\Delta \tilde{H}} - \frac{\tilde{\tilde{U}}^{-1}(e^{-\tilde{\gamma}} - e^{-2\Delta \tilde{H}})X^2}{1 - 2\tilde{\tilde{U}}^{-1} \Delta \tilde{H}} \]

\[ = \frac{-z \tilde{\xi}^2}{(e^{-\tilde{\gamma}} X^2 + 1)^2 + 4X'(e^{-\tilde{\gamma}} X^2 + 1) \cosh \Delta \tilde{H} \cosh \tilde{H} + 2X^2(\cosh 2\tilde{H} + \cosh 2\Delta \tilde{H})} \]

\[ + \log[e^{-\tilde{\gamma}} X^2] \]

\[ = \frac{1}{2} \log[(e^{-\tilde{\gamma}} \xi^2 + 1)^2 + 4\xi(e^{-\tilde{\gamma}} \xi^2 + 1) \cosh \Delta \tilde{H} \cosh \tilde{H} + 2\xi^2(\cosh 2\tilde{H} + \cosh 2\Delta \tilde{H})] \]

\[ + \theta(n-1) \log[e^{-\tilde{\gamma}} \xi^2] \]

\[ \frac{\xi (\xi^2 e^{-\tilde{\gamma}} + 1) \cosh \tilde{H} \sinh \Delta \tilde{H}}{\Delta \tilde{H}} - \frac{-\tilde{\tilde{U}}^{-1}(e^{-\tilde{\gamma}} - e^{-2\Delta \tilde{H}})\xi^2}{1 - 2\tilde{\tilde{U}}^{-1} \Delta \tilde{H}} - \frac{-\tilde{\tilde{U}}^{-1}(e^{-\tilde{\gamma}} - e^{-2\Delta \tilde{H}})\xi^2}{1 + 2\tilde{\tilde{U}}^{-1} \Delta \tilde{H}} \]

\[ = \tilde{\tilde{w}}(\tilde{H}, \Delta H) + z \tilde{\xi}^2 \tilde{w}(H, \Delta H). \]  

We now set \( J_1, \phi_1 \) as

\[ J_1 = -\tilde{H} , \quad J_2 = -\Delta \tilde{H} , \quad \phi_1 = m , \quad \phi_2 = \Delta m \]

in the inversion formulas of many variables (Appendix I). The ferro or antiferro order parameter \( m \) or \( \Delta m \) is related by the following equations,

\[ \frac{m}{N_0} = \frac{M_A + M_B}{N_0} = -\frac{\partial \tilde{w}}{\partial \tilde{H}} , \quad \Delta m = \frac{M_A - M_B}{N_0} = -\frac{\partial \tilde{w}}{\partial \Delta \tilde{H}} . \]

Let us use the inversion formula. We find by using (I·13) and (I·14) that the Gibbs free energy density \( \gamma \) is given by

\[ \tilde{\gamma} = \beta \gamma = \tilde{w} + \tilde{H} m + \tilde{H} \Delta m \]

\[ \approx \tilde{w}(\tilde{H}_0(m, \Delta m), \Delta \tilde{H}_0(m, \Delta m)) + \tilde{H}_0(m, \Delta m)m + \Delta \tilde{H}_0(m, \Delta m)\Delta m , \]

where \( \tilde{H}_0(m, \Delta m), \Delta \tilde{H}_0(m, \Delta m) \) are functions which satisfy the simultaneous equations

\[ \frac{2\xi \cosh \tilde{H}_0 \cosh \Delta \tilde{H}_0 + 2\xi^2 \sinh 2\tilde{H}_0}{4\xi \cosh \tilde{H}_0 \cosh \Delta \tilde{H}_0 + 2(\cosh 2\tilde{H}_0 + \cosh 2\Delta \tilde{H}_0) \xi^2 + 1} , \]

\[ \frac{2\xi \cosh \tilde{H}_0 \sinh \Delta \tilde{H}_0 + 2\xi^2 \sinh 2\Delta \tilde{H}_0}{4\xi \cosh \tilde{H}_0 \cosh \Delta \tilde{H}_0 + 2(\cosh 2\tilde{H}_0 + \cosh 2\Delta \tilde{H}_0) \xi^2 + 1} . \]
The symbol \( \tilde{\omega}_0^{(1)}(\cdot) \) implies the differentiation once with respect to \( \tilde{H}_0 \), etc. Here, we change the order parameters as

\[
(m, \Delta m) \longrightarrow \left( \tilde{H}_0(m, \Delta m), \Delta \tilde{H}_0(m, \Delta m) \right) = (\varphi, \Delta \varphi), \tag{10.2.62}
\]

since \( \varphi = 0 \) when \( m = 0 \) and \( \Delta \varphi = 0 \) when \( \Delta m = 0 \). Then we can rewrite \( \tilde{\gamma} \) using \( \varphi, \Delta \varphi \) as

\[
\tilde{\gamma} = \tilde{\omega}(\varphi, \Delta \varphi) - \tilde{\omega}_0^{(1)}(\varphi, \Delta \varphi) \varphi \varphi - \tilde{\omega}_0^{(1)}(\varphi, \Delta \varphi)_{\varphi \Delta \varphi}, \tag{10.2.63}
\]

where we have defined

\[
\tilde{\omega}(\varphi, \Delta \varphi) = \tilde{\omega}_0(\varphi, \Delta \varphi) + \tilde{\omega}_1(\varphi, \Delta \varphi). \tag{10.2.64}
\]

Note here that if \( \Delta \varphi = 0 \), Eq. (10.2.63) agrees with (10.2.32).

(ii) Staggered magnetization

From (10.2.63), the non-vanishing order parameters for \( H_A = H_B = 0 \) are obtained by solving the simultaneous equations

\[
\begin{pmatrix}
0 \\
0 \\
\end{pmatrix} = \begin{pmatrix}
\frac{\partial \tilde{\gamma}}{\partial m} \\
\frac{\partial \tilde{\gamma}}{\partial \Delta m} \\
\end{pmatrix} = \begin{pmatrix}
\frac{\partial \varphi}{\partial m} & \frac{\partial \Delta \varphi}{\partial m} \\
\frac{\partial \varphi}{\partial \Delta m} & \frac{\partial \Delta \varphi}{\partial \Delta m} \\
\end{pmatrix} \begin{pmatrix}
\frac{\partial \tilde{\gamma}}{\partial \varphi} \\
\frac{\partial \tilde{\gamma}}{\partial \Delta \varphi} \\
\end{pmatrix}. \tag{10.2.65}
\]

Since

\[
\det \begin{pmatrix}
\frac{\partial \varphi}{\partial m} & \frac{\partial \Delta \varphi}{\partial m} \\
\frac{\partial \varphi}{\partial \Delta m} & \frac{\partial \Delta \varphi}{\partial \Delta m} \\
\end{pmatrix} \neq 0, \tag{10.2.66}
\]

we have only to solve

\[
\begin{pmatrix}
0 \\
0 \\
\end{pmatrix} = \begin{pmatrix}
\frac{\partial \tilde{\gamma}}{\partial \varphi} \\
\frac{\partial \tilde{\gamma}}{\partial \Delta \varphi} \\
\end{pmatrix} = \begin{pmatrix}
-\tilde{\omega}_0^{(2)}(\varphi, \Delta \varphi) \varphi \varphi - \tilde{\omega}_0^{(2)}(\varphi, \Delta \varphi)_{\varphi \Delta \varphi} \Delta \varphi + z \tilde{i}^2 \tilde{\omega}_1^{(1)}(\varphi, \Delta \varphi) \\
-\tilde{\omega}_0^{(2)}(\varphi, \Delta \varphi)_{\varphi \Delta \varphi} \varphi - \tilde{\omega}_0^{(2)}(\varphi, \Delta \varphi)_{\varphi \Delta \varphi} \Delta \varphi + z \tilde{i}^2 \tilde{\omega}_1^{(1)}(\varphi, \Delta \varphi) \end{pmatrix}. \tag{10.2.67}
\]

Because Eq. (10.2.67) is a function of \( \nu, T \), the solutions of the order parameters can be written as

\[
\varphi = \varphi(\nu, T), \quad \Delta \varphi = \Delta \varphi(\nu, T). \tag{10.2.68}
\]

Here we define the transition temperature of the antiferromagnetic state by setting \( m \) to be zero. For this purpose the staggered magnetic susceptibility \( \chi_{st} \) is calculated as
\[ \chi_{\text{hi}}^{-1} = \frac{\Delta H}{\Delta m} \bigg|_{\Delta H = 0} = \frac{1}{\beta} \left. \frac{\partial^2 \tilde{\gamma}}{\partial \Delta m^2} \right|_{m = \Delta m = 0} \]

\[ = \frac{1}{\beta} \left[ -\frac{1}{\tilde{\omega}_0^{(2)}(0, 0)_{\delta \delta \varphi \varphi}} \right] \left[ \frac{\partial^2 \tilde{\varphi}}{\partial \Delta m^2} \right]_{\delta \varphi = 0} \]

\[ = \frac{1}{\beta} \left[ -\frac{1}{\tilde{\omega}_0^{(2)}(0, 0)_{\delta \delta \varphi \varphi}} \right] \left[ 1 - z \int_2 \frac{\tilde{\omega}_1^{(2)}(0, 0)_{\delta \varphi \varphi}}{\tilde{\omega}_0^{(2)}(0, 0)_{\delta \delta \varphi \varphi}} \right] \left[ 1 - \frac{1 + 2 \xi_2(\nu, T)}{2 \xi_2(\nu, T)} \left[ 1 - z \int_2 \frac{1 - 10 \xi_1(\nu, T) + 24 \widetilde{U}_c^{-1}(\xi(\nu, T) + \xi_2(\nu, T))}{6(1 + 2 \xi_2(\nu, T))^2} \right] \right] \].

From (10.2.71), the equation \( \chi_{\text{hi}}^{-1} = 0 \) which gives the transition temperature of the antiferromagnetic state \( T_c \) turns out to be

\[ 1 = z \int_2 \frac{1 - 10 \xi_1(\nu, T_c) + 24 \widetilde{U}_c^{-1}(\xi(\nu, T_c) + \xi_2(\nu, T_c))}{6(1 + 2 \xi_2(\nu, T_c))^2}. \]

As we will see below, the difference in the sign factor in front of \( 8 \widetilde{U}_c^{-1} \xi^2 \) in (10.2.42) and \( 24 \widetilde{U}_c^{-1}(\xi + \xi^2) \) in (10.2.72) is the cause of crossover between the ferro and antiferromagnetic states.

(iii) **Relation between free energy and susceptibility**

We have obtained the free energy in (10.2.59). If we expand it around \( m = \Delta m = 0 \), it is written by

\[ \gamma(m, \Delta m) = \gamma_0 + \frac{1}{2} (m \Delta m) \begin{pmatrix} \frac{\partial^2 \gamma}{\partial m \Delta m} & \frac{\partial^2 \gamma}{\partial m \Delta m} \\ \frac{\partial^2 \gamma}{\partial m \Delta m} & \frac{\partial^2 \gamma}{\partial m \Delta m} \end{pmatrix} \begin{pmatrix} m \\ \Delta m \end{pmatrix} \]

\[ = \gamma_0 + \frac{1}{2} (m \Delta m) \begin{pmatrix} \chi^{-1} & 0 \\ 0 & \chi_{\text{hi}}^{-1} \end{pmatrix} \begin{pmatrix} m \\ \Delta m \end{pmatrix} \]

\[ = \gamma_0 + \frac{1}{2} \chi^{-1} m^2 + \frac{1}{2} \chi_{\text{hi}}^{-1} \Delta m^2, \]

where \((\cdots)_0\) implies the value for \( m = \Delta m = 0 \). Note here that the above matrix is diagonal. In other words, the linear transformation for the magnetizations \( M_A \) and \( M_B \) as in (10.2.58) diagonalizes this matrix.

**10.2.3. Numerical calculation**

Now we come to the numerical work. Taking only the lowest term of \( 1/U \) expansion, it is crude to guess the phase diagram but still may be a starting basis of the strong coupling theory just like the Stoner approximation in weak coupling case.

Since we are interested in the general trends of our results, the numerical values of various quantities are chosen rather arbitrary. In particular the Boltzmann constant is set to unity.
(i) Ferromagnetic state

First, from \((10.2.35)\), \(\varphi\) is calculated by solving the equation

\[
\varphi = \frac{2}{d} \left[ 1 - 2\xi(\nu, T) \cosh \varphi - 8 \bar{U}^{-1} \xi(\nu, T)^2 \sinh \varphi \right] \frac{2(2\xi(\nu, T) + \cosh \varphi)(2\xi(\nu, T) \cosh \varphi + 1)}{2(2\xi(\nu, T) + \cosh \varphi)(2\xi(\nu, T) \cosh \varphi + 1)}
\]

\[(10.2.76)\]

\[
\equiv g(\varphi).
\]

\[(10.2.77)\]

Here, the function \(g(\varphi)\) for some temperatures (and for some typical values of other parameters) is shown in Fig. 10.2 for \(d = 3\). From Fig. 10.2, we see that \(\varphi\) gets the non-vanishing value if \(g'(0) > 1\), or if the temperature of the system is below the critical temperature. From this result and from \((10.2.24)\), \((10.2.37)\) and \((10.2.40)\), we show the magnetization \(m\) vs the temperature \(T\) and the inverse susceptibility \(\chi^{-1}\) vs the temperature above \(T_c\) in Fig. 10.3 and Fig. 10.4 respectively. We notice that the inverse susceptibility is convex above the transition temperature. This point is in constrast to the result of the mean field approximation in weak coupling, which is concave (in Stoner theory like \((T - T_c)^2\)). Thus we expect that the linear Curie-Weiss law is realized somewhere in between the strong coupling mean field (our theory) and weak coupling mean field theory, i.e., intermediate region.

(iii) Inclusion of antiferromagnetic state

Next, from \((10.2.24)\), \((10.2.42)\) and \((10.2.72)\), the transition temperature \(T_c\) vs the difference of number density from half filling \(\nu\) and the transition temperature vs \(U\) are shown in Fig. 10.5 and Fig. 10.6 respectively. The reason why we take rather small value for \(U\) in Fig. 10.5 is
that the crossover between ferro and antiferro is realized for small $U$ if we choose $\nu$ to be larger than the lowest allowed value $\nu_c$. In the figures the transition temperature of the ferromagnetic state $T_c(F)$ is defined by setting $\Delta m=0$ (ferro-para boundary) and that of antiferromagnetic state $T_c(AF)$ by $m=0$ (antiferro-para boundary). These two curves cross each other at a certain point.

From (10.2.63), the free energy is calculated and its shapes in the regions A, B, C, D and E (which are shown in Figs. 10.5 and 10.6) are presented in Fig. 10.7. These regions satisfy the following conditions:

A: $T > T_c(F) > T_c(AF)$,
B: $T_c(F) > T > T_c(AF)$,
C: $T_c(F) > T > T_c(AF)$,
D: $T_c(AF) > T > T_c(F)$,
E: $T_c(AF) > T_c(F) > T$.

If we look at Fig. 10.7, we notice that the shapes of the free energy in these regions have the following features.

A: It has a minimum at the origin.
B: It has a minimum at a certain non-vanishing point on the $\varphi$-axis.
C: It has a minimum at a certain non-vanishing point on the $\varphi$-axis, and a saddle point at some non-zero value on the $\Delta \varphi$-axis.

D: It is unstable in the direction of the $\Delta \varphi$-axis.

E: It is unstable in the direction of the $\Delta \varphi$-axis, and has a local minimum at some point on the $\varphi$-axis.

On the basis of the above results, we have also shown in Figs. 10.6 and 10.7 the phase assignments of the regions A~E.

(iii) Extrapolation to zero temperature

Let us make some conjecture about the phase diagram of zero temperature from all the above results. The conjecture is based on the smoothness assumption concerning the extrapolation in the temperature down to zero. The result is shown in Fig. 10.8 and agrees qualitatively with the result that we can suppose from Nagaoka’s theorem.$^{10,14}$

First, we compare our conjectured phase diagram (Fig. 10.8) at zero temperature with the one (Fig. 10.9) obtained by the supposition from Nagaoka’s theorem$^{10,14}$ and the result of mean-field approximation$^{15}$ in weak coupling. Our result (Fig. 10.8) shows that the state at zero temperature prefers the ferromagnetic state rather than the antiferromagnetic state all the more if $U/T$ and $\nu$ get larger. This behavior agrees with what is expected from Nagaoka’s theorem. It also agrees with the weak coupling mean field result qualitatively in the sense that the boundary between ferro and antiferro has a negative slope in $(U/t)-\nu$ plane. But, as we mentioned before, our result is not valid for small $\nu$ or small $U/t$. This is the reason why our results do not reproduce the correct result even for large $U$ that the state is antiferromagnetic for half-filling ($\nu=0$). Therefore we expect the following: Nagaoka’s supposition is reliable for small $\nu$ whereas the weak coupling mean field result is valid for small $U/t$ and our result can be trusted for large $\nu$ and large $U/t$. From this expectation, we anticipate that the state at zero temperature for large $\nu$ and large $U/t$ is ferromagnetic rather than paramagnetic. This point does not agree with Kanamori’s result obtained by the modified weak coupling mean field, which insists that for

![Fig. 10.8. Conjectured phase diagram at zero temperature.](image1)

![Fig. 10.9. Phase diagram by mean-field approximation.](image2)
arbitrary $U/t$ and for $\nu$ above certain value, the state at zero temperature is a paramagnetic state.\textsuperscript{16}$\sim$\textsuperscript{18} For large $U/t$, we think that the inclusion of specific type of diagrams (multiple scattering diagram) in weak coupling expansion, as was done in Ref. 16), will not be sufficient.

Unfortunately, in our result, the line dividing between the ferromagnetic state and the antiferromagnetic state lies in the region where neither $\nu$ nor $U/t$ is large. Thus this line itself is not so reliable. (In particular the regions corresponding to both ends of the curve of Fig. 10.8 are totally unreliable.) Summarizing these facts, the expected phase diagram at zero temperature is shown in Fig. 10.10. In the figure, only the large $U/t$ part (Ferro) has the meaning and the lines have been drawn rather arbitrary.

The conclusions up to now have been obtained by the lower terms of the expansion (10.2.2). The results will be improved if the higher orders of the form $t^n(1/U)^m$ are included. However, for higher order calculation, it is desirable to establish the graphical rules like the high temperature expansion of Ising system which will be presented in Chapter XI.

References

1) For general references of the Hubbard model, see for example A. Montorsi, The Hubbard Model (World Scientific, 1992).
Chapter XI. Higher Orders of Inversion Series

Up to now the inversion series has mainly been used in its lowest non-trivial order which is given by the first two terms of the series. In §10.1 the first three terms are included. We are naturally interested in the higher order terms and the aim of this chapter to elucidate the mathematical structure of the higher orders. The result can be summarized in the form of two theorems which are applicable to the wide class of the theory. The most crucial point in deriving the theorems is to use the variable $J^{(0)}[\phi]$ instead of the original order parameter $\phi$ itself. Here $J^{(0)}[\phi]$ is the lowest term of the inversion series and has the meaning of the “internal field” in the absence of the interaction. See the discussions in §7.2.1.

In the following the model of quantum electrodynamics (QED) is considered first and the chiral symmetry breaking is discussed in a gauge invariant manner by adopting the local operator $\vec{\phi}(x)\phi(x)$ as an order parameter. Here we encounter the notion of the generalized two particle irreducibility extended to the case of the local composite operator.

After discussions are extended to the relativistic $\phi^4$ theory, the ferromagnetic weak coupling series of the Hubbard model is also discussed. The high temperature expansion of the Ising system is then studied. A brief comment on the density functional theory is finally given.

§11.1. QED and $\vec{\phi}(x)\phi(x)$

The rule for the effective action of the local composite operator has been needed for a long time. The problem is of extreme importance: for example in the non-relativistic case, we want to know the free energy $\Gamma$ of the density operator or in the relativistic theory we are particularly interested in the gauge invariant local composite operators\(^{(1), (2)}\) in QED or QCD.

Recently the effective action for a local composite field $\phi(x)^2$ in the case of $\phi^4$ theory has been derived by Okumura.\(^{(3)}\) The essential tool was the inversion formula\(^{(1), (4), (5), (6)}\) explained in Chapter VII. Though the applicability of Okumura’s work is restricted to the special model, several generalizations\(^{(7), (8)}\) have been accomplished and we now know the explicit graph rule of the effective action which is independent of the particular model.

We deal with QED in this section, having in mind the gauge invariant investigation of the strong coupling phase of massless QED\(^{(9)}\) where the gauge invariant local composite operator $\vec{\phi}(x)\phi(x)$ condenses. Our results are summarized in the form of Theorems 11.1 and 11.2 below. Recall here that the non-local object $\vec{\phi}(x)\phi(y)$ is not invariant under the gauge transformation,

$$\phi(x) \rightarrow e^{i\theta(x)}\phi(x), \quad \vec{\phi}(x) \rightarrow e^{-i\theta(x)}\vec{\phi}(x).$$

We have given some calculations using gauge non-invariant operator $\vec{\phi}(x)\phi(y)$ in
§ 7.3.2.

By taking \( \tilde{\phi}(x)\phi(x) \) as the order parameter our method allows us at the same time to study the positronium states in a gauge invariant manner, whose results are summarized in three equations (11·3·4), (11·3·13) and (11·3·16) below. We can analyze these equations in a perturbative way.

In the arguments that follow, the change of the order parameter from \( \phi = \langle \tilde{\phi}(x)\phi(x) \rangle \) to the lowest order term \( J^{(0)}[\phi] \) of the inversion series is crucial and this process has a physical meaning: switching from the variable \( \langle \tilde{\phi}(x)\phi(x) \rangle \) to the dynamical mass.

Let us introduce the generating functional of connected Green's functions \( W[J] \) of QED by the path integral expression

\[
e^{iW[J]} = \int [dA d\phi d\bar{\phi}] e^{iJ[A, \phi, \bar{\phi}]}, \tag{11·1·1}
\]

\[
I[A, \phi, \bar{\phi}] = I[A, \phi, \bar{\phi}] + \int d^4x J(x) \tilde{\phi}(x)\phi(x). \tag{11·1·2}
\]

Here \( I \) is the action of QED defined by (7·3·9). The source \( J(x) \) in (11·1·2) is coupled to the local composite field \( \tilde{\phi}(x)\phi(x) \), which is gauge invariant. Therefore all the quantities appearing in the following formulas are gauge invariant and hence are independent of the gauge parameter of \( \lambda \). Although we study the case of \( \tilde{\phi}(x)\phi(x) \), any other local composite operators can be equally discussed. The purpose of this section is to extend the lowest order study of the chiral symmetry breaking (§ 7.3.3) to general order.

Now the effective action of the local composite operator \( \tilde{\phi}(x)\phi(x) \) is defined through the following Legendre transformation

\[
\Gamma[\phi] = W[J] - \int d^4x J(x) \phi(x), \tag{11·1·3}
\]

\[
\phi(x) = \frac{\delta W[J]}{\delta J(x)} = \langle \tilde{\phi}(x)\phi(x) \rangle. \tag{11·1·4}
\]

Here \( J(x) \) in (11·1·3) is expressed by \( \phi(x) \) through inverting (11·1·4). We note here the identity (A·5):

\[
\frac{\delta \Gamma[\phi]}{\delta \phi(x)} = -J(x). \tag{11·1·5}
\]

So the effective action is obtained by integrating (11·1·5) with respect to \( \phi(x) \). The essential step is to invert (11·1·4) which can be done by the inversion method explained in Chapter VII. We here rewrite the formulas explicitly up to the third order in \( e^2 \).

From (11·1·4), \( \phi(x) \) can be written as a functional of \( J(x) \) as

\[
\phi(x) = \sum_{n=0}^{\infty} \phi^{(n)}[J](x) = \phi^{(0)}[J](x) + \phi^{(1)}[J](x) + \phi^{(2)}[J](x) + \cdots, \tag{11·1·6}
\]

where \( \phi^{(n)}[J](x) \) is of the \( n \)-th order in \( e^2 \) (regarding \( J(x) \) as of order unity). This is the original series. The inverted series is defined as
\[ J(x) = \sum_{i=0}^{\infty} J^{(i)}(\phi)(x) = J^{(0)}(\phi)(x) + J^{(1)}(\phi)(x) + J^{(2)}(\phi)(x) + \cdots. \]  

Here \( J^{(i)}(\phi)(x) \) is of the \( i \)-th order in \( e^2 \) (regarding \( \phi \) as order unity). In order to simplify the equations, we sometimes use the notation \( J_{\phi}(\phi) = J^{(i)}(\phi) \) in the following. Substituting (11.1.7) into (11.1.6), we find

\[
\phi = \sum_{i=0}^{\infty} \phi^{(i)}(\sum_{j=0}^{\infty} J^{(j)}(\phi)) \\
= \phi^{(0)}[J_{\phi}(\phi)] + \left( \phi^{(0)}[J_{\phi}(\phi)] J^{(1)}(\phi) + \phi^{(1)}[J_{\phi}(\phi)] \right) \\
+ \left( \phi^{(0)}[J_{\phi}(\phi)] J^{(2)}(\phi) + \frac{1}{2} \phi^{(0)}[J_{\phi}(\phi)] J^{(1)}(\phi)^2 + \phi^{(1)}[J_{\phi}(\phi)] J^{(1)}(\phi) + \phi^{(2)}[J_{\phi}(\phi)] \right) \\
+ \cdots, \tag{11.1.8}
\]

where we have suppressed coordinate variables and integrations as follows,

\[
\frac{1}{2} \phi^{(0)}[J_{\phi}(\phi)] J^{(1)}(\phi)^2 = \frac{1}{2} \int d^4y_1 \int d^4y_2 \frac{\delta^2 \phi^{(0)}[J_{\phi}(\phi)](x)}{\delta J^{(0)}(\phi)(y_1) \delta J^{(0)}(\phi)(y_2)} J^{(1)}(\phi)(y_1) J^{(1)}(\phi)(y_2). 
\]

This kind of notation is employed in the following. By regarding \( \phi(x) \) as the order of unity and by comparing both sides of (11.1.8) in each order of \( e^2 \), we can determine \( J^{(i)}(\phi) \) as follows,

\[
\phi = \phi^{(0)}[J_{\phi}(\phi)] \implies J^{(0)}(\phi) = \phi^{(0)-1}[\phi], \tag{11.1.9}
\]

\[
J^{(1)}(\phi) = -(\phi^{(0)}[J_{\phi}(\phi)])^{-1} \phi^{(1)}[J_{\phi}(\phi)], \tag{11.1.10}
\]

\[
J^{(2)}(\phi) = -(\phi^{(0)}[J_{\phi}(\phi)])^{-1} \left( \phi^{(2)}[J_{\phi}(\phi)] + \phi^{(1)}[J_{\phi}(\phi)] J^{(1)}(\phi) + \frac{1}{2} \phi^{(0)}[J_{\phi}(\phi)] J^{(1)}(\phi)^2 \right). \tag{11.1.11}
\]

Notice that \( (\phi^{(0)}[J_{\phi}(\phi)])^{-1} \phi^{(1)}[J_{\phi}(\phi)] J^{(1)}(\phi) \) is, for example, the abbreviation of

\[
\int d^4y_1 \int d^4y_2 \left( \frac{\delta \phi^{(0)}[J_{\phi}(\phi)]}{\delta J^{(0)}(\phi)} \right)^{-1}(x,y_1) \frac{\delta \phi^{(1)}[J_{\phi}(\phi)](y_2)}{\delta J^{(0)}(\phi)(y_2)} J^{(1)}(\phi)(y_2). 
\]

Let us expand \( \Gamma(\phi) \) as a sum of \( \Gamma^{(i)}[\phi] \) which is of \( i \)-th order in \( e^2 \):

\[
\Gamma(\phi) = \sum_{i=0}^{\infty} \Gamma^{(i)}[\phi] = \Gamma^{(0)}[\phi] + \Gamma^{(1)}[\phi] + \Gamma^{(2)}[\phi] + \cdots \tag{11.1.12}
\]

Then in each order of \( e^2 \) we have the following identity from (11.1.5),

\[
\frac{\delta \Gamma^{(i)}(\phi)}{\delta \phi(x)} = -J^{(i)}(x). \tag{11.1.13}
\]

\( \Gamma^{(i)}[\phi] \) is obtained by integrating the above identity with respect to \( \phi \). We now explain this process explicitly up to \( i=2 \). From (11.1.4) and (11.1.6), the original series \( \phi^{(0)}[J], \phi^{(1)}[J] \) and \( \phi^{(2)}[J] \) are found easily using Feynman diagrams:

\[
i \phi^{(0)}[J] = \text{\Large \textbullet}, \tag{11.1.14}
\]
\[ i\phi^{(1)}[J] = \begin{array}{c}
\end{array} , \] (11.1.15)

\[ i\phi^{(2)}[J] = \begin{array}{c}
\end{array} + \begin{array}{c}
\end{array} + \begin{array}{c}
\end{array} + \begin{array}{c}
\end{array} , \] (11.1.16)

where the broken line is the photon propagator \( D_0 \) appearing in (7.3.9). Each small dot corresponds to the vertex with a factor \(-ie\gamma_\mu\) and a large dot indicates the insertion of the operator \( \hat{\phi}(x)\phi(x) \) which accompanies the factor \( i \). The solid line with an arrow is the electron propagator \( G_J \) which is defined by

\[ iG_J^{-1}(x, y) = iG_0^{-1}(x, y) + J(x)\delta^4(x - y) \]

\[ = (i\partial - m + J(x))\delta^4(x - y) . \] (11.1.17)

To each fermion loop the factor \(-1\) is attached, of course, and the diagram is divided by the corresponding symmetry factor. We here use the fact that all the diagrams containing fermion loops with odd number of small dots vanish. From (11.1.9) to (11.1.11) the inverted series \( J^{(0)}[\phi] \), \( J^{(1)}[\phi] \) and \( J^{(2)}[\phi] \) are determined as

\[ i\phi(x) = \begin{array}{c}
\end{array} \implies J^{(0)} = J^{(0)}[\phi] , \] (11.1.18)

\[ J^{(1)}[\phi](x) = \begin{array}{c}
\end{array} \] (11.1.19)

\[ J^{(2)}[\phi](x) = \begin{array}{c}
\end{array} \] (11.1.20)

In these graphs the electron propagators are different from (11.1.14) to (11.1.16) and are now \( G_J \) (instead of \( G_o \)) defined by

\[ iG_J^{-1}(x, y) = iG_0^{-1}(x, y) + J^{(0)}[\phi](x)\delta^4(x - y) \] (11.1.21)

where \( J^{(0)}[\phi](x) \) is given by (11.1.18). In (11.1.19) and (11.1.20), it is convenient to define a new kind of propagator

\[ \Delta_2^{-1}(x, y) = \left( \frac{\delta^2 iW^{(0)}[J^{(0)}[\phi]]}{\partial J^{(0)}[\phi](x)\partial J^{(0)}[\phi](y)} \right)^{-1} = -iG_J(x, y)iG_J(y, x)^{-1} \]

\[ = \left( \frac{-1}{\bigcirc} \right)_{xy} . \] (11.1.22)

We call this “the inverse propagator” in what follows. Note that \( \Delta_2(x, y) \) is the bare propagator of the composite operator evaluated at \( J = J^{(0)}[\phi] \); \( \Delta_2(x, y) = -i\bar{\phi}(x)\phi(x)i\bar{\phi}(y)\phi(y)\rangle_{J = J^{(0)}[\phi]} \). There is a space-time integration at each end of
\[ \Delta_2^{-1} \] except for the left end of the first factor \( \Delta_2^{-1} \) in (11.1.19) and (11.1.20) which is fixed to be \( x \). It would be convenient to write \( \Delta_2^{-1} \) diagrammatically as a double line which plays the role of eliminating one composite propagator. Then Eq. (11.1.19), for example, becomes

\[ J^{(1)}[\phi](x) = \[
\]

(11.1.23)

From (11.1.13) and (11.1.18) to (11.1.20), we finally get \( \Gamma^{(0)} \), \( \Gamma^{(1)} \) and \( \Gamma^{(2)} \). The integration over \( \phi \) leads to relatively simple expressions (apart from irrelevant constant terms)

\[ i\Gamma^{(0)}[\phi] = -\frac{1}{2} \text{TrLn}D_0^{-1} + \text{TrLn}G_{\phi}^{-1} - i\Gamma^{(0)}[\phi] \phi , \]

(11.1.24)

\[ i\Gamma^{(1)}[\phi] = \[
\]

(11.1.25)

\[ i\Gamma^{(2)}[\phi] = \]
\[ + \]
\[ + \]
\[ + 
\]

(11.1.26)

Here we have used the relation

\[ - \frac{\delta J^{(0)}[\phi]}{\delta i\phi} = - \left( \frac{\delta i\phi}{\delta J^{(0)}[\phi]} \right)^{-1} = \left[ \begin{array}{c}
\bullet \\
\end{array} \right] = \Delta_2^{-1} \].

(11.1.27)

In order to see the graphical implication, let us rearrange (11.1.26) and use the third expression in (11.1.27) again to represent \( \Delta_2^{-1} \) instead of the fourth expression (the double line):

\[ i\Gamma^{(2)}[\phi] = \]
\[ + \]
\[ + \]
\[ - \]

(11.1.28)

We have now two expressions: (11.1.26) and (11.1.28).

Let us study (11.1.26) first. There are three diagrams which have no \( \Delta_2^{-1} \). These diagrams are just the second order diagrams appearing in \( iW[J] \). The remaining term in (11.1.26) can be produced by the following procedure.

(a-1) Write down the first order diagrams appearing in \( \delta iW[J]/\delta J \), i.e., (11.1.15). As for the propagator, \( G_{\phi} \) has to be used.

(a-2) Connect two diagrams found in (a-1) by \( \Delta_2^{-1} \).

On the other hand, Eq. (11.1.28) looks more complicated. Let us look at the graphs without \( \Delta_2^{-1} \). Then the first term in the parenthesis on the right-hand side of (11.1.28) is a 2-particle reducible (2PR) graph with respect to the electron propagator. Here a 2PR graph is defined as a connected graph in which the amputation of at least one pair of propagators contained in it separates the graph into two pieces. The 2-particle irreducible (2PI) graph is defined in an obvious manner; it is also a connected graph but the amputation of any pairs of propagators in it does not separate the graph into two pieces. The first and second graphs on the right-hand side of (11.1.28) are
examples of 2PI graphs. Here the second term in the parentheses on the right-hand side of (11·1·28) can be obtained as follows (see Fig. 11.3).

(b-1) The first graph in the parentheses on the right-hand side of (11·1·28) is a 2PR graph. Separate the graph into two pieces by cutting a pair of propagators (i.e., 2PR propagators) in it.

(b-2) Join (with a factor \(i\)) the two newly made external propagators in each of the two separated graphs.

(b-3) Connect two joints of the two graphs by \(\Delta_2^{-1}\).

The expression in the parenthesis on the right-hand side of (11·1·28) implies that we have to subtract the above constructed graph from 2PR graph. Roughly speaking we have to subtract from \(\Gamma^{(2)}\) the contribution coming from the graph where \(\bar{\phi}(x)\phi(x)\) appears as an intermediate state. The subtracted part has already been taken into account by choosing \(\bar{\phi}(x)\phi(x)\) as an independent variable. This is the essence of the Legendre transformation. We can say that the resulting expression is irreducible with respect to the local composite operator \(\bar{\phi}(x)\phi(x)\).

How about the higher order terms of \(\Gamma[\phi]\)? Using the inversion formula of \(J^{(3)}[\phi]\), we can calculate \(i\Gamma^{(3)}[\phi]\). The result is just what we expect:

\[
i\Gamma^{(3)} = \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array} \gamma_1^{(3)} + \gamma_2^{(3)} + \gamma_3^{(3)} + \gamma_4^{(3)},
\end{array}
\]

(11·1·29)

\[
\gamma_1^{(3)} = R_2(\begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array}),
\]

(11·1·30)

\[
\gamma_2^{(3)} = R_2(\begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array}),
\]

(11·1·31)

\[
\gamma_3^{(3)} = R_2(\begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array}),
\]

(11·1·32)

\[
\gamma_4^{(3)} = R_2(\begin{array}{c}
\begin{array}{c}
\text{\hspace{1cm}}
\end{array}
\end{array}).
\]

(11·1·33)

We have arranged the graphs in (11·1·29) according to the property of 2PR as in (11·1·28). The definition of \(R_2\) is given in Theorem 11.2 below. Especially the graphs in \(\gamma_1^{(3)}\) are explicitly written down on the right-hand side of (11·1·40). The graphs in \(\gamma_2^{(3)}, \gamma_3^{(3)}\) and \(\gamma_4^{(3)}\) are obtained by \(R_2\) in a similar manner as in \(\gamma_1^{(3)}\). Now we reach two theorems which will be proved in the next section. Theorem 11.1 is the generalization of (11·1·26) and Theorem 11.2 corresponds to (11·1·28). These two theorems are general in the sense that their validity is not restricted to \(\bar{\phi}(x)\phi(x)\) in QED but it applies to the local bilinear operators of any theory.
**Theorem 11.1**

$iT^{[\phi]}$ consists of $iT^{[0][\phi]}$ given in (11.1.24) and all the connected tree diagrams constructed out of the $k$-vertex $v_k$ ($k \geq 0$) and inverse propagator $\Delta_2^{-1}$. Here $v_k$ is defined by

$$v_k(x_1, x_2, \cdots, x_k) = \frac{\delta^k i\bar{W}[J^{[0][\phi]}]}{\delta J^{[0][\phi]}(x_1) \cdots \delta J^{[0][\phi]}(x_k)(x_k)} - \delta_{k,0} \left( -\frac{1}{2} \text{Trln}D_0^{-1} + \text{Trln}G_{10}^{-1} \right) - \delta_{k,1} \otimes - \delta_{k,2} \otimes .$$  \hspace{1cm} (11.1.34)

Explicitly, $v_0 = i\bar{W}[J^{[0][\phi]}] - (-1/2)\text{Trln}D_0^{-1} + \text{Trln}G_{10}^{-1})$. Diagrams appearing in $v_i$ up to the second order in $e^2$ are given in Fig. 11.1. As shown in Fig. 11.1, loops are contained in $v_a$.

Similarly the graph rule of $J^{[\phi]}(x)$ is given as follows; it is the sum of $J^{[0][\phi]}(x)$ defined in (11.1.18) and all the connected tree diagrams constructed with the $k$-vertex $v_k$ ($k \geq 1$), inverse propagator $\Delta_2^{-1}$, and an external line $\Delta_2^{-1}$ which starts from $x$. Examples of the diagrams appearing in $iT^{[\phi]}$ and $J^{[\phi]}(x)$ are given in Figs. 11.2 (a) and (b), respectively. Each end of the vacuum tree diagram is, of course, $v_i$.

We have written down $v_k$ as (11.1.34), in order to stress its diagrammatical role. The fully algebraic expression of (11.1.34) is as follows,

$$v_k(x_1, x_2, \cdots, x_k) = \frac{\delta^k i\bar{W}[J^{[0][\phi]}]}{\delta J^{[0][\phi]}(x_1) \cdots \delta J^{[0][\phi]}(x_k)(x_k)} - \delta_{k,0} i\bar{W}[J^{[0][\phi]}]$$

$$- \delta_{k,1} \frac{\delta i\bar{W}[J^{[0][\phi]}]}{\delta J^{[0][\phi]}(x_1)} - \delta_{k,2} \frac{\delta^2 i\bar{W}[J^{[0][\phi]}]}{\delta J^{[0][\phi]}(x_1) \delta J^{[0][\phi]}(x_2)(x_2)}. \hspace{1cm} (11.1.35)$$

In this form, together with (11.1.22) we find that $v_k$ and $\Delta_2^{-1}$ (as a result, Theorem 11.1 also) is not model dependent.

**Theorem 11.2**

$i\Gamma^{[\phi]}$ and $J^{[\phi]}$ are given by the equations

$$i\Gamma^{[\phi]} = R_2(i\bar{W}[J^{[0][\phi]}]) - i \int d^4 x J^{[0][\phi]}(x) \phi(x), \hspace{1cm} (11.1.36)$$

$$J^{[\phi]}(x) = \int d^4 y \Delta_2^{-1}(x, y) R_2\left( \frac{\delta (i\bar{W}[J^{[0][\phi]}])}{\delta J^{[0][\phi]}(\phi)}(y) \right) + J^{[0][\phi]}(x), \hspace{1cm} (11.1.37)$$

where $R_2$ is the operation to yield diagrams required for $\Gamma^{[\phi]}$ or $J^{[\phi]}(x)$. The

![Diagram](image_url)

**Fig. 11.1.** Diagrams appearing in $v_i$ up to the second order in $e^2$.

![Diagram](image_url)

**Fig. 11.2.** (a) An example of the diagram appearing in $iT^{[\phi]}$. (b) An example of the diagram appearing in $J^{[\phi]}(x)$. 
Chapter XI. Higher Orders of Inversion Series

definition of $R_2$ is summarized in (c-1)~(c-5) below ((c-1)~(c-3) are the same as in
(b-1)~(b-3).):

(c-1) If there are 2PR parts with respect to two electron propagators, separate the
graph into two pieces by cutting 2PR propagators.

(c-2) Join (with a factor $i$) the resulting two external propagators in each of the two
separated graphs.

(c-3) Connect two joints of the two graphs by $\Delta z^{-1}$.

(c-4) Carry out the same procedures (c-1)~(c-3) for the resulting graph obtained in
(c-3) until it produces no new graphs.

(c-5) Sum up all the resulting graphs including the original graph.

The examples of $R_2$ operation on some typical graphs in $W[J^{(0)}]$ are given as

$$R_2\left(\begin{array}{c}
\includegraphics[width=0.2\textwidth]{example1}\n\end{array}\right) = \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example2}\n\end{array} + \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example3}\n\end{array}$$

$$R_2\left(\begin{array}{c}
\includegraphics[width=0.2\textwidth]{example4}\n\end{array}\right) = \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example5}\n\end{array} ,$$

$$R_2 = \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example6}\n\end{array} + \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example7}\n\end{array} + \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example8}\n\end{array} + \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example9}\n\end{array} + \begin{array}{c}
\includegraphics[width=0.2\textwidth]{example10}\n\end{array} .$$

An example of the procedures (c-1)~(c-3) is given in Fig. 11.3. In Fig. 11.4, we
concentrate our attention on the procedure (c-4) and illustrate how the $R_2$ operation
on the graph (a) in Fig. 11.4 produces the graphs given on the right-hand side of

Fig. 11.3. An example of the $R_2$ operation on 2PR
diagram (a). Each procedure (c-1), (c-2) and
(c-3) (or (b-1), (b-2) and (b-3)) acts on the graph
(a), (b) and (c) and it produces (b), (c) and (d),
respectively.

Fig. 11.5. The operation $R_3$ on the graph (a) does
not produce the graph (b) because (a) and (b)
are topologically the same graphs.

Fig. 11.4. The illustration of the procedure (c-4)
acting on the graph (a). The procedures (c-1)
~(c-3) operate on the 2PR part indicated as a
broken line with dots. This process continues
to yield (b), (c) and (d).
Notice that the $R_3$ operation on the graph (a) in Fig. 11.5 does not produce the graph (b). This is because the graph on the right of $\Delta z^{-1}$ in (b) which is nothing but $\delta^2 i W^{(0)}[f^{(0)}]/\partial f^{(0)}(x_1)\partial f^{(0)}(x_2)$ does not appear in $v_x$. The operation $R_3$ only produces the graph in $v_x$. The reason is easily found in the proof of Theorem 11.2 given in § 11.2. Also we see that the operation $R_2$ produces graphs which are “tree” with respect to the inverse propagator $\Delta z^{-1}$. It is easy to confirm that Theorems 11.1 and 11.2 are indeed satisfied for lower order calculations (presented above) of $I^{(0)}$ and $J^{(0)}$ through the inversion method.

Let us investigate the meaning of Theorem 11.2. For this aim, it will be helpful to compare our effective action $I'[\phi]$ with that in which the order parameter is a non-local field $\hat{G}(x, y) = \langle \phi(x) \bar{\phi}(y) \rangle$. It is already known that the effective action $I'[G]$ for the non-local $\hat{G}(x, y)$ is given by (Appendix C.2)

$$iI'[G] = -\frac{1}{2} \text{Tr} \ln D_0^{-1} + \text{Tr} G_0^{-1} G + \text{Tr} \ln G + \kappa_2[G], \tag{11.1.41}$$

where $\kappa_2[G]$ is the sum of all the 2PI vacuum graphs. Owing to the non-locality of $G$ the graphical rule for $I'[G]$ is fairly simplified as (11.1.41) compared with $I'[\phi]$ of the local case. Let us study $I'[G]$ by the inversion method introducing the source term $\int d^4x d^4y f(x, y) \phi(x) \bar{\phi}(y)$ and define $W[J]$. First, $J^{(0)}[G](x, y)$ can be obtained explicitly:

$$\hat{G}(x, y) = \langle \phi(x) \bar{\phi}(y) \rangle = i \left\{ (i \partial - m) \delta^4(x - y) + J^{(0)}[G](x, y) \right\}^{-1}. \tag{11.1.42}$$

The rules for the non-local case are the following: we have to omit (c-2) in Theorem 11.2 and modify (c-3) as (c-3'):

(c-3') Connect the two graphs with $\delta^2 i \hat{r}^{(0)}[G]/\partial G \partial G = (\partial_0 G)^{-1} G^{-1}$. (This is $\Delta z^{-1}$ in the non-local case. Note that we know its explicit form.)

In this case, the examples of $R_3$ operation become

$$R_3 \left( \begin{array}{c} \text{--} \end{array} \right) = \begin{array}{c} \text{--} \\ \text{--} \end{array} + \begin{array}{c} \text{--} \\ \text{--} \end{array} \right] = \begin{array}{c} \text{--} \\ \text{--} \end{array} \right] = 0, \tag{11.1.43}$$

$$R_2 \left( \begin{array}{c} \text{--} \end{array} \right) = \begin{array}{c} \text{--} \\ \text{--} \end{array} \right], \tag{11.1.44}$$

and so forth. So we deduce that after the $R_3$ operation the contribution from 2PR graphs becomes zero and only 2PI graphs survive. This is our way of explaining why we only find 2PI graphs in $\kappa_2[G]$. In the local case, the cancellation as in (11.1.43) does not occur, but we see that the contribution from 2PR graphs to $I'[\phi]$ will be reduced to some extent by the $R_2$ operation. The minus sign in the inverse propagator $\Delta z^{-1}$ is the origin of this reduction. As has been emphasized, $R_3$ operation corresponds to the subtraction of the “$\bar{\phi}(x)\phi(x)$ reducible part” from each 2PR graph.
§ 11.2. Perturbative construction of effective action: proof of theorems

In this section, the proof of Theorems 11.1 and 11.2 is given. For the general proof, however, we do not have to rely on the perturbative inversion series developed in the previous section. Instead, we construct another method of the inversion process through the generating functional and apply it to the proof of the theorems. To evaluate $W[J]$, let us return to (11·1·1) and use (7·3·9). Thus we start from

$$e^{iW[J]} = \int [dA d\phi d\bar{\phi}] e^{i\mu} \times \frac{\int [dA d\phi d\bar{\phi}] e^{i\mu}}{\int [dA d\phi d\bar{\phi}] e^{i\mu}}. \quad (11·2·1)$$

where $I_I$ is given in (7·3·9) and $I^{(0)}_I$ is the free part of $I_I$ obtained by setting $e^2 = 0$.

$$iW[J] = -\frac{1}{2} \text{Tr} \ln D_0^{-1} + \text{Tr} \ln G_{\gamma^{-1}} + \kappa[J], \quad (11·2·2)$$

where $\kappa[J]$ is the sum of all the connected vacuum diagrams with two or more loops. Some of the lower order graphs are given as follows (propagators are denoted as $G_{\gamma}$ which is equal to $G_{\gamma}$ of (7·3·11)),

$$\kappa[J] = \begin{array}{c}
\bigcirc \\
\tiny \begin{array}{cc}
\bigcirc & \bigcirc \\
\bigcirc & \bigcirc
\end{array}
\end{array} + \ldots. \quad (11·2·3)$$

From (11·1·3) and (11·2·2), we have

$$i\tilde{\Gamma}[\phi] = -\frac{1}{2} \text{Tr} \ln D_0^{-1} + \text{Tr} \ln G_{\gamma}^0 + \kappa[J[\phi]] - i \int d^4 x J[J[\phi]](x) \phi(x). \quad (11·2·4)$$

It is true that the above equation gives $\Gamma[\phi]$ if we know $J[\phi]$. This is carried out in a perturbative manner in the following way. Using (11·1·7) and (11·1·12), the zeroth order of (11·2·4) becomes

$$i\tilde{\Gamma}^{(0)}[\phi] = -\frac{1}{2} \text{Tr} \ln D_0^{-1} + \text{Tr} \ln G_{\gamma}^0 - i \int d^4 x J^{(0)}[\phi](x) \phi(x). \quad (11·2·5)$$

Here $G_{\gamma}$ is given in (11·1·21). Equation (11·2·5) has the same form as (11·1·24) but in (11·2·5) the $\phi$ dependence of $J^{(0)}[\phi]$ has not yet been determined. Now we use the identity (11·1·13):

$$- J^{(0)}[\phi](x) = \frac{\delta \tilde{\Gamma}^{(0)}[\phi]}{\delta \phi(x)}
= - J^{(0)}[\phi](x) - \int d^4 y \frac{\delta J^{(0)}[\phi]}{\delta \phi(x)}(\phi(y) + G_{\gamma}(y, x)). \quad (11·2·6)$$

Therefore if the condition

$$\det \left( \frac{\delta J^{(0)}[\phi]}{\delta \phi(x)}(y) \right) \neq 0 \quad (11·2·7)$$

is satisfied, we get $J^{(0)}[\phi](x)$,
\[ i\phi(x) = -iG_{\phi}(x, x) = \quad (11.2.8) \]

Here the propagator is \( G_{\phi} \). This agrees with the result given in (11.1.18). As a result we can use (11.1.27) in what follows. Note that Eq. (11.2.7) is nothing but the condition that the function \( J^{00}[\phi] \) has the inverse or equivalently the condition that \( \phi \) of (11.1.18) can be inverted to get \( J^{00}[\phi] \).

In order to investigate the higher order terms, let us introduce \( \Delta J[\phi] \) as

\[ J[\phi] = J^{00}[\phi] + \Delta J[\phi], \quad \Delta J[\phi] = J^{(1)}[\phi] + J^{(2)}[\phi] + J^{(3)}[\phi] + \cdots \quad (11.2.9) \]

Substituting (11.2.9) into (11.2.4), we have

\[ i\Gamma[\phi] = -\frac{1}{2} \text{Tr} \ln D_0^{-1} + \text{Tr} \ln (G_0^{-1} - ij^{00}[\phi] - i\Delta J[\phi]) \]

\[ -i \int d^4x J^{(0)}[\phi](x)\phi(x) - i \int d^4x \Delta J[\phi](x)\phi(x) + \kappa[J[\phi]]. \quad (11.2.10) \]

The second term on the right-hand side of (11.2.10) is expanded in powers of \( \Delta J \):

\[ \text{Tr} \ln (G_0^{-1} - ij^{00}[\phi] - i\Delta J[\phi]) \]

\[ = \text{Tr} \ln G_{\phi}^{-1} + i\text{Tr} \phi \Delta J[\phi] - \text{Tr} \sum_{j=2}^{\infty} \frac{1}{j} (G_{\phi}(i\Delta J[\phi]))^j, \quad (11.2.11) \]

where we have used (11.2.8). The fourth term on the right-hand side of (11.2.10) is canceled by the second term on the right-hand side of (11.2.11). Using (11.2.5),

\[ i\Gamma[\phi] \]

now becomes

\[ i\Gamma[\phi] = i\Gamma^{(0)}[\phi] - \text{Tr} \sum_{j=2}^{\infty} \frac{1}{j} (G_{\phi}(i\Delta J[\phi]))^j + \kappa[J[\phi]]. \quad (11.2.12) \]

In (11.2.12), the electron propagator is \( G_{\phi}(x, y) \) and \( i\Delta J[\phi] \) acts as a two-point vertex which is inserted into the electron propagator.

The second term on the right-hand side of (11.2.12) consists of the second and higher order terms in \( e^2 \), while the last term has first order terms in \( e^2 \). The crucial thing is that \( i\Delta J[\phi] \) does not appear in \( \Gamma^{(0)}[\phi] \). Consequently we can determine \( \Gamma^{(1)} \) and \( J^{(1)} \) by using (11.2.3). The propagator in \( \kappa[J[\phi]] \) is also expanded in powers of \( i\Delta J \) or \( j^{(k)} \) (\( k \geq 1 \)) to obtain \( i\Gamma^{(1)}[\phi] \), so that the propagator appearing in the following graphs is now \( G_{\phi} \),

\[ i\Gamma^{(1)}[\phi] = \quad \quad (11.2.13) \]

\[ J^{(1)}[\phi](x) = -\frac{\delta i\Gamma^{(1)}}{\delta \phi(x)} = -\int d^4y \frac{\delta J^{(0)}(y)}{\delta \phi(x)} \frac{\delta i\Gamma^{(1)}}{\delta J^{(0)}(y)} = \quad (11.2.14) \]

In (11.2.14), we have used the fact that the \( \phi \) dependence of \( \Gamma^{(1)}[\phi] \) is only through \( J^{(0)}[\phi] \) defined in (11.2.8). Equations (11.2.13) and (11.2.14), of course, coincide with the previous results (11.1.25) and (11.1.23).

Substituting (11.2.14) into (11.2.12), \( i\Gamma^{(0)}[\phi] \) is obtained and then \( J^{(2)} \) is obtained.
by taking the derivative (see (11.1.13)). This process can be continued up to the desired order. In other words we can successively get $I^{(i)}$ and $J^{(i)}$ according to the following order:

$$iI^{(1)} \rightarrow J^{(1)} \rightarrow iiI^{(2)} \rightarrow J^{(2)} \rightarrow iiI^{(3)} \rightarrow J^{(3)} \rightarrow \cdots.$$  

(11.2.15)

Thus we are led to the following Lemma:

**Lemma** Using (11.2.12), $iI^{(j)}[\phi]$ and $J^{(j)}[\phi](x)$ ($j \geq 1$) are recursively derived as follows,

$$iI^{(j)}[\phi]=j\text{-th order of } iI^{(0)}[\phi], J^{(1)}[\phi], \ldots, J^{(j-1)}[\phi].$$  

(11.2.16)

$$J^{(j)}[\phi]=-\frac{\delta I^{(j)}}{\delta \phi}.$$  

(11.2.17)

This Lemma yields the same results given in §11.1 where we have utilized the inversion formula successively.

Now, with the help of Lemma, we prove Theorems 11.1 and 11.2. For each theorem, we should prove that all the required graphs appear and that each topologically different graph has the 'correct weight'. Here we should explain what the 'correct weight' means. The Feynman rule is a statement in which each graph appears once and each graph uniquely corresponds to a definite mathematical expression including its symmetry factor. Both theorems state that $I[\phi]$ is given by the sum of all the required graphs and that one graph appears only once in the sum, that is, there is no extra multiplicative constant attached to the graph. So the statement that a graph has the 'correct weight' means that a graph contributes to $I[\phi]$ with no extra multiplicative constant including the sign factor.

**Proof of Theorem 11.1**

We will prove Theorem 11.1 by the mathematical induction with respect to the order of perturbation in terms of $e^\phi$. First, assume that the statement given in Theorem 11.1 is true for $iI^{(n)}[\phi]$ and $J^{(n)}[\phi]$ ($j \leq n$). Then we show that:

(d-1) Every required graph appears in $iI^{(n+1)}[\phi]$ and in $J^{(n+1)}[\phi]$.

(d-2) Each graph has the correct weight in $iI^{(n+1)}[\phi]$ and in $J^{(n+1)}[\phi]$.

It is stressed here that we have to prove the graph rule for $I[\phi]$ and $J[\phi]$ simultaneously using Lemmas (11.2.16) and (11.2.17); in order to give $iI^{(j)}[\phi]$, the quantities $J^{(0)}[\phi], \ldots, J^{(j-1)}[\phi]$ is required while in order to get $J^{(j)}[\phi]$, the graph rule for $iI^{(j)}[\phi]$ is required. Let us introduce $\bar{\kappa}[\phi]$ as

$$\bar{\kappa}[\phi]=-\text{Tr} \sum_{f=3}^n \frac{1}{f} (G_{j_0}(i\Delta J[\phi]))^j + \kappa[J[\phi]].$$  

(11.2.18)

From (11.1.34) and (11.2.2) and expanding $\kappa[J[\phi]]=\kappa[J^{(0)}[\phi]+\Delta J[\phi]]$ in powers of $\Delta J[\phi]$, $\bar{\kappa}$ can be expressed as

$$\bar{\kappa}[\phi]=\sum_{k=0}^\infty \frac{1}{k!} \int d^4x_1 \cdots \int d^4x_k \Delta J[\phi](x_1) \times \cdots \times \Delta J[\phi](x_k).$$  

(11.2.19)
Here we notice that \( v_0[\phi] = \kappa [J^{(0)}[\phi]] \). In addition, we find the following equation from (11.2.12),

\[
i \Gamma[\phi] = i \Gamma^{(0)}[\phi] + \Delta J \overset{\nearrow}{\rightarrow} \Delta J + \kappa[\phi]. \tag{11.2.20}
\]

(Here the propagators in the second term on the right-hand side is \( G_{I_S} \) and it is assumed that it includes the combinatoric factor and sign.) From the assumption of induction, \( J^{(j)}[\phi] \) \((j \leq n)\) consists of all the \( j \)-th order connected tree diagrams constructed out of the \( k \)-vertex \( v_k \) \((k \geq 1)\), the inverse propagator \( \Delta z^{-1} \), and an external line \( \Delta z^{-1} \). Then after the substitution of \( \sum_{j=0}^n J^{(j)}[\phi] \) for \( \Delta J \) in (11.2.20) we convince ourselves that \( i \Gamma^{(n+1)}[\phi] \) consists of all the \((n+1)\)-th order connected tree diagrams constructed out of the \( k \)-vertex \( v_k \) \((k \geq 1)\) and the inverse propagator \( \Delta z^{-1} \). This is seen more clearly in the equations

\[
i \Gamma[\phi] = i \Gamma^{(0)}[\phi] - \frac{1}{2} \int d^4x_1 \int d^4x_2 \int d^4y_1 \int d^4y_2 \left(f(x_1) \Delta z(x_1, y_1)\right) \times \Delta z^{-1}(y_1, y_2) \left(\Delta z(x_2, x_3) i \Delta J(x_3)\right) + \sum_{k=0}^\infty \frac{1}{k!} \int d^4x_1 \cdots \int d^4x_k \int d^4y_1 \cdots \int d^4y_k \int d^4z_1 \cdots \int d^4z_k \times v_k(x_1, \cdots, x_k) \Delta z^{-1}(x_1, y_1) \times \cdots \times \Delta z^{-1}(x_k, y_k) \times \left(\Delta z(y_1, z_1) i \Delta J[\phi](z_1)\right) \times \cdots \times \left(\Delta z(y_k, z_k) i \Delta J[\phi](z_k)\right), \tag{11.2.21}
\]

where we have inserted \( \Delta z^{-1} \Delta z = 1 \). Notice that \( J^{(j)}[\phi](z_i) \) has \( \Delta z^{-1} \) as an external line from the assumption of induction. (See for example the last expression in (11.2.14).) As a result, the term \( \int d^4x_1(\Delta z(x_1, y_1) J^{(j)}[\phi](z_1)) \) \((j \leq n)\) consists of all the \( j \)-th order connected tree diagrams constructed out of the \( k \)-vertex \( v_k \) \((k \geq 1)\), the inverse propagator \( \Delta z^{-1} \), and an external point (large dot). Thus we have proved (d-1) for \( \Gamma^{(n+1)} \).

Next we prove (d-2) for \( \Gamma^{(n+1)} \). Let us consider a particular graph appearing in \( i \Gamma^{(n+1)}[\phi] \). It appears \( N(\Delta z^{-1}) \) times in the second term on the right-hand side of (11.2.21) with a minus sign. Here \( N(\Delta z^{-1}) \) is the number of the inverse propagator \( \Delta z^{-1} \) in a graph we are considering. This is because we have distinguished one special inverse propagator among these \( N(\Delta z^{-1}) \) inverse propagators and there are \( N(\Delta z^{-1}) \) ways of distinguishing an inverse propagator (Fig. 11.6 (a)). Likewise the diagram in question appears \( N(v) \) times in the third term on the right-hand side of (11.2.21). Here \( N(v) \) represents the number of \( k \)-vertices \( v_k \) in the graph (Fig. 11.6 (b)). For example, \( N(v) = 8 \) and \( N(\Delta z^{-1}) = 7 \) in the Fig. 11.2 (a). At this point the following topological relation valid for the connected tree diagram is essential:

\[
N(v) - N(\Delta z^{-1}) = 1. \tag{11.2.22}
\]

After all, each graph has the correct weight in \( i \Gamma^{(n+1)}[\phi] \) since the combina-
tion (11.2.21) includes every diagram only once.

Now let us come to the remaining half of Theorem 11.1 (rule for $J$). From the fact that the $\phi$ dependence of $iL^{(n+1)}[\phi]$ ($n \geq 0$) is through $J^{(0)}[\phi]$, Eq. (11.2.17) becomes

$$J^{(n+1)}[\phi](x)$$

$$= - \int d^4 y \frac{\delta J^{(0)}(y)}{\delta \phi(x)} \frac{\delta iL^{(n+1)}}{\delta J^{(0)}(y)}$$

$$= \int d^4 y A_2^{-1}(x, y) \left( \frac{\delta A_2^{-1}}{\delta J^{(0)}} \delta iL^{(n+1)} + \sum_k \frac{\delta v_k}{\delta J^{(0)}} \delta iL^{(n+1)} \right)_y. \quad (11.2.23)$$

Equation (11.2.23) exhausts with the correct weight all the tree diagrams having one external point specified by $x$. This is seen as follows. In (11.2.23), $\delta v_k/\delta J^{(0)}$ is nothing but the functional $(k+1)$-derivative of $iW[J^{(0)}]$ by $J^{(0)}$ and the ordinary Feynman rules (with the correct weight) hold for it. Recall that the functional derivative makes one extra external point. The Feynman rules also hold for $\delta iL^{(n+1)}/\delta A_2^{-1}$ and $\delta iL^{(n+1)}/\delta v_k$, because we can regard $A_2^{-1}$ (or $v_k$) as a non-local vertex. For $\delta A_2^{-1}/\delta J^{(0)}$, we note the relation

$$\frac{\delta A_2^{-1}(x, y)}{\delta J^{(0)}(z)} = \int d^4 w A_2^{-1}(x, v) \frac{\delta A_2(v, w)}{\delta J^{(0)}(z)} A_2^{-1}(w, y)$$

$$= - \int d^4 v \int d^4 w A_2^{-1}(x, v)$$

$$\times \left( \frac{\delta^3 iW^{(0)}[\phi]}{\delta J^{(0)}[\phi](v) \delta J^{(0)}[\phi](w) \delta J^{(0)}[\phi](z)} \right) A_2^{-1}(w, y)$$

$$= \int d^4 v \int d^4 w \frac{\varepsilon}{z} \frac{\varepsilon}{w} \frac{\varepsilon}{y} \cdot (11.2.24)$$

Owing to the definition of $v_k$ given in (11.1.34), the first term on the right-hand side of (11.2.23) naturally appears separately since it is excluded in the second term,

$$\frac{\delta v_k(x_1, \cdots, x_k)}{\delta J^{(0)}[\phi](y)}$$

$$= \frac{\delta^{k+1} iW^{(0)}[\phi]}{\delta J^{(0)}[\phi](x_1) \cdots \delta J^{(0)}[\phi](x_k) \delta J^{(0)}[\phi](y)} - \delta_{k,0} \frac{\delta^2 iW^{(0)}[\phi]}{\delta J^{(0)}[\phi](y)}$$

$$- \delta_{k,1} \frac{\delta^2 iW^{(0)}[\phi]}{\delta J^{(0)}[\phi](x_1) \delta J^{(0)}[\phi](y)} - \delta_{k,2} \frac{\delta^2 iW^{(0)}[\phi]}{\delta J^{(0)}[\phi](x_1) \delta J^{(0)}[\phi](x_2) \delta J^{(0)}[\phi](y)}$$

$$= v_{k+1}(x_1, \cdots, x_k, y) - \delta_{k,2} \frac{\delta^3 iW^{(0)}[\phi]}{\delta J^{(0)}[\phi](x_1) \delta J^{(0)}[\phi](x_2) \delta J^{(0)}[\phi](y)}. \quad (11.2.25)$$

The graphical representation on the right-hand side of (11.2.23) is shown in Fig. 11.7. In these discussions, it should be noticed that we have shown not only (d-1) but also (d-2). Since we have already verified that Theorem 11.1 is satisfied for the lower order of $iL^{(n)}[\phi]$ and $iJ^{(n)}[\phi]$, the proof of Theorem 11.1 is completed.

In order to help the understanding, we have sometimes used diagrams in the proof.
of Theorem 11.1, but as we have emphasized the proof does not depend on the diagrams. This is to say, Theorem 11.1 does not depend on specific models. Once we choose a Lagrangian (or a Hamiltonian) and a source term $J$, the generating functional of Green's functions $W[J]$ is defined. Then we can introduce $v_k$ and $A^{-1}$ as in (11.1.35) and (11.1.22), respectively. Thus Theorem 11.1 can be proved by only using the character which is independent of the model. Actually we will see some examples of this theorem for other models in the following section.

**Proof of Theorem 11.2**

Now Theorem 11.2 is proved by paying attention to the relation with Theorem 11.1. We have to show that the operation $R_2$ applied to $\delta iW[J^{(0)}]/\delta J^{(0)}$ (or $iW[J^{(0)}]$) produces all the connected tree diagrams constructed out of the $k$-vertex $v_k$ and the inverse propagator $A^{-1}$ and with (or without) an external point. This is verified by considering the reverse procedure of $R_2$. Statement (d-1) is true since any connected tree diagram constructed with $k$-vertex $v_k$ and the inverse propagator $A^{-1}$ and with (or without) an external point can be traced back (apart from the weight) to its original diagram appearing in $\delta iW[J^{(0)}]/\delta J^{(0)}$ (or $iW[J^{(0)}]$) with the help of the reverse procedure of $R_2$. How about (d-2) in this case? The important fact is that the operation of $R_2$ applied to $iW[J^{(0)}]$ (or $\delta iW[J^{(0)}]/\delta J^{(0)}$) produces a particular diagram only once so that we can uniquely recover graphs of $iW[J^{(0)}]$ (or $\delta iW[J^{(0)}]/\delta J^{(0)}$) from those of $R_2(iW[J^{(0)}])$ (or $R_2(\delta iW[J^{(0)}]/\delta J^{(0)})$. That is why the condition (d-2) is satisfied in the case of Theorem 11.2.

Let us illustrate this fact by an example. In Fig. 11.8 we show diagrams for which the reverse procedure of $R_2$ does not seem to exist at first sight. Consider the two diagrams (a') and (b') of Fig. 11.8. Here A, B, C and D are diagrams which are topologically different from each other. The diagrams (a') and (b') are the same graphs except for the direction of an arrow in these right half parts. The difference in the direction of the arrow is the key to recovering the original diagram uniquely. Owing to the direction of an arrow, (a') cannot be traced back to (b). In this case the arrow determines the way to recover the original diagram. Therefore the reverse procedure of $R_2$ exists. (The proof given here is actually model dependent. For
example, if we employ $\phi^4$ theory as a model the proof here fails, because there is no arrow on the propagator. This fact is quite natural since the statement of Theorem 11.2 is model dependent, in contrast to Theorem 11.1. It turns out, however, that in order to find the generalized form of Theorem 11.2, we have only to change the definition of the $R_2$ operator, which will be discussed in § 11.5. With this example in mind, the identification is easily done for other complicated diagrams. The remaining terms (outside of the operation $R_2$) in Theorem 11.2 play a role to fix the zeroth order terms in $I[\phi]$ or $J[\phi]$. It is easy to check that they work correctly. So the proof of Theorem 11.2 is completed.

We can now see the reason that the $R_2$ operation on the graph (a) in Fig. 11.5 does not produce the graph (b). Indeed in the graph (b), there is a graph $\delta^2 \i W[J^{(0)}[\phi]]/\delta J^{(0)}[\phi](x_1)\delta J^{(0)}[\phi](x_2)$ on the right of $\Delta_2^{-1}$ which does not exist in $\nu_2$. The $R_2$ operation rule is constructed so that the same graphs appearing in Theorem 11.1 are produced by the $R_2$ operation to $W[J^{(0)}[\phi]]$. That is why the $R_2$ operation does not produce the graph (b).

§ 11.3. Applications

11.3.1. Massless QED — change of order parameter —-

The theorems we have obtained can readily be applied to the study of chiral symmetry breaking of massless QED in a gauge invariant manner since the source term we have employed is a gauge invariant one: $\int d^4x J(x)\overline{\psi}(x)\psi(x)$. Indeed this is one of the reasons why we are interested in the local composite operator.

The problem was first discussed by Ukita, Komachiya and Fukuda. A calculation along this line has been performed by Kondo et al. They take $\phi$ as an order parameter and perform the lowest order calculation by the inversion method which has been given in § 7.3.3. Recently, Inagaki and Fukuda, Okumura, and Hondou suggested that it is more convenient if we employ $J^{(0)}$ rather than $\phi$ itself as an order parameter. Here we follow this suggestion and investigate the problem in terms of $J^{(0)}[\phi]$.

Let us take $J(x)$ as a constant $J$ which independent of the space-time coordinate. Then $\phi(x)$ is also independent of $x$. From (11.1.18) or (11.2.8), $J^{(0)}[\phi]$ is given as

$$
\phi = -i\text{tr} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k + J^{(0)}[\phi]}
$$

$$
= 4J^{(0)} \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + (J^{(0)}[\phi])^2},
$$

where we have set the mass $m=0$ and the integration in the second equation of (11.3.1) is the Wick rotated one. Let us introduce a cutoff $\Lambda$ for the integration in (11.3.1), then

* Miransky proposed another way of studying the chiral symmetry breaking by constructing the effective potential for the gauge invariant operator $\overline{\psi}(x)\psi(x)$. However, the Schwinger-Dyson equation for the non-local operator $\overline{\psi}(x)\psi(y)$ in the ladder approximation has also been employed to get the effective potential. Therefore his approach is not a gauge invariant one.
\[ \phi = \frac{J^{(0)}[\phi]}{4\pi^2} \left[ A^2 - (J^{(0)}[\phi])^2 \ln \left( \frac{A^2 + (J^{(0)}[\phi])^2}{(J^{(0)}[\phi])^2} \right) \right]. \quad (11.3.2) \]

If we regard \( \phi \) as a small variable, \( J^{(0)}[\phi] \) can be expressed as

\[ J^{(0)}[\phi] = \frac{4\pi^2}{A^2} \phi + \frac{(4\pi)^2}{A^2} \phi^3 \ln \frac{A^2 + (4\pi^2)^2 \phi^2}{(4\pi^2)^2 \phi^2} + \cdots. \quad (11.3.3) \]

Equation (11.3.2) allows us to use \( J^{(0)}[\phi] \) as an order parameter since \( \phi = 0 \) or \( \phi \neq 0 \) corresponds to \( J^{(0)}[\phi] = 0 \) or \( J^{(0)}[\phi] \neq 0 \), respectively. As we have found in §11.2, all the dependence on \( \phi \) contained in \( J[\phi] \) is through \( J^{(0)}[\phi] \). Even \( J^{(0)}[\phi] \) can be expressed with \( J^{(0)}[\phi] \) in spite of the fact that it has the term \( J^{(0)}[\phi] \phi \) appearing in \( J^{(0)}[\phi] \). This is because \( \phi \) is expressed as an explicit function of \( J^{(0)}[\phi] \) as given in (11.3.2). Moreover, \( J^{(0)}[\phi] \) is nothing but the mass term appearing in the propagator \( G_{\phi} \), when the chiral symmetry is broken, so that in an example here the change of variable from \( \phi \) to \( J^{(0)}[\phi] \) corresponds to the change of \( \phi \phi' \) to the dynamical mass.

Now we set \( J = 0 \) in (11.1.5) which can explicitly be written as (11.1.37) owing to Theorem 11.2. As a result, the equation to determine \( J^{(0)}[\phi] \) becomes

\[ -J^{(0)}[\phi](x) = \int d^4 y \Delta^{-1}(x, y) R_2 \left( \frac{\delta(i W[J^{(0)}[\phi]])}{\delta J^{(0)}(y)} - \text{Tr} \ln G_{\phi}^{-1} \right). \quad (11.3.4) \]

The diagrams appearing on the right-hand side of (11.3.4) are shown in Fig. 11.9 up to the second order in \( e^2 \). The lowest order calculation of the chiral symmetry breaking of massless QED can be performed by substituting the first term in Fig. 11.9 into (11.3.4). In this case, the symmetry breaking solution in terms of \( \phi \) with the help of (11.3.2) reproduces the one given in §7.3.3.

The higher order terms are explicitly and straightforwardly written down by Theorem 11.2. One of the merit of our rule is that it allows us to write down these higher order terms in a systematic way.

11.3.2. Excited states

Using on-shell expansion explained in Chapter II, we can determine not only the ground state \( |0\rangle \) but also excited states \( |i\rangle \) and scattering matrix elements among them. The ground state has already been investigated in §11.3.1 by setting \( J = 0 \) in (11.1.5). Now we apply our theorems to the on-shell equation (2.1.5). Before doing this, we generalize our source term a little bit. The exited state \( |i\rangle \) obtained as the solution of the on-shell equation is the bound state which couples to the source term; in our case considered up to now the state \( |i\rangle \) has the quantum number of \( \bar{\psi}(x)\psi(x) \), in other words, \( \langle i|\bar{\psi}(x)\psi(x)|0\rangle \neq 0 \). The new source term is chosen in such a way that we can study the positronium states \( ^2S_1 \) and \( ^1S_0 \) at the same time. Let us replace \( \int d^4 x f(x) \bar{\psi}(x)\psi(x) \) by

![Fig. 11.9. Diagrams appearing in the first term on the right-hand side of (11.3.4) up to the second order in \( e^2 \).](image-url)
\[\int d^4x \left( J(x) \bar{\phi}(x) \psi(x) + J_5(x) \bar{\phi}(x) \gamma^5 \psi(x) + J_\mu(x) \bar{\phi}(x) \gamma^\mu \psi(x) \right). \]  
(11.3.5)

Note that the \(^1S_0\) state couples to \(\bar{\phi}(x) \gamma^5 \psi(x)\) and \(^3S_1\) to \(\bar{\phi}(x) \gamma^\mu \psi(x)\). \(W[J]\) in (11.1.1) becomes \(W[J, J_5, J_\mu]\) and the Legendre transformation is defined as

\[\Gamma[\phi, \phi_5, \phi_\mu] = W[J, J_5, J_\mu] - \int d^4x \left( J(x) \phi(x) + J_5(x) \phi_5(x) + J_\mu(x) \phi_\mu(x) \right), \]  
(11.3.6)

\[\phi(x) = \frac{\delta W[J]}{\delta J(x)} , \quad \phi_5(x) = \frac{\delta W[J]}{\delta J_5(x)} , \quad \phi_\mu(x) = \frac{\delta W[J]}{\delta J_\mu(x)}. \]  
(11.3.7)

For notational convenience, we write \(J_i = (J(x), J_5(x), J_\mu(x))\) and \(\phi_i = (\phi(x), \phi_5(x), \phi_\mu(x))\) and use the notation \(i = 1, 5, \mu\) in the following. The Feynman rules are now slightly different from the one given in § 11.1. In any diagrams the propagator is \(G_{J_i}^{(0)}\) in the diagrams of \(\Gamma[\phi_i]\) or \(J_i[\phi_i]\) and is given as

\[iG_{\Gamma_{J_i}}(x, y) = iG_0^{-1}(x, y) + \left( J_3^{(0)}(x) + J_5^{(0)}(x) \gamma_5 + J_\mu^{(0)}(x) \gamma^\mu \right) \delta^4(x - y). \]  
(11.3.8)

To each large dot referring to the insertion of \(\bar{\phi}(x) \phi(x), \bar{\phi}(x) \gamma^5 \phi(x), \bar{\phi}(x) \gamma^\mu \psi(x)\), there is a factor \((i, i\gamma_5, i\gamma_\mu)\). With these redefinitions the theorems we have obtained hold.

The \(n\)-th functional derivative of \(\Gamma[\phi_i]\) with respect to \(\phi_i\) can be written down by the following theorems.

**Theorem 11.3**

\[\delta^n \Gamma[\phi_i]/\delta \phi_{i_1} \cdots \delta \phi_{i_n} (n \geq 1)\] consists of \(\delta^n \Gamma^{(0)}[\phi_i]/\delta \phi_{i_1} \cdots \delta \phi_{i_n}\) and all the connected tree diagrams constructed out of the \(k\)-vertex \(\nu_k\) \((k \geq 1)\), the inverse propagator \(A^{-1}\) and \(n\) external lines \((-A^{-1})\). Here \(\nu_k\) \((k \geq 1)\) and \(A^{-1}\) are defined by the obvious extension of (11.1.34) and (11.1.22), respectively, corresponding to the change of the source term: \(J \rightarrow J_i\).

**Theorem 11.4**

\[\delta^n \Gamma[\phi_i]/\delta \phi_{i_1} \cdots \delta \phi_{i_n} (n \geq 1)\] is given by the following equation,

\[\delta^n \Gamma[\phi_i]/\delta \phi_{i_1} \cdots \delta \phi_{i_n} = R_{\Gamma_i} \left( \delta^n \bar{\Gamma}[J_i^{(0)}] / \delta J_5^{(0)} \cdots \delta J_\mu^{(0)} \right) (-A^{-1}_{j_{i_1}}) \cdots (-A^{-1}_{j_{i_n}}) + \delta^n \Gamma^{(0)}[\phi_i]/\delta \phi_{i_1} \cdots \delta \phi_{i_n}, \]  
(11.3.9)

where the summation and the space-time integration are implied for repeated indices and for notational convenience we have introduced \(\bar{\Gamma}\) as

\[i\bar{\Gamma}[J_i^{(0)}] = i\Gamma[J_i^{(0)}] - \text{Tr} \ln G_{J_i^{(0)}}. \]  
(11.3.10)

We only give the outline of the proof of Theorems 11.3 and 11.4. Using the same argument given in (11.2.23), we can prove Theorem 11.3 by mathematical induction. In this case, the number of the differentiation is taken as the induction variable. Then the proof of Theorem 11.4 is automatically completed, because the proof of Theorem 11.4 is based on Theorem 11.3 and is equivalent to the proof of Theorem 11.2 from Theorem 11.1. According to Theorem 11.4, the second derivative of the effective action is
\[ \frac{\delta^2 i\bar{\Gamma}[\phi_1]}{\delta\phi_{1i}\delta\phi_{1s}} = R_2 \left( \frac{\delta^2 i\bar{\Gamma}[J_i(0)]}{\delta J_i(0)\delta J_i(0)} \right) \times \left( -\Delta_{-1}^{-1} \right)_{i,ij} \left( -\Delta_{-1}^{-1} \right)_{js} + \left( -\Delta_{-1}^{-1} \right)_{i,ts}. \] 

(11.3.11)

Let us introduce the notation \((\cdots)_0\) which implies \((\cdots)\) evaluated at the stationary solution \((\phi^{(0)})_i\) obtained by setting \(J_i=0\). Then the propagator \(G_{J_0}\) inside \((\cdots)_0\) becomes \(G_{J_0}\) where \(J_0=J_i(0)[(\phi^{(0)})_i]\). All the diagrams containing fermion loops with odd number of \(\gamma_\mu\) can be omitted. Matrix elements \((\delta^2 i\bar{\Gamma}/\delta\phi\delta\phi_\mu)_0\) and \((\delta^2 i\bar{\Gamma}/\delta\phi_5\delta\phi_\mu)_0\) have at least one fermion loop with an odd number of \(\gamma_\mu\), so that they vanish. The inverse propagator has the diagonal form

\[ (\Delta_{-1}^{-1})_0 = \begin{pmatrix} (\Delta_{-1}^{-1})_{11} & 0 & 0 \\ 0 & (\Delta_{-1}^{-1})_{5s} & 0 \\ 0 & 0 & (\Delta_{-1}^{-1})_{\mu\nu} \end{pmatrix}. \]

(11.3.12)

Thus we obtain the following two sets of equations for (2.1.5):

\[ \left( D_{4,1} E_{5,1} \right) (\Delta\phi_1) = 0, \]

(11.3.13)

\[ D_{5,1} D_{5,1} (\Delta\phi_5) = 0, \]

(11.3.14)

\[ D_{4,i} = (\Delta_{-1}^{-1})_{ii} + E_{4,i}, \quad (i=1, 5) \]

(11.3.15)

\[ E_{4,i} = (\Delta_{-1}^{-1})_{ii} R_2 \left( \frac{\delta^2 i\bar{\Gamma}[J_i(0)]}{\delta J_i(0)\delta J_i(0)} \right)_0 (\Delta_{-1}^{-1})_{ii}, \quad (i = 1, 5) \]

(11.3.16)

\[ \left( (\Delta_{-1}^{-1})_{\mu\nu} + (\Delta_{-1}^{-1})_{\mu\tau} R_2 \left( \frac{\delta^2 i\bar{\Gamma}[J_i(0)]}{\delta J_i(0)\delta J_i(0)} \right)_0 (\Delta_{-1}^{-1})_{\nu\tau} \right) \Delta\phi_\nu = 0. \]

This is the gauge invariant bound state equation in the channels defined by \(\phi_1\) \((i=1, 5, \mu)\). Note that Eq. (11.3.13) or (11.3.16) gives a gauge invariant answer to the energy eigenvalue of the excited states even if we approximate the kernel by expanding it in powers of \(e^2\); each term is independent of the gauge parameter \(\lambda\). This is in sharp contrast with the conventional Bethe-Salpeter equation where one uses as \(\Delta\phi\) a gauge non-invariant non-local operator such as \(\phi(x, y) = \langle \phi(x) \tilde{\phi}(y) \rangle\). The lowest order diagrams appearing in \(R_2 \left( \delta^2 i\bar{\Gamma}[J_i(0)]/\delta J_i(0)\delta J_i(0) \right)_0\) in (11.3.13) are given in Fig. 11.10. The Goldstone mode associated with the chiral symmetry breaking appears as a constant solution of (11.3.13) in the case \(\phi_1^{(0)} = \langle \tilde{\phi}\phi \rangle \neq 0\) and/or \(\phi_5^{(0)} = \langle \tilde{\phi}\gamma_5\phi \rangle \neq 0\). The solution of (11.3.13) and (11.3.16) gives the positronium states \(^1\!S_0\) and \(^3\!S_1\), respectively.

§ 11.4. Case of QCD

The chiral symmetry breaking in QCD when the quark mass is zero is an interesting subject. The results of the previous sections can be straightforwardly extended to QCD without any essential change. The Lagrangian of QCD is given in (4.1.1)
with the colour singlet source term $J(x)\bar{q}^A(x)q^A(x)$ added to it. One convinces oneself that the results presented in the form of Theorems 11.1 and 11.2 do not depend on the details of the interaction. Therefore we do not reproduce the discussions about QCD here. We merely remind the reader of the fact that we have already studied in § 7.4 the chiral symmetry breaking in QCD. There, some of the higher order graphs have been summed up by the technique of renormalization group.

§ 11.5. $\phi^4$ model

11.5.1. Local composite operator

The $\phi^4$ theory with $\phi(x)^2$ as an order parameter has been investigated in detail in Ref. 3. Here we discuss the problem along the line presented in the previous sections which is slightly different from the original treatment.\(^3\) (In Ref. 3, several other forms of the theorem are shown.)

As has been mentioned in § 11.2, the definition of $R_2$ has to be modified in order to apply Theorem 11.2 to other models. Let us take an Hermitian field $\phi$ and consider the effective action of the local composite operator $\phi(x)^2$ for $\phi^4$ theory. This will be sufficient to see how to generalize Theorem 11.2 to the bosonic case. Here a particular set of diagrams has an important role to write down the definition of $R_2$. In order to see it we return to the proof of Theorem 11.2 and investigate Fig. 11.8 again. In the bosonic case there is no arrow on the propagator and we cannot distinguish (a') and (b'). The operation $R_2$ produces twice as much as the required diagram. This problem can be avoided, for example, by a change of the definition of $R_2$ as follows: (c-5) appearing just below Theorem 11.2 has to be altered as:

\[(c-5')\] Sum up all the topologically different resulting graphs only once including the original graphs. Here the summation is taken for all the graphs on which $R_2$ operated.

With the above definition of $R_2$, new $R_2$ does not operate on each graph but on the total sum of the graphs (for example, $W[J^{(0)}]$). Then Theorem 11.2 agrees with Theorem 11.1. However, it is preferable if we can introduce $R_2$ for a small subset of $W[J^{(0)}]$. The precise meaning of the statement such as the subtraction of the "$\phi(x)^2$-reducible part" is clarified by the definition of the subset of diagrams. Let us call the subset of diagrams defined by (e-1)~(e-4) as a 2PR set.

(e-1) If there are 2PR parts in a graph, separate the graph into two pieces by cutting 2PR propagators.

(e-2) Connect two graphs. Notice that there are two ways to connect two graphs. One leading to the original graph and the other to the exchange graph.

(e-3) Carry out the same procedures (e-1), (e-2) for the resulting graph obtained in (e-2) until it produces no new graphs.

(e-4) Sum up all the topologically different resulting graphs only once.

For example, (a) and (b) in Fig. 11.8 (the loop (A-C-D-B) and (A-D-C-B)) and the loop
A-C-B-D make up one 2PR set. Then $R_2$ operates not on each graph but on a 2PR set as a whole and with this definition Theorem 11.2 holds for $\phi^4$ theory.

In $\phi^4$ case, we find cancellations of some graphs appearing in $\Gamma[\langle \phi(x)\phi(x) \rangle]$ which is obtained by a direct use of Theorem 11.1 or 11.2 modified for $\phi^4$ theory. In order to investigate the cancellation, let us introduce terminologies 1VR and 1VI which represent the character of graphs. The 1VR (1-vertex reducible) vertex is defined as a 4-point vertex in a connected 2PR diagram deletion of which results in a separation of the graph. The 1VI graph is the connected graph without any 1VR vertices while the 1VR graph is a graph in which at least one 1VR vertex is present. By definition, the term represented by

\[
\begin{array}{c}
\includegraphics[scale=0.5]{1VI_graph.png}
\end{array}
\]  

(11.5.1)

is 1VI because the graph is 2PI. For later convenience, we assume that the trivial skeleton (Trln term) is not 1VR or 1VI.

Then we find out that there is no 1VR graph in $\Gamma'$, which can be stated as a theorem:

**Theorem 11.5**

$$R_2(1\text{VR graph})=0.$$  \hspace{1cm} (11.5.2)

Examples of $R_2$ operation on some 1VR graphs are given as follows,

$$R_2\left(\begin{array}{c}
\includegraphics[scale=0.5]{1VR_graph1.png}
\end{array}\right) = \begin{array}{c}
\includegraphics[scale=0.5]{1VR_graph2.png} + \includegraphics[scale=0.5]{1VR_graph3.png} = 0,
\end{array}$$  \hspace{1cm} (11.5.3)

$$R_2\left(\begin{array}{c}
\includegraphics[scale=0.5]{1VR_graph4.png}
\end{array}\right) = \begin{array}{c}
\includegraphics[scale=0.5]{1VR_graph5.png} + \includegraphics[scale=0.5]{1VR_graph6.png} + \underbrace{\left(\includegraphics[scale=0.5]{1VR_graph7.png} + \includegraphics[scale=0.5]{1VR_graph8.png}\right)}_{\text{1VI graphs}}.
\end{array}$$  \hspace{1cm} (11.5.4)
Proof

If a graph A in Fig. 11.11 does not have any 1VR vertex, we call the part of the graph surrounded by the broken lines the 1VI piece. In a 1VR graph there are at least two 1VI pieces. Here the $R_2$ operation on the 1VI piece and other part of the graph can be done independently except for the symmetry factor. If there is no symmetry factor, the cancellation is simple. Suppose that 4-point vertex combined with A is a 1VI piece in the following equation,

$$R_2 (\text{B}\text{A}) = \text{B}\text{A} + \text{B}\text{A}$$

$$= 0 .$$  \hspace{1cm} (11.5.5)

Here the part of a graph surrounded by broken dotted lines means the summation of the result of $R_2$ operation on the part of the graph. In the second term on the right-hand side of (11.5.5) the denominator and the factor attached to the left of the 1VI piece is the same. Multiplication of these two terms gives delta function and the minus of the second term coincides with the first term on the right-hand side of (11.5.5). Thus theorem is justified in this case.

In general, we have to examine the symmetry factor related to the 1VI piece. Let us see (11.5.4) as an example. Using the definition $\sigma C_r = n!/(n-r)!r!$, the second term on the right-hand side of (11.5.4) is given by $(-\sigma C_4)$ times as much as the first term because of the fact that one of the four identical 1VI pieces is specified in the second term in contrast to the first term. By the same reason the sum of the third and fourth term which are in the parenthesis is $\sigma C_2$ times as much as the first term. By the same argument the contribution of the first six terms in (11.5.4) is given by

$$(1-\sigma C_1 + \sigma C_2 - \sigma C_3 - \sigma C_4) = 0 .$$

The 7-th term is also zero by the same cancellation mechanism which we have encountered for the first six terms.

Generally, in the case that $N$ identical 1VI pieces in a graph form $N$-fold symmetry, graphs generated by the $R_2$ operation on the original graph cancel out by the mechanism of the identity

$$(1-1)^N = 1 - \sigma N C_1 + \sigma N C_2 - \cdots + (-1)^{N} \sigma N C_N = 0 ,$$

which contains the information on how many 1VI pieces we have chosen. Since we have considered all the cases for the 1VR graph in terms of the 1VI piece, Theorem 11.5 holds for any case. So the proof of Theorem 11.5 is completed.
11.5.2. **Non-local composite operator**

We have already mentioned that the rule is known for the effective action of the non-local objects; \( I[\langle \phi(x_1) \rangle, \langle \phi(x_1)\phi(x_2) \rangle, \ldots, \langle \phi(x_1)\cdots\phi(x_N) \rangle] \) up to \( N=4 \). (The results are presented in Appendix C up to \( N=3 \).) These results are easily reproduced as the inversion series with the aid of similar cancellation mechanism we have shown in the previous section. In this case, the relation between order parameters \( \langle \phi(x) \rangle, \langle \phi(x)\phi(y) \rangle, \langle \phi(x)\phi(y)\phi(z) \rangle \) and their conjugate valuables \( J^{(0)}(x) \) \( J^{(0)}(x, y) \) \( J^{(0)}(x, y, z) \) is simple. That is why we can write down the effective action by order parameter itself, not by \( J^{(0)}[\phi] \). An example has been given in (11.1.41)~(11.1.44) for the case \( N=2 \). In general case, including the case of local composite operator, however, the relation is not so simple and the change of the order parameter from \( \phi \) to \( J^{(0)}[\phi] \) is essential to obtain the rule of the effective action.

§ 11.6. **Itinerant electron model**

In this section we give the rules of the higher order terms of the itinerant electron model discussed in Chapter X. The full order rules of the effective action for the itinerant electron model are first presented by Okumura. We will re-express it in terms of the statement used in this chapter. Let us first give the effective action up to the fourth order of the perturbative series using the notation of § 10.1,

\[
F = F^{(0)} + F^{(1)} + F^{(2)} + F^{(3)} + F^{(4)} + \cdots ,
\]

\[
F^{(0)} = \sum_x \frac{J^{(0)}(x)}{Z} \phi_x - \sum_{x, \sigma} \text{Tr} \ln [G_{\sigma}^{(0)}]^{-1},
\]

\[
F^{(1)} = U \sum_x \phi_x \phi_x = \frac{U}{2} \sum_{x, \sigma} \phi_x \phi_{x-\sigma} = \quad \text{Diagram 1},
\]

\[
F^{(2)} = \quad \text{Diagram 2},
\]

\[
F^{(3)} = \quad \text{Diagram 3},
\]

\[
F^{(4)} = \quad \text{Diagram 4} + \quad \text{Diagram 5} + \quad \text{Diagram 6} + \quad \text{Diagram 7} + \quad \text{Diagram 8} + \quad \text{Diagram 9} + \quad \text{Diagram 10} + \quad \text{Diagram 11} + \quad \text{Diagram 12}
\]

+ \left( \quad \text{Diagram 13} + \quad \text{Diagram 14} \right)

+ \left( \quad \text{Diagram 15} + \quad \text{Diagram 16} \right)

\]
Here the representation of the graph in this section is somewhat different from the one in Chapter X. The large dot in the above figures corresponds to the black dot in Chapter X. The four-point vertex is explicitly written as a small dot in contrast to the case of Chapter X. The rule of $\phi^4$ model and itinerant electron model is basically the same. The difference of the two models arises from the spin and the arrow.

**Theorem 11.6**

$F[\phi]$ consists of $F^{(0)}[\phi]$ given in (11.6.2) and all the connected tree diagrams constructed out of $k$-vertex $v_k$ ($k \geq 0$) defined in (11.6.7) below and the inverse propagator $\Delta_k^{-1}$. Similarly $J[\phi]$ is the sum of $J^{(0)}[\phi]$ given in (10.1.23) and the connected tree diagrams constructed with $k$-vertex $v_k$ ($k \geq 1$), the inverse propagator $\Delta_k^{-1}$ and also $\Delta_k^{-1}$ is attached to the external point.

Here $v_k[J^{(0)}]$ and $\Delta_k^{-1}$ are defined as follows,

$$ v_k[J^{(0)}](x_1, \sigma_1, x_2, \sigma_2, \ldots, x_k, \sigma_k) = \frac{\delta^k W[J^{(0)}[\phi]]}{\delta f_{x_1, \sigma_1}[\phi]\ldots\delta f_{x_k, \sigma_k}[\phi]} + \delta_{k,0} W^{(0)}[J^{(0)}[\phi]] $$

$$ - \delta_{k,1} \frac{\delta W^{(0)}[J^{(0)}[\phi]]}{\delta f_{x_1, \sigma_1}[\phi]} + \delta_{k,2} \frac{\delta^2 W^{(0)}[J^{(0)}[\phi]]}{\delta f_{x_1, \sigma_1}[\phi]\delta f_{x_2, \sigma_2}[\phi]}, $$

$$(\Delta_k^{-1})_{x_1, \sigma_1, x_2, \sigma_2} = -\left(\frac{\delta^2 W^{(0)}[J^{(0)}[\phi]]}{\delta f_{x_1, \sigma_1}[\phi]\delta f_{x_2, \sigma_2}[\phi]}\right)^{-1}.$$

Inverse propagator $\Delta_k^{-1}$ is a $2 \times 2$ matrix with respect to the spin degrees of freedom and it has no non-diagonal elements:

$$ \Delta_k^{-1} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} $$

(11.6.9)

where the first and second part of the row (and the column) correspond to the spin up state and down state, respectively.

**Theorem 11.7**

$$ F[\phi] = R_2(W[J^{(0)}[\phi]]) - \sum_{x, \sigma} J^{(0)}_{x, \sigma} \phi_{x, \sigma}, $$

(11.6.10)

$$ J_{x, \sigma}[\phi] = \sum_{x', \sigma'} (\Delta_k^{-1})_{x, \sigma; x', \sigma'} R_2\left(\frac{\delta(W[J^{(0)}[\phi]] - W^{(0)})}{\delta f_{x', \sigma'}[\phi]}\right) + J^{(0)}_{x, \sigma}, $$

(11.6.11)

where $R_2$ is the operation to yield diagrams required for $F[\phi]$ or $J_x[\phi]$. The definition of $R_2$ is summarized in (1)~(5) below:
(1) If there are 2PR parts with respect to two propagators, separate the graph into two pieces by cutting 2PR propagators.

(2) Join (with a factor $i$) the resulting two external propagators in each of the two graphs.

(3) Connect two joints of the two graphs by $A_k^{-1}$.

(4) Carry out the same procedures (1)~(3) for the resulting graph obtained in (3) until it produces no new graphs.

(5) Sum up all the resulting graphs including the original graph.

An example of $R_2$ operation on a graph in $W[J^{(0)}]$ is given as follows,

$$
R_2 \left( \begin{array}{c}
\text{graph 1} \\
\text{graph 2}
\end{array} \right) = \begin{array}{c}
\text{graph 1} \\
\text{graph 2}
\end{array} \begin{array}{c}
\text{graph 3} \\
\text{graph 4}
\end{array} \begin{array}{c}
\text{graph 5} \\
\text{graph 6}
\end{array}.
\right)
$$

(11.6.12)

Let us consider the cancellation problem: there is a cancellation mechanism after we have applied Theorem 11.6 or 11.7 as we have seen in § 11.5. For example, the following graph appears in $W[J]$:

$$
\begin{array}{c}
\text{graph 7}
\end{array}
$$

On the other hand, there is no such term in (11.6.4). According to Theorem 11.6, the second order terms appearing in the effective action are evaluated as

$$
F^{(2)}[\phi] = R_2 \left( \begin{array}{c}
\text{graph 1} \end{array} \right) + R_2 \left( \begin{array}{c}
\text{graph 2} \end{array} \right) + R_2 \left( \begin{array}{c}
\text{graph 3} \end{array} \right)
$$

(11.6.13)

The second and third term on the right-hand side of (11.6.13) vanish. Indeed

$$
R_2 \left( \begin{array}{c}
\text{graph 8}
\end{array} \right) = \begin{array}{c}
\text{graph 9} \\
\text{graph 10}
\end{array} \begin{array}{c}
\text{graph 11} \\
\text{graph 12}
\end{array} \begin{array}{c}
\text{graph 13} \\
\text{graph 14}
\end{array}.
$$

(11.6.14)

The first and second term on the right-hand side of (11.6.14) are equal except for the sign. The same is true for the third term on the right-hand side of (11.6.13). The above cancellation mechanism is similar to that given in § 11.5. Notice here that

$$
\begin{array}{c}
\text{graph 15}
\end{array}
$$

(11.6.15)

is a 1VI graph as in (11.5.1). In this way the following theorem holds:
THEOREM 11.8

\[ R_s(1VR\ graph) = 0. \quad (11.6.16) \]

§ 11.7. Ising model

The linked cluster expansion for the Ising model has been developed by many people.\(^{14}\) Their technique to sum up the graphs which we call renormalization is well established. However the rule of the effective action or the Helmholtz free energy has not been known up to now. In the conventional treatment, we investigate Gibbs free energy as a stationary point of some functional. One of the functionals, which previous workers defined, looks like the Helmholtz free energy but it is not the functional of magnetization \( m \) and is different from the object we are going to investigate below. We will discuss the relation between the effective action and the functional defined in the previous works later in this section.

The key to write down the rule is the change of the order parameter from magnetization \( m \) to its conjugate variable \( H^{(0)}[m] \) which is the lowest term of the perturbative inversion series of magnetic field \( H \). Physically \( H^{(0)}[m] \) is the lowest value of the internal magnetic field due to non-zero \( m \). Rules of the \( \Gamma[m] \) and \( H[m] \) are given as Theorems 11.9 ~ 11.11 below. From Theorem 11.11, we find that there is no one line reducible (1LR) graph in the effective action.

Let us introduce the Hamiltonian of the Ising model:

\[ -\beta \mathcal{H} = \sum_{ij} K_{ij} S_i S_j + \sum_i H_i S_i. \quad (11.7.1) \]

Here \( \beta = 1/k_B T \), \( K_{ij}/\beta \) is the exchange interaction between the nearest-neighbor sites \( i, j \), and \( H_i \) is the non-dimensional magnetic field which plays the role of a source. The spin \( S_i \) takes two values, \( S_i = \pm 1 \). Then the generating functional of the Green's function, \( W[H] \), which is related to Gibbs free energy \( G[H] \) as \( G[H] = -(1/\beta) W[H] \), is given as follows,

\[ W[H] = \ln \text{Tr} e^{-\beta \mathcal{H}}. \quad (11.7.2) \]

In order to study the phase transition, we perform the Legendre transformation:

\[ \Gamma[m] = W[H] - \sum_i H_i m_i, \quad (11.7.3) \]

\[ m_i = \frac{\partial W}{\partial H_i} = \langle S_i \rangle, \quad (11.7.4) \]

where \( m_i \) is the magnetization at the site \( i \) and the effective action \( \Gamma \) defined here is related to the Helmholtz free energy as \( F[m] = -\Gamma/\beta \).

In the linked-cluster expansion we regard \( K_{ij} \) as a small parameter and make a perturbative series in \( K_{ij} \) as

\[ W[H] = \ln \left\{ \exp \sum_{t,j} K_{t,j} \frac{\delta}{\delta H_t} \frac{\delta}{\delta H_j} \prod_k (2 \cosh H_k) \right\}. \quad (11.7.5) \]

Let us define \( M_{n,t} \) as
\[ M_{n,i} = \frac{d^n}{dH_i^n} \ln \prod_j (2 \cosh H_j) = \begin{cases} \sum_j \ln (2 \cosh H_j), & n = 0, \\ \frac{d^n}{dH_i^n} \ln (2 \cosh H_i), & n > 0. \end{cases} \] (11.7.6)

Then \( W[H] \) and \( m_i \) are given diagrammatically as follows,

\[ W[H] = \begin{array}{c}
\begin{array}{c}
0 \\
\frac{1}{2}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\frac{1}{2}
\end{array}
\begin{array}{c}
1 \\
1
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\frac{1}{2}
\end{array}
\begin{array}{c}
2 \\
2
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\frac{1}{4}
\end{array}
\begin{array}{c}
2 \\
2
\end{array}
\end{array} + O(K^3),
\] (11.7.7)

\[ m_i[H] = \begin{array}{c}
\begin{array}{c}
1 \\
i
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\frac{1}{2}
\end{array}
\begin{array}{c}
2 \\
i
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\frac{1}{2}
\end{array}
\begin{array}{c}
2 \\
i
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\frac{1}{2}
\end{array}
\begin{array}{c}
3 \\
i
\end{array}
\end{array} + O(K^3),
\] (11.7.8)

where a circle with a number \( n \) denotes \( M_{n,i} \) and a line \( K_{i,j} \). We call any circle as the vertex in the following. Symmetry factor is explicitly written for later convenience. Hereafter we employ the notation that the superscript \( (n) \) represents the order of the perturbation as in §11.1. In general, the number in the circle is the sum of the number of lines incident to that circle and the number of the differentiation with respect to \( H_i \). When we calculate \( m_i = \delta W/\delta H_i \), the contribution of the number of the differentiation to the number in a circle is at most one. If the number in a circle is larger than the number of lines incident to that circle, the circle corresponds to the external point.

Inverted series is now found as

\[ m_i = \begin{array}{c}
\begin{array}{c}
1
\end{array}
\end{array} \implies H_i^{(0)} = \tanh^{-1} m_i, \] (11.7.9)

\[ H_i = H_i^{(0)} - \frac{1}{2} \begin{array}{c}
\begin{array}{c}
2 \\
1
\end{array}
\end{array} - \frac{1}{2} \begin{array}{c}
\begin{array}{c}
2 \\
3 \\
2
\end{array}
\end{array} - \frac{1}{2} \left\{ \frac{1}{2} \begin{array}{c}
\begin{array}{c}
3 \\
2 \\
2
\end{array}
\end{array} + \frac{1}{3!} \begin{array}{c}
\begin{array}{c}
4 \\
3
\end{array}
\end{array} \right\} \]

\[ - \frac{1}{2} \left\{ \frac{1}{2} \begin{array}{c}
\begin{array}{c}
2 \\
3 \\
2
\end{array}
\end{array} + \frac{1}{2^2} \left( \begin{array}{c}
\begin{array}{c}
3 \\
4 \\
2 \\
2
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
3 \\
3
\end{array}
\end{array} - \frac{1}{2} \begin{array}{c}
\begin{array}{c}
3 \\
2
\end{array}
\end{array} \right) \right\} \]

\[ + \left( \frac{1}{2^3} \begin{array}{c}
\begin{array}{c}
5 \\
2
\end{array}
\end{array} + \frac{1}{2^2} \left( \begin{array}{c}
\begin{array}{c}
2 \\
1
\end{array}
\end{array} - \begin{array}{c}
\begin{array}{c}
3 \\
2
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
3 \\
2
\end{array}
\end{array} - \frac{1}{2} \begin{array}{c}
\begin{array}{c}
3 \\
2
\end{array}
\end{array} \right) \right) \]
Chapter XI. Higher Orders of Inversion Series

\[ + \frac{1}{2^2} \begin{array}{cc}
3 & 3 \\
3 & 3
\end{array} + \frac{1}{2} \begin{array}{cc}
2 & 4 \\
4 & 2
\end{array} + \frac{1}{4!} \begin{array}{cc}
5 & 4 \\
4 & 5
\end{array} \right) + O(K^6). \quad (11\cdot7\cdot10) \]

Here

\[ \frac{-1}{2} \]

represents \(-(M_2)^{-1}\) which we call the inverse vertex and it plays the same role as the inverse propagator \(\Delta_2^{-1}\) of \(\S\ 11.1\). On the right-hand side of the above equations we have dropped the subscript \(i\) because we can easily identify the external point. An inverse vertex has the same index with the vertices on both sides. To make things clear, we give an example:

\[ - \frac{1}{2^2} \begin{array}{cc}
3 & 3 \\
2 & 2
\end{array} \]

\[ = \frac{1}{2^2} \sum_{i,j} \frac{-1}{M_{a,i}} M_{b,i}(K_{i,j})^2 M_{b,j} \frac{-1}{M_{a,j}} M_{a,j}(K_{j,i})^2 M_{a,i}, \]

where the number in a circle is the sum of the number of lines incident to the circle and the number of inverse vertices attached to the circle. It is easy to check that the result given in \((7\cdot3\cdot21)\) is reproduced by Eqs. \((11\cdot7\cdot9)\) and \((11\cdot7\cdot10)\) if one imposes the translational invariance condition (i.e., independent of the index \(i\)).

By noting \(\delta \Gamma[m]/\delta m_i = -H_i\), the effective action \(\Gamma[m]\) is obtained by integrating \((11\cdot7\cdot9)\) and \((11\cdot7\cdot10)\),

\[ \Gamma^{(0)} = 0 - \sum_i H_i^{(0)} m_i, \quad (11\cdot7\cdot11) \]

\[ = \Gamma^{(0)} + \frac{1}{2} \begin{array}{cc}
1 & 1 \\
1 & 1
\end{array} + \frac{1}{4} \begin{array}{cc}
2 & 2 \\
2 & 2
\end{array} + \frac{1}{6} \begin{array}{cc}
2 & 2 \\
2 & 2
\end{array} + \frac{1}{3!} \begin{array}{cc}
3 & 3 \\
3 & 3
\end{array} + \frac{1}{8} \begin{array}{cc}
2 & 2 \\
2 & 2
\end{array} + \frac{1}{2^3} \left( \begin{array}{cc}
2 & 4 \\
4 & 2
\end{array} + \begin{array}{cc}
2 & 3 \\
3 & 2
\end{array} \right) \]

\[ + \frac{1}{2^2} \begin{array}{cc}
2 & 2 \\
2 & 2
\end{array} + \frac{1}{2^3} \left( \begin{array}{cc}
2 & 4 \\
4 & 2
\end{array} + \begin{array}{cc}
2 & 3 \\
3 & 2
\end{array} \right) + O(K^6) \quad (11\cdot7\cdot12) \]

Our diagrammatical rule differs from the existing works of linked cluster expansion, because they did not calculate the Helmholtz free energy itself. Let us have a look at what people have been doing. They define a functional \(\Phi[\tilde{M}_n]\) where \(\tilde{M}_{n,i}\) is a temporarily defined quantity: it is a magnetization \(m_i[H]\) but with the replacement
of the factor $M_{k,i}$ ($k=1 \sim \infty$) corresponding to the external point of each graph by $M_{k+n,i}$. Here $n$ is an arbitrary positive integer. The graph rule of $\Phi[\tilde{M}_i]$ is characterized by 1-vertex irreducible (1VI) graphs (which will be explained in the next paragraph). The relation between $W[H]$ and $\Phi[\tilde{M}_i]$ is given by

$$W[H] = \sum_i \tilde{M}_{0,i} + \Phi[\tilde{M}_i] - \sum_i \sum_{n=1}^\infty G_{n,i} \tilde{M}_{n,i}, \quad \text{(11 \cdot 7 \cdot 13)}$$

where the function $G_{n,i}$ plays the role of a generalized 1-body effective field.\(^*)\) The functional $\Phi[\tilde{M}_i]$ resembles the effective action $\Gamma[m]$ because $\tilde{M}_{1,i}$ is $m_i$ and $G_{1,i}$ is $H^{(1)}$. However there is no correspondence between $\tilde{M}_{n,i}$ (for $n \neq 1$) and $m_i$ or between $G_{n,i}$ and $H^{(n)}$. Thus to get a rule for $\Gamma[m]$ is another task.

In order to explain 1VI, we first define 1-vertex reducibility. If a graph is divided into some disconnected parts by removing a vertex from the graph, we call the vertex the 1-vertex reducible (1VR) part.\(^**)\) If a graph has at least one 1VR part, we call the graph a 1VR graph. Any 1VI graph is a graph that has no 1VR part. From (11 \cdot 7 \cdot 12), we find that there are some 1VR graphs in the Helmholtz free energy.

We will only give results of the inversion in Theorems 11.9 and 11.10 below. The proof is similar to the one given in § 11.2, see also Refs. 7) and 8).

**Theorem 11.9**

$\Gamma[m]$ consists of $\Gamma^{(0)}[m]$ given in (11 \cdot 7 \cdot 11) and all the connected tree diagrams constructed out of $k$-vertex $v_k$ ($k \geq 0$) defined in (11 \cdot 7 \cdot 14) below and the inverse vertex $-(M_2)^{-1}$.

Similarly $H[m]$ is the sum of $H^{(0)}[m]$ given in (11 \cdot 7 \cdot 9) and the connected tree diagrams constructed with $k$-vertex $v_k$ ($k \geq 1$), the inverse vertex $-(M_2)^{-1}$ and also $-(M_2)^{-1}$ is attached to the external point.

Here the definition of $v_k[H^{(0)}]$ is similar to (11 \cdot 1 \cdot 34),

$$v_k[H^{(0)}](i_1, i_2, \cdots, i_k) = \frac{\delta^k W[H^{(0)}][m]}{\delta H^{(0)}[m]_{i_1} \cdots \delta H^{(0)}[m]_{i_k}} - \delta_{k,0} W[H^{(0)}][m]$$

$$\quad - \delta_{k,1} \frac{\delta W[H^{(0)}][m]}{\delta H^{(0)}[m]_{i_1}} - \delta_{k,2} \frac{\delta^2 W[H^{(0)}][m]}{\delta H^{(0)}[m]_{i_1} \delta H^{(0)}[m]_{i_2}}. \quad \text{(11 \cdot 7 \cdot 14)}$$

From the definition (11 \cdot 7 \cdot 14), 0-vertex $v_0$ is given as $v_0 = W[H^{(0)}] - W^{(0)}[H^{(0)}]$. If we identify the inverse vertex $-(M_0)^{-1}$ with double line, examples of diagrams appearing in $\Gamma[m]$ and $H[m]$ are already found in Fig. 11.2.

**Theorem 11.10**

$$\Gamma[m] = R_1(W[H^{(0)}][m]) - \sum_i H_i[m], \quad \text{(11 \cdot 7 \cdot 15)}$$

$$H_i[m] = -(M_2)^{-1}_i R_2\left(\frac{\delta(W[H^{(0)}][m] - W^{(0)})}{\delta H^{(0)}_i[m]}\right) + H^{(0)}_i, \quad \text{(11 \cdot 7 \cdot 16)}$$

where $R_1$ is the operation to yield diagrams required for $\Gamma[m]$ or $H_i[m]$. The

\(^*)\) See for example Ref. 18).

\(^***)\) In linked cluster expansion 1VR part is called articulation point.
definition of \( R_i \) is summarized as in (1)~(5) below.

(1) If there are 1VR parts, separate the graph into two pieces by cutting away 1VR vertex. If there are several different ways to separate the graph into two pieces by cutting away a 1VR vertex, we should carry out the procedures (1) ~ (3) for each.

(2) Assign the appropriate external vertex \( M_k \) to each of the two resulting graphs. Here \( k \) of \( M_k \) is the sum of the number of incident lines and incident inverse vertices (i.e., flowing into the vertex in question) and one which is caused by the operation (1). For the graph of \( H_i[m] \), there is one external vertex corresponding to \( i \). We have to add one more for that vertex of course.

(3) Connect two graphs by an inverse vertex \(- (M_2)^{-1}\).

(4) Carry out the same procedures (1)~(3) for the resulting graph obtained in (3) until it produces no new graphs.

(5) Sum up all the resulting graphs including the original graph.

Examples of \( R_i \) operation on some typical graphs in \( W[H^{(0)}] \) and \( \delta (W[H^{(0)}] - W^{(0)}[H^{(0)}]) / \delta H_i^{(0)} \) are given as follows,

\[
R_1 \left( \frac{1}{2^3} \begin{array}{c}
2 \hline \\
4 \hline \\
2
\end{array} \right) = \frac{1}{2^3} \left( \begin{array}{c}
2 \hline \\
4 \hline \\
2 \\
\frac{-1}{2}
\end{array} \right) + \frac{1}{2^3} \left( \begin{array}{c}
3 \hline \\
2 \hline \\
2
\end{array} \right),
\]

(11.7.17)

\[
R_2 \left( \frac{1}{2^3} \begin{array}{c}
2 \hline \\
5 \hline \\
2
\end{array} \right) = \frac{1}{2^3} \left( \begin{array}{c}
2 \hline \\
5 \hline \\
2
\end{array} \right) + \frac{1}{2^3} \left( \begin{array}{c}
4 \hline \\
2 \hline \\
3 \\
\frac{-1}{2}
\end{array} \right) + \frac{1}{2^3} \left( \begin{array}{c}
3 \hline \\
2 \hline \\
3 \\
\frac{-1}{2}
\end{array} \right)
\]

(11.7.18)

An example of the procedures (1)~(3) is given in Fig. 11.12. In Fig. 11.13, the process (4) is demonstrated for the case of (11.7.18).

Now let us consider the cancellation problem: there seems to be still a cancellation mechanism after we have applied Theorem 11.9 or 11.10. For example, the following graph appears in \( W[H] \):

\[
\frac{1}{2} \begin{array}{c}
1 \hline \\
2 \hline \\
1
\end{array}.
\]

On the other hand, there is no such term in (11.7.12). According to Theorem 11.9 or 11.10, the second order terms appearing in the effective action are evaluated as

---

* In case the external vertex \( M_k \) which we have assigned in the process (2) is \( M_2 \) and in case there is no incident lines to the vertex, we regard that the way of cutting we have done in (1) is not appropriate because there is no \( M_2 \) in \( v_k \) \( (k = 2) \). The definition of \( R_i \) is given so as to satisfy the rule given in Theorem 11.9. We give an example in Fig. 11.13 (d) as one of such a case.
Fig. 11.12. An example of \( R_1 \) operation on 1VR graph (a). Each procedure (1), (2), and (3) acts on the graph (a), (b), (c) and it produces (b), (c) and (d), respectively.

Fig. 11.13. The illustration of the procedure (4) acting on the graph (a). The procedures (1) \( \sim \) (3) operating on the 1VR part indicated as a broken line. Notice that the graph (d) does not appear on the right-hand side of (11.6·8), because it contradicts with the footnote of rule (2).

Fig. 11.14. Illustration of 1LR graph. At least one of the graphs located on each side of the line, A or B, is not \( M_1 \).

\[
\Gamma^{(2)}[m] = \frac{1}{4} \begin{array}{ccc}
\end{array} + \frac{1}{2} \begin{array}{ccc}
\end{array} + \frac{1}{2} \begin{array}{ccc}
\end{array} + \frac{1}{2} \begin{array}{ccc}
\end{array} .
\]

(11·7·19)

The second and third term on the right-hand side of (11·7·19) cancel each other. The cancellation takes place for other graphs in \( \Gamma[m] \). In order to explain it, we introduce a new terminology: we call a line in a graph one line reducible (1LR) part if the graph is divided into two pieces when one eliminates the line in question from the graph and if at least one of the resulting two separated graphs is not \( M_1 \). We call a graph 1LR if the graph have 1LR part. The 1LR graph is illustrated in Fig. 11.14. 1LR graph is a graph that does not have 1LR part. There is one exception to this statement: we, for later convenience, do not include the graph

\[
\frac{1}{2} \begin{array}{ccc}
\end{array} .
\]

(11·7·20)

in 1LI graph.

**THEOREM 11.11**

\[
R_1(1LR \text{ graph}) = 0 .
\]

(11·7·21)

This rule is special to this model and to the source term \( \Sigma_i H_i S_i \). Owing to Theorems 11.10 and 11.11, there is no 1LR graph in \( \Gamma[m] \). The proof of Theorem 11.11 is similar to the one given in § 11.5.1. Notice that

\[
R_1(\frac{1}{2} \begin{array}{ccc}
\end{array} ) = \frac{1}{2} \begin{array}{ccc}
\end{array} .
\]

(11·7·22)

because of the definition of \( R_1 \). After we obtain the representation of \( \Gamma[m] \), we can perform a renormalization of
the vertex given, for example, by Bloch and Langer.\textsuperscript{16}) In this case we do not have to introduce a temporarily defined quantity $\bar{M}_{n,t}$. We have only to sum up the vertex as a function of $m$ using the technique of Bloch and Langer. The important point is that in spite of the fact that our aim is the free energy written by $m$ instead of $H$, we can still sum up the higher order terms by a similar technique as the one introduced for the free energy written by $H$. Summing up higher order terms requires exact rule for which our theorem will be helpful.

\section*{§ 11.8 Density functional theory}

In § 8.2, the density functional theory has been formulated in terms of the Legendre transformation. We can start from the generating functional $I[n]$ and apply the on-shell expansion scheme. The essential point is of course the inversion between the source $J(x)$ and the expectation value $n(x)$ of the density operator. Here the probe is introduced as in (8·2·2) which has the same structure as the probe given in (11·1·2) when we discussed QED. Therefore the full order rule of the inversion and also the rule to calculate $I[n]$ is similar as in § 11.1 with a slight modification due to the difference in the interaction vertex. We believe that it will not be necessary to reproduce the details here. When $J(x)$ is independent of $x$, it is the chemical potential and the rule in this case is for the inversion between the chemical potential and the number.

References

8) S. Yokojima, Doctoral thesis (Keio University, 1995).
12) M. Hondou, Master thesis, Keio Univ. 1995, see also Chapter X.
Chapter XII. Non-Equilibrium Generating Functional \(W[J_1, J_2]\) and \(\Gamma[\phi_1, \phi_2]\)

The purpose of this chapter is to apply the method of the Legendre transformation, or the generating functional to time-dependent non-equilibrium processes. In Chapter IX, we have already applied inversion method to non-equilibrium superconducting phenomenon but below we are going to discuss the subject both by more general terminology and by a model theory.

The central concern is the time evolution of the expectation value of small number of selected dynamical variables. These are of course the macrovariables, or the order parameters, which are observed in the experiments. The Legendre transformation is, as stated in the Introduction, one of the systematic and convenient ways of obtaining the equation of motion for these variables.

For this purpose we need the density operator \(\bar{\rho}(t)\) as a function of time assuming that its initial value \(\bar{\rho}_i\), whether it is a pure or a mixed state, is given at some time \(t = t_i\). In the usual experimental situation, \(\bar{\rho}_i\) is given by the equilibrium distribution specified by the Hamiltonian at \(t = t_i\) and after that the system is brought into the non-equilibrium state by changing the parameter in the Hamiltonian. Since all the time evolution is governed, strictly speaking, by the Hamiltonian, the above situation will exhaust any of the non-equilibrium processes. Our approach presented in this chapter is the formalism which takes into account such a situation and everything is calculated as a function of \(t_i\) and \(\bar{\rho}_i\).

After introducing the definitions of two generating functionals, together with their important properties, on-shell expansion of these functionals is studied. Next subject is the classical and macroscopic limit and then the model calculation is presented illustrating the use of inversion method for non-equilibrium processes. Finally the adiabatic inversion method is studied in a formal language. In the following discussions, except for §§ 12.5 and 12.6, we first formulate the theory by assuming that \(\bar{\rho}\) can be any distribution, equilibrium or non-equilibrium. In §§ 12.5 and 12.6, \(\bar{\rho}\) is restricted to be an equilibrium distribution.

§ 12.1. Definition of \(W[J_1, J_2]\) and \(\Gamma[\phi_1, \phi_2]\)

Let us now consider the system whose Hamiltonian operator is written as

\[
\bar{H} = \bar{H}_0 + g\bar{H}_i,
\]  

(12.1.1)

where \(\bar{H}_0\) is the free part and \(\bar{H}_i\) is the interaction part and the factor \(g\) is inserted to represent a coupling constant. Since we want to study dynamical non-equilibrium processes, a time-dependent external force \(J(t)\) is introduced which couples to some physical quantity \(\bar{O}\) of the system. This \(J(t)\) can be either a fictitious source to be set zero in the end or a non-vanishing actual external parameter. Thus the Hamiltonian of the system changes with time. It is expressed as

\[
\bar{H}(t) = \bar{H} - J(t)\bar{O}.
\]  

(12.1.2)
Then the expectation value \( \langle \tilde{O} \rangle_t \) is now given as follows,

\[
\langle \tilde{O} \rangle_t = \text{Tr} \{ \tilde{\rho} \tilde{K}_t \langle \tilde{O} \rangle_t \},
\]

\[
\tilde{K}_t = T \exp \left\{ -\frac{i}{\hbar} \int_{t_i}^t ds \tilde{H}(s) \right\},
\]

where \( \tilde{K}_t \) is the time evolution kernel and the symbol \( T \) implies the time ordering operator and \( \tilde{K}_t^* \) is the adjoint of \( \tilde{K}_t \). The matrix \( \tilde{\rho} \) is an arbitrary density operator of the initial time \( t_i \) which need not necessarily be an equilibrium distribution.

Our interest is to calculate \( \langle \tilde{O} \rangle_t \) to clarify its time dependence. For example, we want to know how the expectation value \( \langle \tilde{O} \rangle_t \) changes with time if the force \( J(t) \) is increased in strength from zero to some constant value \( J \). It is clear that \( \langle \tilde{O} \rangle_t \) depends not only on the final value \( J \) but also on the way how \( J(t) \) approaches \( J \).

Below we first keep the initial time \( t_i \) to be finite and follow the system for any finite positive time interval \( t - t_i \). The conventional approach takes \( t_i = -\infty \) since the discussion becomes simple in this case. This choice, however, is not suited for the discussion of the time evolution of the system if one wants to know the density operator \( \tilde{\rho}(t) \) at any instant of time under the condition that \( \tilde{\rho}(t) \) is given at \( t_i \).

We are also interested in the role of the interaction term \( \tilde{g} \tilde{H}_t \) which acts to distribute the energy supplied through \( J(t)\tilde{O} \) among all the degrees of freedom of the system. The energy redistribution is carried out after a sufficient elapse of time and the system will approach a new equilibrium. We are interested in the temperature, for example, of this final state.

To answer these questions of the dynamical phenomena of a macroscopic system, it is necessary to develop the field theoretical method to calculate various quantities for \textit{finite time interval}. In order to discuss the problem systematically, the method of generating functional and its Legendre transform is quite suitable. We can develop the perturbative formula, for example, for studying the expectation value of any physical observables of the system once the Hamiltonian of the system is given.

Let us recall here the use of equilibrium Gibbs free energy \( W[J] \) which is introduced as

\[
e^{-\beta W[J]} = \text{Tr} e^{-\beta (\tilde{H} - \tilde{J} \tilde{O})}.
\]

The response \( \phi \) is given by

\[
\phi = -\frac{\partial W[J]}{\partial J},
\]

which is the equilibrium expectation value of \( \tilde{O} \). Through the Legendre transformation, the corresponding Helmholtz free energy \( \Gamma[\phi] \) is written as

\[
\Gamma[\phi] = W[J] + J\phi,
\]

where \( J \) is expressed by \( \phi \) through inverting \( (12.1.6) \). The response \( \phi = \langle \tilde{O} \rangle_s \) is also obtained by solving the equation,

\[
\frac{\partial \Gamma[\phi]}{\partial \phi} = J.
\]
We try to extend these equilibrium generating functions to the non-equilibrium ones which determine the expectation values of the physical quantities in the dynamical processes. There are two types of the non-equilibrium generating functionals $W[J_1, J_2]$ and $\Gamma[\phi_1, \phi_2]$ which are the extensions of Gibbs' and Helmholtz's free energy (see § 7.1) in the equilibrium case respectively.

The precise definitions of $W[J_1, J_2]$ and $\Gamma[\phi_1, \phi_2]$ are given as follows. The generating functional $W[J_1, J_2]$ is first defined by introducing two kinds of real valued sources $J_i(t)$ and $J_i(t)$,

$$e^{(i\hbar)W[J_1, J_2]} = \text{Tr}\{\hat{\mathcal{R}}^t \hat{\rho}_i(\hat{\mathcal{R}}^t)^*\}, \quad (12.1.9)$$

$$\hat{\mathcal{R}}^t = \text{Exp}\left[-\frac{i}{\hbar} \int_{t_i}^{t_r} dt \{\hat{H} - J_i(t)\hat{O}\}\right]. \quad (i=1,2) \quad (12.1.10)$$

The final time $t_r$ here is taken to be sufficiently large satisfying $t_i < t < t_r$ where $t$ is the time we are looking at the system.

The double path formulation of non-equilibrium theory has a long history, starting from Schwinger's works. For an extensive investigation, see Refs. 5 and 7. Here we have in mind the application of inversion method to non-equilibrium processes so that the Feynman rule for these cases is inevitable. Apart from the formal discussions, we study below the diagrammatic expansion of non-equilibrium generating functional.

The essential feature of the non-equilibrium generating functional is the presence of two kinds of sources $J_i$ and $J_d$. The appearance of these two parameters is due to the fact that the density matrix $\hat{\rho}(t)$ develops in time on both sides as $\hat{\rho}(t) = \hat{K}_i \hat{\rho}_i \hat{K}_i^*$. Note also that, because of the cyclic character of $\text{Tr}$ operation, $W$ is identically zero if $J_1 = J_2$, which is the reason why we need two kinds of source. Since $J_1 \neq J_2$ in (12.1.9), the time evolution of $\hat{\rho}_i$ is not physical. So that $W[J_1, J_2]$ itself is not a physical quantity in contrast to the equilibrium Gibbs free energy $W[J]$ of (12.1.5) which is a physical one in the sense that it is the free energy of the system with Hamiltonian $\hat{H} - J\hat{O}$. In this sense it is important to note that there is no generating functional of equilibrium type for the non-equilibrium processes. However this does not invalidate the use of $W[J_1, J_2]$; the functional $W[J_1, J_d]$ does play the role of the generating functional, as is seen below.

Second non-equilibrium generating functional is defined by the double Legendre transformation,

$$\Gamma[\phi_1, \phi_2] = W[J_1, J_2] - \sum_{i=1}^{2} \int_{t_i}^{t_r} dt \ J_i(t) \frac{\delta W[J_1, J_2]}{\delta J_i(t)}, \quad (12.1.11)$$

$$\phi_i(t) = (-1)^{i+1} \frac{\delta W[J_1, J_2]}{\delta J_i(t)}, \quad (i=1,2) \quad (12.1.12)$$

where $t$ is the time and $\delta/\delta J_i(t)$ signifies the functional derivative. Then the physically observed expectation value of $\hat{O}(t)$ with $t > t_i$ is given by

$$\phi(t) = \langle \hat{O}(t) \rangle = \left. \frac{\delta W[J_1, J_2]}{\delta J_i(t)} \right|_{J_1 = J_2 = 0}$$
The equation of motion of \( \phi(t) \) is obtained as follows. We note here the inverted relation of (12·1·12),

\[
\frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_i(t)} = (-1)^i J_i(t), \quad (i = 1, 2)
\]  

(12·1·14)

which comes from the definitions (12·1·11) and (12·1·12). In (12·1·13) we have assumed that \( J_{1,2} \) are fictitious sources which are made to vanish at the end. In case a physical source coupled to \( \hat{O} \) is really present, the artificial source term \( J_i \) has to be set to a physical source \( J(t); J_1(t) = J_2(t) = J(t) \). If a real source \( J(t) \) is absent, we are considering the case where the non-equilibrium process is realized because the initial density matrix is not equal to the equilibrium distribution. Let us consider the latter case for simplicity. Then we are led to the equation of motion of \( \phi(t) \),

\[
\frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t)} = \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_2(t)} = 0.
\]  

(12·1·15)

The solution to (12·1·15) satisfies \( \phi_1(t) = \phi_2(t) = \phi(t) \) because of the symmetry under 1 \( \leftrightarrow \) 2. Therefore we can use another type of equation of motion,

\[
0 = \left. \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_i(t)} \right|_{\phi_1(t) = \phi_2(t) = \phi(t)}.
\]  

(12·1·16)

This has a similar form of the equation of motion for the coordinate variable \( q \) in classical analytical dynamics which is obtained by the stationary condition on the action functional \( I[q]; \delta I[q]/\delta q(t) = 0 \). Because of this analogy, \( \Gamma \) is also called the effective action here.

However we cannot express (12·1·16) by a stationary condition on some action functional \( F[\phi] \) of single argument \( \phi \) which satisfies

\[
\left. \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t)} \right|_{\phi_1 = \phi_2 = 0} = \frac{\delta F[\phi]}{\delta \phi(t)},
\]  

(12·1·17)

\[
\frac{\delta^2 F[\phi]}{\delta \phi(t) \delta \phi(s)} = \frac{\delta^2 F[\phi]}{\delta \phi(s) \delta \phi(t)}. \quad (12·1·18)
\]

Non-existence of \( F[\phi] \) is seen as follows\(^{50,6} \); we get from (12·1·17) and (12·1·18)

\[
\frac{\delta^2 F[\phi]}{\delta \phi(t) \delta \phi(s)} = \delta \left( \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_i(t)} \left|_{\phi_1 = \phi_2 = 0} \right. \right)
\]

\[
= \left[ \frac{\delta^2 \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t) \delta \phi_1(s)} + \frac{\delta^2 \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t) \delta \phi_2(s)} \right] \left|_{\phi_1 = \phi_2 = 0} \right.
\]

(12·1·19)

and \( \delta^2 F[\phi]/\delta \phi(s) \delta \phi(t) \) is obtained by exchanging \( t \leftrightarrow s \) in (12·1·19). However this result contradicts with (12·1·18) because in general

\[
\left. \frac{\delta^2 \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t) \delta \phi_2(s)} \right|_{\phi_1 = \phi_2 = 0} + \left. \frac{\delta^2 \Gamma[\phi_1, \phi_2]}{\delta \phi_1(s) \delta \phi_2(t)} \right|_{\phi_1 = \phi_2 = 0}.
\]  

(12·1·20)
Note that \([\delta^2 W/\delta J_i(t)\delta J_j(s)]\) is equal to \(\langle \bar{Q}(s)\bar{Q}(t)\rangle\) for \(J_i = 0\), which is not symmetric under the exchange \(t \leftrightarrow s\) since \(\langle \bar{Q}(t), \bar{Q}(s)\rangle \neq 0\) in general. Related to this property, \(\delta^2 \Gamma/\delta \phi_i(t)\delta \phi_j(s)\) is not symmetric under \(t \leftrightarrow s\). For example, if we have the friction term \(\eta \phi(t)\) in (12.1.16), the term \(\langle \delta/\delta \phi(s)(\eta \phi(t))\rangle = \eta (d/dt) \delta(t-s)\) is not symmetric under the exchange \(t \leftrightarrow s\). Therefore there is no generating functional \(F[\phi]\) which has single variable as its argument for the non-equilibrium statistical mechanics. Only for the equilibrium case does the generating functional exist.

We remind here the relation between the equation of motion and its solution for the case of non-vanishing physical source, \(J_1 = J_2 = 0\). \(\phi(t)\) given in (12.1.13) is the solution of (12.1.16). If we set \(J_1 = J_2 = J\), they become

\[
\phi(t) = \frac{\delta W[J_1, J_2]}{\delta J_1(t)} \bigg|_{J_1 = J_2 = J}, \tag{12.1.21}
\]

\[
-J(t) = \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_i(t)} \bigg|_{\phi_1 = \phi_2 = \phi}, \tag{12.1.22}
\]

which are the solution and the equation of motion under the presence of the physical source \(J(t)\) respectively. We get (12.1.22) by solving (12.1.21) with respect to \(J(t)\), i.e., inversion of (12.1.21). Equation (12.1.22) clearly shows that \(J(t)\) acts as a force conjugate to \(\phi(t)\).

The information on the initial conditions has to be retained in the inversion process but we can alternatively drop it by adding separately the initial conditions

\[
\phi(t_i) = \text{Tr} \bar{\rho}_i \bar{\Omega}, \quad \phi(t_i) = \text{Tr} \bar{\rho}_i \bar{\Omega}, \quad \text{etc.,} \tag{12.1.23}
\]

to (12.1.16) or (12.1.22). Note that in general the equation of motion (12.1.16) itself depends on the initial state \(\bar{\rho}_i\), the temperature \(T\) of the initial state for example. The usual Newton's classical equation of motion, on the other hand, is the microscopic equation of motion and does not depend on the initial state and all the information of the initial state is supplied through the initial conditions.

\section{12.2. Relations involving \(W[J_1, J_2]\) and \(\Gamma[\phi_1, \phi_2]\)\)

\subsection{12.2.1. Identities of second derivative}

We note two important identities which hold for the second derivative of \(W\) or \(\Gamma\),

\[
\sum_{i,j=1}^n \int_{t_i}^{t_{i+1}} ds \frac{\delta^2 \Gamma}{\delta \phi_i(t) \delta \phi_j(s)} (-1)^{i+j+1} \frac{\delta^2 W}{\delta J_i(s) \delta J_j(t')} = \delta_{ij} \delta(t-t'), \tag{12.2.1}
\]

\[
\sum_{i,j=1}^n \left( \frac{\delta^2 W}{\delta J_i(t) \delta J_i(t')} \right)_{J_1 = J_2} = 0. \tag{12.2.2}
\]

The first identity is obtained by differentiating (12.1.14) by \(\phi_i(t')\). The second one is a consequence of the definition of \(W[J_1, J_2]\) given in (12.1.9). In order to see this, let us take the derivative of (12.1.12) keeping in mind the form (12.1.9),

\[
\frac{\delta^2 W}{\delta J_i(t) \delta J_i(t')} = \frac{i}{\hbar} \langle \bar{\Omega}(t) \bar{\Omega}(t') \rangle, \quad \frac{\delta^2 W}{\delta J_i(t) \delta J_j(t')} = -\frac{i}{\hbar} \langle \bar{\Omega}(t') \bar{\Omega}(t) \rangle, \tag{12.2.3}
\]
\[
\frac{\delta^2 W}{\delta j_1(t) \delta j_1(t')} = -\frac{i}{\hbar} \langle \hat{O}(t) \hat{O}(t') \rangle, \quad \frac{\delta^2 W}{\delta j_2(t) \delta j_2(t')} = \frac{i}{\hbar} \langle \hat{T} \hat{O}(t) \hat{O}(t') \rangle. \tag{12.2.4}
\]

Here, after the differentiation \(J_1=J_2\) is assumed and \(\hat{T}\) denotes the anti-time ordering and \(\hat{O}(t)\) is the Heisenberg operator defined by

\[
\hat{O}(t) = \hat{K}_t \hat{O} \hat{K}_t,
\]

where \(\hat{K}_t\) is given in (12.1.4) and the expectation value is defined by \(\langle \cdots \rangle = \text{Tr} \rho_1 \cdots\). Because the sum of the above four equations is identically zero owing to the definition of \(T\) and \(\hat{T}\), Eq. (12.2.2) follows.

The same relation as (12.2.2) holds for \(\Gamma\) also. This can be seen as follows. We rewrite (12.1.14) as

\[
\left( \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t)} \right)_{\phi_1(t) = \phi_2(t) = \phi(t)} + \left( \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_2(t)} \right)_{\phi_1(t) = \phi_2(t) = \phi(t)} = 0. \tag{12.2.5}
\]

Let us differentiate (12.2.5) by \(\phi(t')\) then

\[
\sum_{i,j=1,2} \left( \frac{\delta^2 \Gamma}{\delta \phi_i(t) \delta \phi_j(t')} \right)_{\phi_i = \phi_j} = 0. \tag{12.2.6}
\]

12.2.2. Expansion of \(W\) or \(\Gamma\) in powers of \(J^{-}\) or \(\phi^{-}\)

We first define \(W[J_1, J_2, J_3]\) by introducing another source \(J_3\) in the imaginary time path,

\[
e^{i\hbar W[J_1, J_2, J_3]} = \text{Tr} \{ \hat{K}^{J_1} \hat{\rho}_{J_3}(\hat{K}^{J_3})^* \}, \tag{12.2.7}
\]

\[
\hat{\rho}_{J_3} = \text{Tr}_\tau \exp \left[ -\frac{1}{\hbar} \int_0^\hbar d\tau \{ \hat{H} - J_3(\tau) \hat{O} \} \right], \tag{12.2.8}
\]

where \(\text{Tr}_\tau\) implies the \(\tau\)-ordering. The corresponding \(\Gamma\) is also defined as follows,

\[
\Gamma[\phi_1, \phi_2, \phi_3] = W[J_1, J_2, J_3] - \int_{t_1}^\infty dt_1 f_1(t_1) \phi_1(t_1) - \int_{t_1}^\infty dt_2 f_2(t_2) \phi_2(t_2) - \frac{1}{i} \int_0^\hbar d\tau J_3(\tau) \phi_3(\tau). \tag{12.2.9}
\]

Here we have introduced

\[
\frac{\delta W}{\delta f_i(t)} = (-)^{i+1} \phi_i, \quad (i = 1, 2), \quad \frac{\delta W}{\delta f_3(\tau)} = \frac{1}{i} \phi_3(\tau). \tag{12.2.10}
\]

The following change of variables is performed at this point:

\[
J^{(+)} = \frac{1}{2} (J_1 + J_2), \quad J^{(-)} = J_1 - J_2 \tag{12.2.11}
\]

or equivalently

\[
J_1 = J^{(+)} + \frac{1}{2} J^{(-)}, \quad J_2 = J^{(+)} - \frac{1}{2} J^{(-)}. \tag{12.2.12}
\]

We have the same relations for \(\phi^{(+)}\) and \(\phi^{(-)}\). In the following we consider
$W[J^{(+)}], J^{(-)}, J_3]$ and $\Gamma[\phi^{(+)}, \phi^{(-)}, \phi_3]$. It is easy to get the following relations,

$$\frac{\delta W}{\delta J^{(-)}(t)} = \phi^{(+)}(t), \quad \frac{\delta W}{\delta J^{(+)}(t)} = \phi^{(-)}(t),$$

$$J_1 \phi_1 - J_2 \phi_2 = J^{(+)} \phi^{(-)} + J^{(-)} \phi^{(+)}.$$  \hspace{1cm} (12.2.13)

Thus we can write

$$\Gamma[\phi^{(+)}, \phi^{(-)}, \phi_3] = W - \int_{t_1}^{t_2} dt J^{(+)}(t) \frac{\delta W}{\delta J^{(+)}(t)}$$

$$- \int_{t_1}^{t_2} dt J^{(-)}(t) \frac{\delta W}{\delta J^{(-)}(t)} - \int_0^{t_2} d\tau J_3(\tau) \frac{\delta W}{\delta J_3(\tau)}.$$

Now we expand $W$ or $\Gamma$ in powers of $J^{(-)}$ or $\phi^{(-)}$. Since these variables are unphysical ones being set to be zero in the end, we need expansion coefficient which is linear in $J^{(-)}$ or $\phi^{(-)}$ in practical problems. Then the following relation is easily obtained,

$$W[J^{(+)}], J^{(-)}=0, J_3] = W_\delta[J_3].$$ \hspace{1cm} (12.2.14)

Here $W_\delta[J_3]$ is related to the imaginary time free energy as

$$W_\delta[J_3] = \frac{\hbar}{i} \ln \text{Tr} \rho J^t.$$

But together with (12.2.14), the second equation of (12.2.13) tells us that

$$\phi^{(-)} \to 0 \quad \text{as} \quad J^{(-)} \to 0.$$  \hspace{1cm} (12.2.15)

On the other hand the identity of the Legendre transformation

$$\frac{\delta \Gamma}{\delta \phi^{(+)}(t)} = -J^{(-)}(t)$$

implies that in this limit $\Gamma$ loses the dependence on $\phi^{(+)}$. Thus in the limit $J^{(-)} \to 0$, we have a second imaginary time free energy,

$$\Gamma[\phi^{(+)}, \phi^{(-)}=0, \phi_3] = W_\delta[J_3] - \int_0^{t_2} d\tau J_3(\tau) \frac{\delta W_\delta[J_3]}{\delta J_3(\tau)} = \Gamma_\delta[\phi_3].$$ \hspace{1cm} (12.2.16)

Consider next the linear term in $J^{(-)}$ or $\phi^{(-)}$. By definition

$$\frac{\delta W}{\delta J^{(-)}(t)} \bigg|_{J^{(-)}=0} = \phi^{(+)}(t) \bigg|_{J^{(-)}=0}, \quad \frac{\delta \Gamma}{\delta \phi^{(-)}(t)} \bigg|_{\phi^{(-)}=0} = -J^{(+)}(t) \bigg|_{\phi^{(-)}=0},$$

so that the following dual forms are obtained,

$$W[J^{(+)}], J^{(-)}, J_3] = W_\delta[J_3] + \int_{t_1}^{t_2} dt J^{(-)}(t) \phi^{(+)}(t) + O[J^{(-)}]^2, \hspace{1cm} (12.2.16)$$

$$\Gamma[\phi^{(+)}, \phi^{(-)}, \phi_3] = \Gamma_\delta[\phi_3] - \int_{t_1}^{t_2} dt \phi^{(+)}(t) J^{(+)}(t) + O[\phi^{(-)}]^2, \hspace{1cm} (12.2.17)$$

where on the right-hand side of these equations, $\phi^{(+)}(t)$ or $J^{(+)}(t)$ is actually
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\[
\phi^{(+)}(t) = \phi^{(+)}(J^{(-)} = 0, J^{(+)}; t), \quad J^{(+)}(t) = J^{(+)}(\phi^{(-)} = 0, \phi^{(+)}; \phi_5; t). \quad (12.2.18)
\]

It can be shown that the expansion coefficients of higher orders are expressed by the multiple retarded anti-commutators of the operator \( \hat{\mathcal{O}} \). On the other hand the Tailor expansion in terms of \( \phi^{(+)} \) brings about the multiple retarded commutator which has a real physical meaning and will be reproduced in the next subsection.

We have seen that in the limit when \( J^{(-)} \) or \( \phi^{(-)} \) goes to zero the imaginary time free energy is reproduced. But another important limit exists where the equilibrium free energy is recovered. This is the case when

\[
\phi_1(t) = \phi_2(t) = \phi_3(t) = \text{const}, \quad \text{i.e.,} \quad \phi^{(+)}(t) = \phi_3(t) \equiv \phi = \text{const}, \quad \phi^{(-)}(t) = 0.
\]

Obviously the above case is transformed to \( J \) variables as follows,

\[
J_1(t) = J_2(t) = J_3(t) = \text{const}', \quad \text{i.e.,} \quad J^{(+)}(t) = J_3(t) \equiv J = \text{const}', \quad J^{(-)}(t) = 0.
\]

Thus we get

\[
J^{(+)}(\phi^{(-)} = 0, \phi^{(+)} = \phi_3 \equiv \phi) = J_3(\phi^{(-)} = 0, \phi^{(+)} = \phi_3 \equiv \phi) = \frac{\delta \Gamma_3[\phi]}{\delta \phi}. \quad (12.2.19)
\]

In this way we arrive at

\[
\frac{\delta \Gamma}{\delta \phi^{(-)}(t)} \bigg|_{\phi^{(-)} = 0, \phi^{(+)} = \phi_3 \equiv \phi} = \frac{\delta \Gamma_3[\phi]}{\delta \phi}. \quad (12.2.20)
\]

Corresponding obvious equation for \( W \) is

\[
\frac{\delta W}{\delta f^{(-)}(t)} \bigg|_{J^{(-)} = 0, J^{(+)} = J_3} = \frac{\delta W_3}{\delta f}. \quad (12.2.21)
\]

In the next section we discuss the on-shell expansion of \( \Gamma \) which is the expansion of \((\delta \Gamma/\delta \phi^{(-)}(t))|_{\phi^{(-)} = 0}\) in powers of \( \phi^{(+)} \). We will see that multiple retarded commutator emerges and the expansion relates two different density matrixes corresponding, for example, to the condensed or un-condensed ground state.

\[\S\text{ 12.3. On-shell expansion of } \Gamma[\phi_1, \phi_2]\]

On-shell expansion is a technique for extracting physical quantities from the generating functional \( \Gamma[\phi_1, \phi_2] \). The purpose of the present section is to apply the same technique as used in Chapter II for the zero temperature effective action \( \Gamma[\phi] \) to the non-equilibrium generating functional \( \Gamma[\phi_1, \phi_2] \). By applying on-shell expansion to \( \Gamma[\phi_1, \phi_2] \), we will see the following: starting from one particular (for example the uncondensed) density matrix, on-shell expansion leads to, when all the expansion terms are summed up, another density matrix corresponding to a possible equilibrium density matrix different from the starting one. The new density matrix is obtained by the unitary transformation which has the form of multiplying the coherent state to the old density matrix. This is the analog of the coherent state appeared in the on-shell expansion of \( \Gamma[\phi] \) in zero temperature case as we have seen in Chapter II.

We concentrate below on the real time generating functional \( \Gamma[\phi_1, \phi_2] \). The
relation between the real and imaginary time on-shell equation will be discussed in § 12.3.3.

12.3.1. Case of Hermite field

Consider a field theoretical system described by the Hermitian scalar field $\phi(x)$. We have in mind the phonon field, photon field or the Yukawa meson (Klein-Gordon) field, etc. Let us introduce the canonically conjugate momentum field $\Pi(x)$ satisfying $[\Pi(x), \phi(y)] = (i/\hbar)\delta^3(x-y)$. Then the standard Hamiltonian has the structure

$$\hat{H} = \int d^4x \left\{ \frac{1}{2} \Pi(x)^2 + \frac{1}{2} \phi(x)\omega(-\nabla)\phi(x) + H_I[\phi] \right\}. \quad (12\cdot3\cdot1)$$

Here $\omega(-\nabla)$ is the bare dispersion relation of the field $\phi$ and $H_I$ represents the unharmonic interaction term. The corresponding Lagrangian or the action functional $I[\phi]$ is given as ($\partial_t = \partial/\partial t$),

$$\tilde{I}[\phi] = \int d^4x \left\{ \frac{1}{2} (\partial_t\phi(x))^2 - \frac{1}{2} \phi(x)\omega(-\nabla)\phi(x) - H_I[\phi] \right\}. \quad (12\cdot3\cdot2)$$

In the Heisenberg representation, the following relations hold:

$$[\Pi(t, x), \phi(t', x') = \frac{1}{i} \delta^3(x-y). \quad (12\cdot3\cdot3)$$

Now take the operator $\tilde{\phi}(x)$ as $\tilde{O}$. Then we are going to study the expectation value,

$$\langle \tilde{\phi}(x) \rangle_t = Tr \rho_t U(t, t_t) \phi(x) U(t, t_t) \cdot \quad (12\cdot3\cdot4)$$

The solution to (12·1·15) always satisfies the relation $\phi_1(x) = \phi_2(x)$ which is written as $\phi^{(0)}(x)$. Then (12·1·15) takes the form

$$\left( \frac{\delta I[\phi_1, \phi_2]}{\delta \phi^{(0)}_1(x)} \right)_{\phi_1 = \phi_2 = \phi^{(0)}} = 0. \quad (12\cdot3\cdot5)$$

Let us perform our on-shell expansion. For this purpose we expand $I[\phi_1, \phi_2]$ around $\phi^{(0)}$ writing $\phi_1(x) = \phi_2(x) = \phi^{(0)}(x) + \Delta \phi(x)$,

$$0 = \left( \frac{\delta I[\phi_1, \phi_2]}{\delta \phi^{(0)}_1(x)} \right)_{\phi_1 = \phi_2 = \phi^{(0)}} + \sum_{i=1,2} \int_{t_1}^{t} d^4y \left( \frac{\delta^2 I}{\delta \phi^{(0)}_i(x) \delta \phi^{(0)}(y)} \right)_{\phi^{(0)}} \Delta \phi(y)$$

$$+ \frac{1}{2!} \sum_{i_1, i_2} \int_{t_1}^{t} d^4y_1 d^4y_2 \left( \frac{\delta^3 I}{\delta \phi^{(0)}_i(x_1) \delta \phi^{(0)}_i(y_1) \delta \phi^{(0)}_i(y_2)} \right)_{\phi^{(0)}} \Delta \phi(y_1) \Delta \phi(y_2) + \cdots. \quad (12\cdot3\cdot6)$$

We further expand $\Delta \phi$ as

$$\Delta \phi(x) = \Delta \phi^{(1)}(x) + \Delta \phi^{(2)}(x) + \Delta \phi^{(3)}(x) + \cdots, \quad (12\cdot3\cdot7)$$

assuming that $\Delta \phi^{(n)}$ is of the order $(\Delta \phi^{(1)})^n$. Then we get our on-shell expansion by requiring that (12·3·6) holds in each power of $\Delta \phi^{(1)}$. The zero-th order vanishes because of (12·3·5) and for the first order we get the mode determining equation,
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\[ 0 = \int_{-\infty}^{\infty} d^4 y \left( \Gamma^{(0)}_{11}(x, y) + \Gamma^{(0)}_{12}(x, y) \right) \delta \phi^{(1)}(y), \] (12.3.8)

\[ \Gamma^{(0)}_{ij}(x, y) = \frac{\delta^2 \Gamma}{\delta \phi_i(x) \delta \phi_j(y)}. \]

Here and in what follows we take $t_i \to -\infty$ for simplicity. Equation (12.3.8) is the
generalization of the mode determining equation of the small oscillation (2.1.5). (In
(2.1.5), the suffixes $i, j$ are for the components of $\phi$ field whereas here they distinguish
the time paths.)

Now the following identities are noted, which are functional analog of (12.2.1) and
(12.2.2),

\[ \sum_{i_1} \int d^4 y \Gamma^{(2)}_{111}(x, y)(-1)^{i_2 + i_4 + 1} W^{(2)}_{111}(y, z) = \delta_{i_1, i_4} \delta^4(x - z), \] (12.3.9)

\[ \sum_{i_1, i_2} (W^{(2)}_{ij}(x, y))_{j_1 = j_2} = 0, \] (12.3.10)

\[ W^{(2)}_{ij}(x, y) = \frac{\delta^2 W}{\delta f_i(x) \delta f_j(y)}. \] (12.3.11)

By using these relations we can derive

\[ -\delta^4(x - z) = \int d^4 y \left( \Gamma^{(2)}_{11}(x, y) + \Gamma^{(2)}_{12}(x, y) \right) \left( W^{(2)}_{11}(y, z) + W^{(2)}_{12}(y, z) \right)_{j_1 = j_2 = i}. \] (12.3.12)

Indeed this relation follows by choosing $i_1 = i_3 = 1$ in (12.3.9) and by the repeated use of (12.3.10). However $W^{(2)}_{11} + W^{(2)}_{12}$ is the retarded Green's function,

\[ (W^{(2)}_{11}(y, z) + W^{(2)}_{12}(y, z))_{j_1 = j_2 = i} = \langle W^{(2)}_{x}(y, z) \rangle_{i} = \frac{i}{\hbar} \theta(\tau - z) \langle \phi(y), \phi(z) \rangle_{i}, \] (12.3.13)

where we have defined $\langle \cdots \rangle = \text{Tr} \rho_i(\cdots)$. Therefore the relation $(\Gamma^{(2)}_{11} + \Gamma^{(2)}_{12})_o = -(W^{(2)}_{x})_{j_1 = i}$ implies that Eq. (12.3.8) determines the pole of $W^{(2)}_{x}$. For constant $\phi^{(0)}$, $(W^{(2)}_{x}(x, y))_o$ is a function of $x - y$, therefore in Fourier space (12.3.8) takes the form

\[ (\Gamma^{(2)}_{11}(\omega, p) + \Gamma^{(2)}_{12}(\omega, p))_o \Delta \phi^{(1)}(\omega, p) = 0. \] (12.3.14)

The dispersion relation $\omega = \omega(p)$ can be fixed by requiring that we have non-vanishing
$\Delta \phi^{(1)}$ and in this case $\Delta \phi^{(1)}$ has the support on the shell defined by $\omega = \omega(p)$ in
four-dimensional space of $p = (\omega, p)$. This is the reason why we call (12.3.8) the
on-shell equation and our scheme the on-shell expansion. Because the Hamiltonian
or the action given in (12.3.2) is symmetric under $\omega \leftrightarrow -\omega$, $\Gamma^{(2)}(\omega, p)$ is a function of
$\omega^2$. Therefore we can write in the vicinity of the shell

\[ (\Gamma^{(2)}_{11}(\omega, p) + \Gamma^{(2)}_{12}(\omega, p))_o = Z^{-1}(\omega^2 - \omega^2(p)), \] (12.3.15)

where $Z$ is the wave function renormalization factor, i.e. the inverse of the residue of
the pole of $W^{(2)}_{x}$, of the corresponding mode. In $x$-space, by using the notation $px$
\[ \begin{align*}
= \omega t - p \cdot x, \\
\langle \Gamma^{(3)}_{11}(x-y) + \Gamma^{(3)}_{12}(x-y) \rangle_0 &= \frac{1}{(2\pi)^4} \int d^4p \exp(-ip(x-y)) \langle \Gamma^{(3)}_{11}(\omega, p) + \Gamma^{(3)}_{12}(\omega, p) \rangle_0 \\
&= -Z^{-1}(\partial^2 + \omega^2(-\nabla_x)) \delta^4(x-y) \\
&= -Z^{-1}f(\partial_x) \delta^4(x-y). 
\end{align*} \]
(12.3.16)

Here, as indicated, the differentiation applies to the coordinate \(x\) and \(\delta^4(x-y)\) is the four-dimensional Dirac \(\delta\)-function. There are two independent solutions to (12.3.14), each having an undetermined constant \(C^{(\pm)}\):

\[ \Delta \phi^{(1)}(\omega, p) = C(p) \delta(\omega^2 - \omega^2(p)) \]
\[ = \frac{C(\omega = \omega(p), \pm p)}{2\omega(p)} \delta(\omega - \omega(p)) + \frac{C(\omega = -\omega(p), \pm p)}{2\omega(p)} \delta(\omega + \omega(p)). \]
(12.3.17)

Let us define

\[ C^{(\pm)}(p) = \frac{C(\omega = \pm \omega(p), \pm p)}{(2\pi)^4 \sqrt{2\omega(p)}}. \]
(12.3.18)

Then, in the coordinate space we have

\[ \Delta \phi^{(1)}(x) = \frac{1}{(2\pi)^4} \int d^4p \exp(-ipx) \Delta \phi^{(1)}(\omega, p) \]
\[ = \int \frac{d^3p}{\sqrt{2\omega(p)}} \left[ C^{(+)}(p) \exp(-ip^{(0)}x) + C^{(-)}(p) \exp(ip^{(0)}x) \right]. \]
(12.3.19)

where \(\omega(p) = \omega(-p)\) is assumed and \(p^{(0)}x = \omega(p)t - p \cdot x\). We will see below that \(\Delta \phi^{(1)}(x)\) is the wave function (plane wave) of the excited mode. This is shown by deriving another form of \(\Delta \phi^{(1)}(x)\) using the technique of formula due to LSZ. (12.3.9)

(Here \(\Delta \phi^{(1)}(x)\) is a simple plane wave since we have taken \(\delta(x)\) as \(\delta\). If the composite operator \(\hat{\delta}(x)\delta(y)\), for example, is adopted then \(\Delta \phi^{(1)}(x)\) has the dependence on the internal coordinate besides \(\exp(ip^{(0)}x)\)).

For the second or higher orders the required relations are

\[ \sum_{i=1,2} \int d^4y \langle \Gamma^{(3)}_{11}(x,y) \rangle_0 \Delta \phi^{(2)}(y) \]
\[ + \frac{1}{2!} \sum_{i=3,4} \int d^4y_1 d^4y_2 \langle \Gamma^{(3)}_{11}(x,y_1,y_2) \rangle_0 \Delta \phi^{(2)}(y_1) \Delta \phi^{(1)}(y_2) = 0, \]
(12.3.20)

\[ \sum_{i=1,2} \int d^4y \langle \Gamma^{(3)}_{11}(x,y) \rangle_0 \Delta \phi^{(3)}(y) \]
\[ + \frac{1}{2!} \sum_{i=3,4} \int d^4y_1 d^4y_2 \langle \Gamma^{(3)}_{11}(x,y_1,y_2) \rangle_0 \left( \Delta \phi^{(1)}(y_1) \Delta \phi^{(2)}(y_2) + \Delta \phi^{(2)}(y_1) \Delta \phi^{(1)}(y_2) \right) \]
\[ + \frac{1}{3!} \sum_{i=5} \int d^4y_1 d^4y_2 d^4y_3 \langle \Gamma^{(3)}_{11}(x,y_1,y_2,y_3) \rangle_0 \Delta \phi^{(3)}(y_1) \Delta \phi^{(1)}(y_2) \Delta \phi^{(1)}(y_3) = 0, \]
(12.3.21)

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After some calculations, $\Delta \phi^{(n)}$ can be expressed by $\Delta \phi^{(1)}$ in a compact form,

$$
\Delta \phi^{(n)}(x) = \frac{1}{n!} \int d^4 y_1 \cdots d^4 y_n d^4 z_1 \cdots d^4 z_n (W^{(n+1)}_R)_{0}(x, y_1, \ldots, y_n) \\
\times \left( W^{(2)}_R \right)_{0}^{-1}(y_1, z_1) \left( W^{(2)}_R \right)_{0}^{-1}(y_2, z_2) \cdots \left( W^{(2)}_R \right)_{0}^{-1}(y_n, z_n) \\
\times \Delta \phi^{(1)}(z_1) \cdots \Delta \phi^{(1)}(z_n),
$$

(12.3.22)

$$
W^{(n+1)}_R(x, y_1, \ldots, y_n) \\
= \sum_{i_1, \ldots, i_n} \left( \frac{\delta^{n+1} W}{\delta J_i(x) \delta J_{i_1}(y_1) \cdots \delta J_{i_n}(y_n)} \right)_{j_1 = j_3} \\
= \left( \frac{i}{\hbar} \right)^n \mathrm{Tr} \left( \rho_i \sum_{P(y_1, \ldots, y_n)} \theta(t_x, t_{y_1}, \ldots, t_{y_n}) \left[ \left[ \phi(x), \phi(y_1), \ldots, \phi(y_n) \right] \right] \right) \\
= \left( \frac{i}{\hbar} \right)^n \langle R(\phi(x) \phi(y_1) \cdots \phi(y_n)) \rangle,
$$

(12.3.23)

$$
\theta(t_x, t_{y_1}, \ldots, t_{y_n}) = \theta(t_x - t_{y_1}) \theta(t_{y_1} - t_{y_2}) \cdots \theta(t_{y_{n-1}} - t_{y_n}).
$$

Here $\sum_{P(y_1, \ldots, y_n)}$ implies the sum over all possible permutation of $\{y_1, \ldots, y_n\}$. The arrow on $W^{(2)}_R$ indicates that it operates to the left. Equation (12.3.22) expresses the fact that among $n+1$ lines $n$ lines are amputated by the inverse of the retarded Green's function.

Now the above formulas are rewritten by the operator form through the reverse use of the LSZ reduction technique\(^{8,9}\) (see Appendix D) and we get another physical interpretation of our expansion scheme. In particular infinite series of on-shell expansion can be summed up into a coherent state of the excitation mode. Consider first $\Delta \phi^{(1)}(x)$. We show that it is related to the wave function of the excited mode. For this purpose let us rewrite $\Delta \phi^{(1)}(x)$ using (12.3.12) and (12.3.16),

$$
\Delta \phi^{(1)}(x) = - \int d^4 x' \int d^4 y \Delta \phi^{(1)}(x') \sum_{i=1,2} I^{(3)}_i(x' - y) \sum_{j=1,2} W^{(3)}_{ij}(y - x) \\
= Z^{-1} \int d^4 x' \Delta \phi^{(1)}(x') f(\vec{\partial}_x) i \langle R(\hat{\phi}(x') \hat{\phi}(x)) \rangle.
$$

(12.3.24)

(12.3.25)

We have used the fact that since the factor $\Delta \phi^{(1)}(x')$ is present we can use the expression (12.3.16) for $I^{(3)}$ in (12.3.24). Now Eq. (12.3.8) is equivalent to

$$
f(\vec{\partial}_x) \Delta \phi^{(1)}(x') = 0,
$$

(12.3.26)

and the partial integration over $\int d^4 x'$ in (12.3.25) is performed. The boundary term at spacial infinity is assumed to vanish by utilizing the wave packet regularization for the plane wave. We keep the boundary term at $t = \pm \infty$ by using the identity

$$
A \partial_t^2 B = \partial_t (A \partial_t B) + (\partial_t^2 A) B, \quad A \partial_t B \equiv A \partial_t B - (\partial_t A) B.
$$

(12.3.27)

By (12.3.26) we get, using the notation $y = (y^0, \mathbf{y})$, the following expression. Note that we have taken $t_i = -\infty$. 


\[ \Delta \phi^{(1)}(x) = Z^{-1} \int d^4 y \partial_\alpha \left( \Delta \phi^{(1)}(y)^* \partial_\beta \right) \rho(y) \phi(x) \phi(x) \rangle \]

\[ = iZ^{-1} \left( \lim_{y_\alpha \to \infty} - \lim_{y_\alpha \to -t_1} \right) \int d^3 y \Delta \phi^{(1)}(y)^* \partial_\beta \rho(y) \phi(x) \phi(x) \rangle. \]

We note here that \( \lim_{y_\alpha \to \infty} \) makes vanishing contribution because of the presence of \( \theta \)-function in \( W_\alpha^{(2)} \) and also that at equal time the fields \( \phi(t, x) \) commute among themselves. Thus we arrive at

\[ \Delta \phi^{(1)}(x) = \rho \{ \phi(x), \hat{A} \}, \quad (12.3.28) \]

\[ \hat{A} = -iZ^{-1} \int d^3 y \left( \Delta \phi^{(1)}(y)^* \hat{H}(y) - (\partial_\alpha \Delta \phi^{(1)}(y)) \rho(y) \phi(x) \phi(x) \rangle \right)_{y_\alpha = t_1}. \quad (12.3.29) \]

In momentum representation \( \hat{A} \) takes a simple form. Let us expand \( \hat{\phi} \) and \( \hat{H} \) in terms of the creation and annihilation operators,

\[ \hat{\phi}(t_1, x) = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3 p}{\sqrt{2\omega(p)}} \left( \hat{a}(p)e^{-ip_0x_1} + \hat{a}(p)^+ e^{ip_0x_1} \right), \quad (12.3.30) \]

\[ \hat{H}(t_1, x) = \frac{i}{(2\pi)^{3/2}} \int d^3 p \sqrt{\frac{\omega(p)}{2}} \left( \hat{a}(p)e^{-ip_0x_1} - \hat{a}(p)^+ e^{ip_0x_1} \right), \quad (12.3.31) \]

where \( p_0 x_1 = \omega(p)t_1 - p \cdot x \) and

\[ \left[ \hat{a}(p), \hat{a}(k)^+ \right] = \delta^3(p-k), \quad (12.3.32) \]

while other commutators are zero. Now inserting (12.3.19), (12.3.30) and (12.3.31) into the definition (12.3.29), we get

\[ \hat{A} = a^+ - a, \quad (12.3.33) \]

\[ a^{(t)} = Z^{-1}(2\pi)^{3/2} \int \frac{d^3 p}{\sqrt{2\omega(p)}} C^{(2)}(p) \hat{a}(p)^{\dagger}. \quad (12.3.34) \]

At this point we assume that the initial density matrix to be the equilibrium one: \( \rho_1 = \exp(-\beta \hat{H}) \). Then \( \hat{\phi} \) does not change the number of particles corresponding to \( a \) or \( a^+ \). This is seen as follows. Since \( t_1 = -\infty \), \( \hat{\phi}(t_1, x) \) corresponds to in-field of LSZ formalism (see Appendix D) and \( a^{(t)} \) annihilates or creates the mode which is an eigenstate of the total Hamiltonian. Recall also that it is defined by the pole of the full order Green's function \( W_\alpha^{(2)} \).

Now \( \Delta \phi^{(1)}(x) \) can be looked upon as a linear combination of the wave function of the state (which is not normalized) containing one excited mode annihilated or created by \( a \) or \( a^+ \). In order to see this, let us write (12.3.28) explicitly in the number representation using (12.3.33),

\[ \Delta \phi^{(1)}(x) = \sum_n \rho_{nn} \langle n | \phi(x), a^+ - a | n \rangle \]

\[ = \sum_n \rho_{nn} \left\{ -\sqrt{n} \langle n | \phi(x) | n - 1 \rangle + \sqrt{n + 1} \langle n | \phi(x) | n + 1 \rangle \right. \]

\[ \left. + \sqrt{n + 1} \langle n + 1 | \phi(x) | n \rangle - \sqrt{n} \langle n - 1 | \phi(x) | n \rangle \right\}. \quad (12.3.35) \]
Here the summation over the indices other than $n$ is suppressed and the following notations have been used,

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^*|n\rangle = \sqrt{n+1}|n+1\rangle.$$  

The above result is the generalization of the zero temperature case to finite temperature where the excited modes and the thermal background are present at the same time. Indeed we can show that (12.3.35) reduces to the known expression if we keep only the ground state $|0\rangle$ in the sum. Using $a|0\rangle = \langle 0|a^* = 0$, we see that $\Delta \phi^{(1)}(x)$ is written as

$$\Delta \phi^{(1)}(x) = \langle 0|\phi(x)|1\rangle + \text{c.c.},$$

where c.c. implies the complex conjugate. The above expression is precisely the wave function of the mode for the case of Hermite field.

Consider next $\Delta \phi^{(2)}(x)$ which can be handled in a similar manner:

$$\Delta \phi^{(2)}(x)$$

$$= \int d^4y_1 \int d^4y_2 iZ^{-1} \Delta \phi^{(1)}(y_1) f(\bar{\phi}(y_1)) iZ^{-1} \Delta \phi^{(1)}(y_2) f(\bar{\phi}(y_2)) \langle R(\phi(x)|\phi(y_1)\phi(y_2))\rangle.$$  

(12.3.36)

The integration over $y_2$ is done first. Following the same process as we have done above, the partial integration leads to

$$\int d^4y_2 iZ^{-1} \Delta \phi^{(1)}(y_2) f(\bar{\phi}(y_2)) \langle R(\phi(x)|\phi(y_1)\phi(y_2))\rangle$$

$$= iZ^{-1} \int d^4y_2 \partial y_2 [\Delta \phi^{(1)}(y_2) \bar{\phi}(y_2) \langle R(\phi(x)|\phi(y_1)\phi(y_2))\rangle]$$

$$= iZ^{-1} \int d^4y_2 (\lim_{y_2 \to -\infty} - \lim_{y_2 \to +\infty}) \Delta \phi^{(1)}(y_2) \bar{\phi}(y_2) \langle R(\phi(x)|\phi(y_1)\phi(y_2))\rangle$$

$$= -iZ^{-1} \int d^4y_2 \Delta \phi^{(1)}(y_2) \bar{\phi}(y_2) \langle [R(\phi(x)|\phi(y_1))\phi(y_2)]|_{y_2 = \pm t}, \bar{\phi}(y_2)\rangle.$$  

(12.3.37)

The remaining integration of $y_1$ can be done similarly with the result

$$\Delta \phi^{(3)}(x) = \frac{1}{2!} \langle [\langle [\phi(x), \bar{\phi}], A] + \bar{A}\rangle.$$  

(12.3.38)

Looking at the above expressions, it is an easy task to guess the results for general $\Delta \phi^{(n)}(x)$. In fact by using the mathematical induction technique, we can show the following form, see Ref. 11):

$$\Delta \phi^{(n)}(x) = \frac{1}{n!} \langle [[\ldots[[\phi(x), \bar{\phi}], \bar{A}], \ldots], \bar{A}\rangle.$$  

(12.3.39)
Now it is a simple matter to sum up over \( n \) and we get

\[
\Delta \phi(x) = \sum_{n=1}^{\infty} \Delta \phi^{(n)}(x) = \text{Tr} \left( \rho_i \exp(-\hat{A}) \hat{\phi}(x) \exp(\hat{A}) \right) = \text{Tr} \left( \exp(\hat{A}) \rho_i \exp(-\hat{A}) \hat{\phi}(x) \right).
\]

(12.3.40)

Usually the initial density matrix is written by \( \tilde{\rho}(x) \) and \( \hat{\phi}(x) \) so that, by noting the definition of (12.3.29) of \( \hat{A} \), we get the c-number shift of the initial variables,

\[
\exp(\hat{A}) \rho_i \left( \tilde{\rho}(x), \hat{\phi}(x) \right) \exp(-\hat{A}) = \rho_i \left( \tilde{\rho}(x) - \Pi_c(x), \hat{\phi}(x) - \phi_c(x) \right) ,
\]

(12.3.41)

\[
\Pi_c(x) = Z^{-1} \left( \partial_x \Delta \phi^{(1)}(x) \right)_{t_i} ,
\]

(12.3.42)

\[
\phi_c(x) = Z^{-1} \left( \Delta \phi^{(1)}(x) \right)_{t_i} .
\]

(12.3.43)

The initial coordinate is shifted as it should:

\[
\Delta \phi(t_i, x) = \text{Tr} \left( \rho_i \left[ \hat{\phi}(t_i, x) + [\hat{\phi}(t_i, x), -iZ^{-1} \hat{A}] \right] \right)
\]

\[
= \text{Tr} \left( \rho_i \left[ \hat{\phi}(t_i, x) + (-iZ^{-1})i \Delta \phi^{(1)}(t_i, x) \right] \right)
\]

(12.3.44)

\[
= \text{Tr} \left( \rho_i \hat{\phi}(t_i, x) \right) + Z^{-1} \Delta \phi^{(1)}(t_i, x) .
\]

(12.3.45)

In the momentum representation

\[
\exp(\hat{A}) \rho_i \left( \hat{a}(p), \hat{a}^\dagger(p) \right) \exp(-\hat{A}) = \rho_i \left( \hat{a}(p) - \hat{C}^{(+)p}(p), \hat{a}^\dagger(p) - \hat{C}^{(+)p}(p) \right) ,
\]

\[
\hat{C}^{(\pm)}(p) = Z^{-1}(2\pi)^{3/2} \frac{C^{(\pm)}(p)}{\sqrt{2\omega(p)}}.
\]

(12.3.46)

Note that \( \exp(-\hat{A}) \) coincides with the familiar operator which brings about the coherent state.

Now we have at hand a novel way of searching for the correct condensed state; vary \( \hat{C}^{(\pm)}(p) \) in such a way that \( \Delta \phi(x) \) becomes constant in time. Then we get the density matrix corresponding to the condensed state. This is illustrated for superfluid \(^4\)He in the next subsection and application of this technique to other real physical systems is under way.

12.3.2. **Non-Hermite case — superfluid \(^4\)He ——**

Let us take the system of \(^4\)He where the complex (i.e., non-Hermite) field operator \( \hat{\phi}(x) \) of \(^4\)He has a non-vanishing expectation value below the temperature \( T_c \) corresponding to the onset of Bose condensation. The model Hamiltonian is the usual one\(^{19} \).
\[
\hat{H} = \int d^3 x \hat{\phi}^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \hat{\phi}(x) \\
+ \frac{1}{2} \int d^3 x d^3 y \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(y) U_0(x-y) \hat{\phi}(y) \hat{\phi}(x),
\]

\[
U_0(x-y) = U_0(y-x), \quad [\hat{\phi}(t, x), \hat{\phi}^\dagger(t, y)] = \delta(x-y).
\]

Here \( U_0(x-y) \) is the assumed repulsive potential of the Helium atom and \( \mu \) the chemical potential. In the following we take for simplicity a local form \( \delta(x-y) \) for \( U_0(x-y) \). Below we set \( \phi^{(1)}(x) = \langle \hat{\phi}^{(1)}(x) \rangle \) and introduce the notation,

\[
\hat{\phi}^a = (\hat{\phi}^i, \hat{\phi}^j), \quad \phi^a = (\phi^i, \phi^j). \quad (a = 1, 2)
\]

(Do not mix the suffix \( \alpha \) with the suffix \( i \) or \( j \) which discriminates the branch of the two real time paths.) We need two kinds of sources \( J_i, \bar{J}_i \) \( (i = 1, 2) \) and define

\[
\hat{H}_i(x) = \hat{H} - \int d^3 x [J_i(x) \hat{\phi}^i(x) + \bar{J}_i(x) \hat{\phi}(x)].
\]

(i) Case \( \hat{\phi} = \hat{\phi}^a \)

Let us take a stationary homogeneous solution \( \phi^a = \langle \hat{\phi}^a(x) \rangle \). (For \( T \leq T_c \), there are two solutions.) Then the on-shell conditions take the form

\[
(i\hbar \partial_t + \mathcal{Q}(-\nabla)) \Delta \phi^{(1)}(x) = 0, \quad (-i\hbar \partial_t + \mathcal{Q}(-\nabla)) \Delta \phi^{(1)}(x) = 0.
\]

Here \( \mathcal{Q}(-\nabla) \) is the complete dispersion relation including the corrections due to the interaction. The solution in Fourier space is written as

\[
\Delta \phi^{(1)} = \int d^3 p C^{(2)}(p) \exp(\mp ip^{(0)} x),
\]

where \( p^{(0)} x = \mathcal{Q}(p) t - p \cdot x \).

In the formula (12.3.22), owing to the presence of the on-shell projection \( \Delta \phi^{(1)} \), \( W^{(2)}_{R} \) can be replaced by its pole part,

\[
\begin{cases}
W^{(2)}_{R}(x, y) = \Delta^{-1}(i\hbar \partial_x + \mathcal{Q}(-\nabla_x)) \delta^4(x-y), \\
W^{(2)}_{R}(x, y) = \Delta^{-1}(-i\hbar \partial_x + \mathcal{Q}(-\nabla_x)) \delta^4(x-y).
\end{cases}
\]

Here \( \sqrt{Z} \) is the wave function renormalization factor of the \(^4\text{He} \) field.

Inserting (12.3.50), (12.3.52) into (12.3.22), the reverse use of the LSZ reduction formula (Appendix D), as was done in the previous chapter, leads to the following expression:

\[
\Delta \phi^{a(n)}(x) = \frac{1}{n!} \langle [\ldots [\hat{\phi}^a(x), \hat{A}], \ldots], \hat{A} \rangle,
\]

\[
\hat{A} = Z^{-1} \int d^3 y \left( \Delta \phi^{(1)}(y) \hat{\phi}^i(y) - \Delta \phi^{(1)}(y) \hat{\phi}(y) \right)_{y^{(0)} = t_i}.
\]

Let us rewrite \( \hat{A} \) by expanding \( \hat{\phi}^{(1)} \) in terms of the creation and annihilation operators,
\[ \hat{\phi}^{(t)}(t_f, x) = \frac{1}{(2\pi)^{3/2}} \int d^3 p \hat{\sigma}(p)^{(t)} e^{-ip^0 x_f}, \] (12.3.54)

where \( p^0 x_f = Q(p) t_f - p \cdot x \). Now inserting (12.3.51) and (12.3.54) into the definition (12.3.53), we get

\[ \hat{A} = a^+ - a, \] (12.3.55)

\[ a^{(t)} = Z^{-1}(2\pi)^{3/2} \int d^3 p C^{(t)}(p) \hat{\sigma}(p)^{t}. \] (12.3.56)

Assuming the equilibrium initial density matrix, we have the following expression for the wave function analogous to (12.3.35),

\[
\Delta \phi^{a,(n)}(x) = \sum_n \rho_{nm} \langle n | [\hat{\phi}^{(t)}(x), a^+ - a] | m \rangle
\]

\[ = \sum_n \rho_{nm} \{ -\sqrt{n} \langle n | \hat{\phi}^{(t)}(x) | n-1 \rangle + \sqrt{n+1} \langle n | \hat{\phi}^{(t)}(x) | n+1 \rangle + \sqrt{n+1} \langle n+1 | \hat{\phi}^{(t)}(x) | n \rangle - \sqrt{n} \langle n-1 | \hat{\phi}^{(t)}(x) | n \rangle \}. \] (12.3.57)

Now we can sum up \( \Delta \phi^{a,(n)}(x) \) into an exponential form to get \( \Delta \phi^a(x) \) as follows,

\[ \Delta \phi^a(x) = \sum_{n=1}^{\infty} \Delta \phi^{a,(n)}(x) \]

\[ = \text{Tr} \left( \rho_x [\hat{\phi}^{t}, \hat{\phi}^{t}] e^{-\hat{A}^{\ast} \hat{\phi}^a(x) e^{\hat{A}}} \right) \]

\[ = \text{Tr} \left( \rho_x [\hat{\phi}^{t}, \hat{\phi}^{t}] \hat{\phi}^a(x) \right), \] (12.3.58)

\[ \hat{\phi}^{t} = \hat{\phi} - Z^{-1} \Delta \phi^{(t)}(t_f), \quad \hat{\phi}^{t} = \hat{\phi}^{t} - Z^{-1} \Delta \phi^{(t)}(t_f). \] (12.3.59)

Equation (12.3.58) tells us that \( \Delta \phi^a(x) \) is the same as \( \langle \hat{\phi}^a(x) \rangle \) but with initial operator inside \( \rho_x \) shifted by the amount \( -Z^{-1} \Delta \phi^{(t)}(t_f, x) \) which is a c-number. This is reminiscent of the shift of boundary conditions under the on-shell variation in classical analytical dynamics, see the discussion leading to Fig. 1.2. However only the shift of the initial value comes in the formula here compared with the case of the classical mechanics where the change of \( q(t) \) at both \( t = t_f \) and \( t = t_0 \) appear. The reason is that we have closed time path for the case of finite temperature while the time flows straightly from \( t = -\infty \) to \( +\infty \) in zero temperature case.

Just like the case of zero temperature discussed in § 4.3, the constant solution of non-equilibrium equation of motion coincides with the stationary solution of the equilibrium free energy. This result provides us with a novel method of finding condensed, i.e., inequivalent, solution. See Ref. 11) for details.

(ii) Case \( \hat{O} = \hat{\phi}^a \hat{\phi}^a \)

Next the pairing condensation is discussed. In superfluid \(^4\text{He}, \) many people pointed out that not only \( \phi^a \) but also \( \phi^a \phi^a \) may condense, see § 14.2. Now the result of the application of the on-shell expansion to the paring theory is briefly summarized below. We will see that the Bogoliubov angle naturally comes in our formalism.
For this purpose we do not write the \( J_5 \) dependence and the pairing is taken up in momentum representation \( \langle \hat{\phi}(-\mathbf{p}) \hat{\phi}^*(\mathbf{p}) \rangle, \langle \hat{\phi}^*(\mathbf{p}) \hat{\phi}^*(-\mathbf{p}) \rangle \) by adding the source term to the Hamiltonian as follows,

\[
\hat{H}_{\text{tr}} = \hat{H} - \int d^3p \left( J_{1\text{tr}}(t, \mathbf{p}) \hat{\phi}^*(\mathbf{p}) \hat{\phi}^*(-\mathbf{p}) + J_{2\text{tr}}(t, \mathbf{p}) \hat{\phi}(-\mathbf{p}) \hat{\phi}(\mathbf{p}) \right). 
\]

The argument goes through in a similar way as the case of \( \langle \hat{\phi}^a \rangle \). We define \( W[J] \) which has the property

\[
\frac{\delta W[J]}{\delta J_{1\text{tr}}(t, \mathbf{p})} = \Phi_1(t, \mathbf{p}), \quad \frac{\delta W[J]}{\delta J_{2\text{tr}}(t, \mathbf{p})} = \Phi_1^*(t, \mathbf{p}).
\] (12.3.60)

Then the equation which governs the time development of the order parameter is written as

\[
\left( \frac{\delta \Gamma}{\delta \Phi_1^{(1)}(t, \mathbf{p})} \right)_{\Phi_1 = \Phi_2 = 0} = 0. 
\] (12.3.61)

On-shell expansion around the uncondensed solution \( \Phi^{(0)} \) is gotten by writing

\[
\Phi^a(t, \mathbf{p}) = \Phi^{(0)} + \Delta \Phi^a(t, \mathbf{p}).
\]

We use the notations,

\[
\Phi^a = (\Phi^0, \Phi^1, \Phi^2) , \quad \Phi(t, \mathbf{p}) = \hat{\phi}(t, -\mathbf{p}) \hat{\phi}(t, \mathbf{p}), \quad \Phi^*(t, \mathbf{p}) = \hat{\phi}^*(t, \mathbf{p}) \hat{\phi}^*(t, -\mathbf{p}).
\]

Then \( \Delta \Phi^a(t, \mathbf{p}) \) is obtained, after some algebra, as follows,

\[
\Delta \Phi^a(t, \mathbf{p}) = \Phi^{(1)}(t, \mathbf{p}) + \Phi^{(2)}(t, \mathbf{p}) \ldots
\]

\[
= \text{Tr} \left( e^{i \Delta \phi_{\text{tr}}(t, \mathbf{q})} \rho_1[\hat{\phi}, \hat{\phi}^*] e^{-i \Delta \phi_{\text{tr}}(t, \mathbf{q})} \hat{\phi}^a(t, \mathbf{p}) \right)
\]

\[
= \text{Tr} \left( \rho_1[\hat{\phi}^0, \hat{\phi}^0^*] \hat{\phi}^a(t, \mathbf{p}) \right).
\]

Here the following notations are employed,

\[
\hat{\phi}^0 = \cosh \theta_\phi \hat{\phi}(\mathbf{k}) - \exp(i \arg \phi_\phi) \sinh \theta_\phi \hat{\phi}^*(\mathbf{k}),
\]

\[
\hat{\phi}^0^* = \cosh \theta_\phi \hat{\phi}^*(\mathbf{k}) - \exp(i \arg \phi_\phi^*) \sinh \theta_\phi \hat{\phi}(\mathbf{k}),
\]

\[
\Delta \phi_{\text{tr}}(t, \mathbf{q}) = Z^{-1}(\Delta \phi^{(1)}(t, \mathbf{q}) \hat{\phi}^*(t, \mathbf{q}) \hat{\phi}^*(t, -\mathbf{q}) - \Delta \phi^{(1)}(t, -\mathbf{q}) \hat{\phi}(t, \mathbf{q}) \hat{\phi}(t, -\mathbf{q}) - \Delta \phi^{(1)}(t, -\mathbf{q}) \hat{\phi}(t, -\mathbf{q}) \hat{\phi}(t, \mathbf{q}) - \Delta \phi^{(1)}(t, \mathbf{q}) \hat{\phi}^*(t, \mathbf{q}) \hat{\phi}^*(t, -\mathbf{q}) - \Delta \phi^{(1)}(t, -\mathbf{q}) \hat{\phi}^*(t, -\mathbf{q}) \hat{\phi}^*(t, \mathbf{q}))
\]

\[
\theta_\phi = |\phi_\phi|, \quad \theta_\phi^* = |\phi_\phi^*|.
\]

The angle \( \theta_\phi \) is nothing but the Bogoliubov angle which is determined by requiring that \( \Delta \Phi(t, \mathbf{p}) \) is independent of \( t \). As in the case of \( \langle \phi^a \rangle \), this will coincide with the condition of minimizing equilibrium free energy.

We summarize our findings of this subsection. On-shell expansion naturally changes the initial density matrix into

\[
e^{C \hat{\phi}^0 - C^* \hat{\phi}^0} \rho_1 e^{-C \hat{\phi}^0 + C^* \hat{\phi}^0}, \quad e^{C \hat{\phi}^0^* - C^* \hat{\phi}^0^*} \rho_1 e^{-C \hat{\phi}^0^* + C^* \hat{\phi}^0^*},
\]

which causes the shift of the operator \( \hat{\phi} \) of the initial state by \( c \)-number \( C^{(1)} \) or the
rotation of the pair field by the amount \( \theta \). It is our claim that \( C^{(\tau)} \) or \( \theta \) can be obtained by the requirement that \( \langle \hat{\phi} \rangle_\tau \) or \( \langle \hat{\phi} \hat{\phi} \rangle_\tau \) be independent of \( \tau \), which coincides with the value fixed by minimizing the equilibrium free energy. The above form of the tranformed density matrix implies that the new state is constructed by adding an infinite number of the unstable modes present in the uncondensed state in a coherent way.

There have been controversy\(^{129}\) about the presence or absence of the gap in the excitation mode when the pairing occurs. By using the exact identity presented in § 3.5, we can show in full order that the gap does not exist, see § 14.2 and Ref. 11).

12.3.3. Relation between real and imaginary time on-shell expansion

The scheme of on-shell expansion, in particular the on-shell equation, can be performed in the imaginary time formalism also. Examples have been given in §§ 10.1.5 and 10.1.6. Here we discuss the relation between the real and imaginary time scheme. For this purpose let us start from the three time path expressions (12.2.7)–(12.2.9).

(i) Stationary solution

Setting \( J_i = 0 \) (\( i = 1, 2, 3 \)), the expectation values \( \phi_i \) are determined by the stationary condition of \( \Gamma \),

\[
\frac{\delta \Gamma}{\delta \phi_i(x)} = 0. \quad (i = 1, 2, 3) \tag{12.3.62}
\]

Note here that when \( i = 1, 2, x = (t, x) \) and for \( i = 3, x \) represents \( x = (\tau, x) \). This type of notation will be used in the following. Now the solution to the above equations always satisfies \( \phi_1(x) = \phi_2(x) = \phi^{(0)}(x) \) so that it is denoted by \( \phi^{(0)}(x) \). Then (12.3.62) is written explicitly as

\[
\left( \frac{\delta \Gamma}{\phi_i(x)} \right)_{(\ast)} = 0, \tag{12.3.63}
\]

where \((\ast)\) implies that we evaluate the preceding quantity at \( \phi_1(x) = \phi_2(x) = \phi^{(0)}(x) \). Equation (12.3.63) is the equation of motion for the order parameter. The \( x \)-independent constant solution \( \phi^{(0)}(x) \) of (12.3.63) coincides with the initial equilibrium values for these parameters, \( \phi_1 = \phi_2 = \phi_3 = \phi^{(0)} \).

(ii) Excitation spectrum

The method of on-shell expansion explained in § 12.3.1 is now studied in the three path form. We seek a new solution to (12.3.63) in the vicinity of \( \phi^{(0)} \) by writing

\[
\phi_i(x) = \phi^{(0)} + \Delta \phi_i(x), \tag{12.3.64}
\]

\[
\phi_3(x) = \phi^{(0)} + \Delta \phi_3(x). \tag{12.3.65}
\]

Now (12.3.62) is evaluated at (12.3.64) or (12.3.65) and take the initial time \( t_i = -\infty \). Then the on-shell equation takes the following form. For \( i = 1 \) of (12.3.62), we get

\[
0 = \sum_{i=1,3} \int_{-\infty}^{\infty} d^4 y \left( \frac{\delta^2 \Gamma}{\delta \phi_1(x) \delta \phi_1(y)} \right)_0 \Delta \phi_1(y) + \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} d^3 y \left( \frac{\delta^2 \Gamma}{\delta \phi_1(x) \delta \phi_3(y)} \right)_0 \Delta \phi_3(y). \tag{12.3.66}
\]
Here \((\cdots)_0\) implies that \((\cdots)\) is evaluated at the solution \(\phi^{(0)}\). Actually the second term on the right-hand side of (12.3.66) is zero since the time coordinate of \(y\) is \(t_t - it\) therefore the time difference of \(x\) and \(y\) is infinity in the limit \(t_t = -\infty\). In order to see this fact, let us consider the following simple integral in the limit \(T \to \infty\),

\[
I \equiv \int_{-\infty}^{\infty} dx f(x) \exp\{ig(x)T\}.
\]  

(12.3.67)

Two cases are studied separately:

(i) \(g(x)\) has the stationary point

In this case the integral is dominated by the stationary point \(x = x_0\). Expanding \(g(x)\) around \(x = x_0\),

\[
I \sim f(x_0) \sqrt{\frac{2\pi}{g''(x_0)T}} \exp\{ig(x_0)T\} + O(T^{-3/2}).
\]

(12.3.68)

(ii) \(g(x)\) has no stationary point

We can change the integration variable from \(x\) to \(y = g(x)\),

\[
I = \int_a^b dy (g'(x))^{-1} f(x) \exp(iyT)
\]

(12.3.69)
with \(a, b\) some constant. In cases \(a\) and \(b\) are finite, the integral goes to zero with the oscillatory behavior for large \(T\). Indeed by the partial integration,

\[
I = \frac{1}{iT} \left( g'(x) \right)^{-1} f(x) \exp(iyT) \bigg|_{y=a}^{y=b} - \frac{1}{iT} \int_a^b dy \frac{d}{dy} \left( (g'(x))^{-1} f(x) \right) \exp(iyT).
\]

(12.3.70)

The second term on the right-hand side is \(O(T^{-2})\) in general. If \(a\) and/or \(b\) are infinite \(I\) will go to zero more rapidly.

In the actual cases we have to study the Feynman diagram of \((\delta^2\Gamma/\delta(x)\delta(y))_0\) with the real part of \(x - y\) going to infinity. If it is shown that \((\delta^2\Gamma/\delta(x)\delta(y))_0\) vanishes in the same limit, we can say that \((\delta^2\Gamma/\delta(x)\delta(y))_0\) vanishes as \(x - y \to \infty\), since the second derivative of \(\Gamma\) and \(W\) are the inverse matrices of each other. Now the general structure of the Feynman diagram tells us that \((\delta^2\Gamma/\delta(x)\delta(y))_0\) contains the multiple integral over the momenta like

\[
I \equiv \int_{-\infty}^{\infty} dp_1 \int_{-\infty}^{\infty} dp_2 \cdots f(p_1, p_2, \cdots) \exp\{ig(p_1, p_2, \cdots)T\}.
\]

(12.3.71)

Although the complete analysis of the limit \(T \to \infty\) is difficult, the answer will be similar to the above example of the single integral. Thus (12.3.66) takes the form

\[
\int_{-\infty}^{\infty} d^4y (\Gamma_1(x, y) + \Gamma_2(x, y)) \Delta\phi(y) = 0,
\]

(12.3.72)

where we have introduced \(\Gamma_0(x, y) = (\delta^2\Gamma/\delta(x)\delta(y))_0\). This coincides with the on-shell equation discussed in §12.3.1 where (12.3.8) was derived by considering only (12.3.64). For \(i = 3\), (12.3.62) becomes
\[ 0 = \int_0^\infty \int_{-\infty}^\infty d\tau d^3y \left( \frac{\delta^2 \Gamma}{\delta \phi_2(x) \delta \phi_3(y)} \right)_0 \Delta \phi_0(y) + \sum_{i=1,2} \int_{-\infty}^\infty d^4y \left( \frac{\delta^2 \Gamma}{\delta \phi_2(x) \delta \phi_i(y)} \right)_0 \Delta \phi_i(y). \]  

(12.3.73)

By the same reason as above the second term on the right-hand side vanishes and we get

\[ 0 = \int_0^\infty \int_{-\infty}^\infty d\tau d^3y \Gamma_{33}(x, y) \Delta \phi_0(y). \]

(12.3.74)

Recall here that \( \Gamma_{11} + \Gamma_{12} \) is the inverse of retarded function and \( \Gamma_{33} \) is the \( \tau \)-causal function. It is known that both are the analytic continuation of each other so that the eigenvalues obtained by solving (12.3.72) and (12.3.74) are the same. In the following we use (12.3.72) as the mode determining equation.

§ 12.4. Classical and macroscopic limit: reparametrization of \( J^{(\cdot)} \)

In this section the classical and macroscopic limit of \( W \) or \( \Gamma \) is studied. For this purpose we first define the Hamiltonian of \( N \)-particle system and the generating functional \( W \) taking the initial density matrix to be completely arbitrary. The diagrammatical rule of \( W \) in this case is explained in Appendixes E and F based on the work of Refs. 13) and 14). We will see that the effect of the initial density matrix appears as external lines of Feynman diagrams. We are interested in two specific parameters \( \hbar \) and \( N \) and take the limit \( \hbar \to 0^{(\cdot)} \) and \( N \to \infty \).  

In order to make it easy to extend our formula to field theoretical case, our system is supposed to consist of \( N \) degrees of freedom and to interact through the potential \( V(\vec{q}) \) with the vector notation \( \vec{q} = (\vec{q}_1, \cdots, \vec{q}_N) \) and the Hamiltonian is taken as

\[ \hat{H} = \hat{H}_0 + V(\vec{q}), \]

(12.4.1)

\[ \hat{H}_0 = \sum_{k=1}^N \left( \frac{\vec{p}_k^2}{2m_h} + \frac{1}{2} m_h \omega_k^2 \vec{\hat{q}}_k^2 \right). \]

(12.4.2)

The initial distribution of the state is represented by an arbitrary density matrix \( \hat{\rho}_i^N \). The generating functional \( W[\vec{J}_i, \vec{J}_2] \) is defined as follows, by choosing \( \vec{q} \) as an operator \( \hat{O} \) of (12.1.10),

\[ e^{i(i/N)W[\vec{J}_1, \vec{J}_2]} / \text{Tr} \hat{\rho}_i^N = \text{Tr} \left( \hat{K}^{i} \hat{\rho}_i^N (\hat{K}^{i})^\dagger \right) / \text{Tr} \hat{\rho}_i^N, \]

(12.4.3)

\[ \hat{K}^{i} = \text{Exp} \left[ -\frac{i}{\hbar} \int_{t_1}^{t_2} dt \{ \hat{H} - \vec{J}_i(t) \cdot \vec{q} \} \right], \quad (i=1, 2) \]

(12.4.4)

where \( \vec{J}_i(t) \cdot \vec{q} = \sum_{k=1}^{N} J_i^k(t) Q^k \) (\( i=1, 2 \)). (In the following \( k \) runs from 1 to \( N \) and \( i=1, 2 \).) The system is driven by external force \( \vec{J}(t) \) and its time-dependent Hamiltonian is expressed as

\[ \hat{H}(t) = \hat{\bar{H}} - \vec{J}(t) \cdot \vec{q}. \]

(12.4.5)

In Appendixes E and F, from the definition of \( W \) in (12.4.3) and adopting the coordinate representation, we rewrite \( W \) in path integral form. In Appendix E, \( W_0[\vec{J}_1, \vec{J}_2] \) is explicitly calculated where \( W_0 \) is \( W \) in the absence of \( V(\vec{q}) \). Using the
result thus obtained the diagrammatical rule is derived in Appendix F by expanding $W$ in powers of $V(\tilde{q})$. The final form is given in (F.16). Here let us proceed in a formal way.

Now in the limit $\hbar \to 0$, we expect to get the classical non-equilibrium generating functional $W_0$. However the classical limit of conventional $W[J_1, J_2]$ is not finite. Let us explain it briefly. Introducing $J^{(\pm)}=(1/2)(J_1+J_2)$, $J^{(-)}=(J_1-J_2)$, $W[J_1, J_2]$ is expanded in powers of $J^{(-)}$ as follows,

\[
W[J_1, J_2]=\sum_{k=1}^{N} \int_{t_1}^{t_2} dt \frac{\delta W}{\delta J^{(-)}(t)} \bigg|_{J^{(-)}=0} \cdot J^{(-)}(t) + \frac{1}{2} \sum_{k, l=1}^{N} \int_{t_1}^{t_2} dt \int_{t_1}^{t_2} ds \frac{\delta^2 W}{\delta J^{(-)}(t) \delta J^{(-)}(s)} \bigg|_{J^{(-)}=0} J^{(-)}(t) J^{(-)}(s) + \ldots
\]

(12.4.6)

\[
= \sum_{k=1}^{N} \int_{t_1}^{t_2} dt \langle q_k(t) \rangle \hat{h} J^{(-)}(t)
+ \frac{1}{2} \sum_{k, l=1}^{N} \int_{t_1}^{t_2} dt \int_{t_1}^{t_2} ds \frac{i}{\hbar} \text{Tr} \left[ \hat{\rho}_1 \cdot \frac{1}{2} \left[ \tilde{q}_k(t), \tilde{q}_l(s) \right]_s \right]_{\text{conn}} J^{(-)}(t) J^{(-)}(s)
+ \ldots
\]

(12.4.7)

where $[\hat{A}, \hat{B}]_s = \hat{A} \hat{B} + \hat{B} \hat{A}$. The notation $\tilde{q}_k(t)$ implies the Heisenberg operator at time $t$. The above form is obtained by an explicit calculation by inserting $J_{1,2}=J^{(\pm)} \pm (1/2)J^{(-)}$ into (12.4.3). The first term in (12.4.7) is finite of course but the second or higher term in (12.4.7) is not finite in the limit $\hbar \to 0$ since $\text{Tr} \left[ \hat{\rho}_1 \left[ \tilde{q}_k(t), \tilde{q}_l(s) \right]_s \right]$ is finite. Therefore $W[J_1, J_2]$ needs the rescaling of $J^{(-)}$ in order to ensure the classical limit. Thus we define $\bar{W}[J^{(-)}, J^{(+)}]$ as

\[
\bar{W}[J^{(-)}, J^{(+)}] = \frac{1}{\hbar} W[J_1, J_2],
\]

(12.4.8)

where the source $J_i(t)$ is now rewritten by

\[
J_1(t)=J^{(+)}(t)+\frac{\hbar}{2} J^{(-)}(t),
\]

\[
J_2(t)=J^{(+)}(t)-\frac{\hbar}{2} J^{(-)}(t).
\]

(12.4.9)

We point out here that the above definition of $J^{(-)}$ differs from the definition of $J^{(-)}$ we have been using by a factor $\hbar$. In this way we get finite classical generating functional defined as

\[
W_0[J^{(-)}, J^{(+)}] = \lim_{\hbar \to 0} \bar{W}[J^{(-)}, J^{(+)}].
\]

(12.4.10)

These reparametrizations of $J^{(-)}$ and $W$ are proved to be crucial to ensure the smooth connection of $\bar{W}[J^{(-)}, J^{(+)}]$ and $W_0[J^{(-)}, J^{(+)}]$ in the limit $\hbar \to 0$.

If we put further $J^{(+)}_h=J^{(+)}$, $J^{(-)}_h=J^{(-)}/N$, then the source term becomes

\[
if_1 \int df^{(-)}(t)(1/N) \sum_{k=1}^{N} q_k(t) \text{ so that the generating functional for the center of mass type is obtained. The large } N \text{ limit is also discussed by this extra factor } 1/N \text{ for } J^{(-)}.
\]
Recall that such a reparametrization is performed to the unphysical source $J^{(-)}$ only.

12.4.1. **Classical limit of $W[J_1, J_2]$**

With observations presented above, we take explicitly the classical limit of $W$ and see that the result coincides with the classical non-equilibrium generating functional, which involves the average over the initial position and momentum. In order to simplify the notation, we take here a system of one degree of freedom and write $J_i(t) = J_i(t)$ with $i = 1, 2$. The redefined generating functional $\bar{W}[J^{(-)}, J^{(+)看不见}]]$ is then written as $\bar{W}[J_1, J_2] = \hbar \bar{W}[J^{(-)}, J^{(+)看不见}]]$, where the source $J_i(t)$ is defined by

$$
\begin{align*}
J_1(t) &= J^{(+)}(t) + \frac{\hbar}{2} J^{(-)}(t), \\
J_2(t) &= J^{(+)}(t) - \frac{\hbar}{2} J^{(-)}(t).
\end{align*}
$$

(12.4.11)

By (F.2), $\bar{W}[J^{(-)}, J^{(+)看不见}]]$ can be represented as

$$
e^{\bar{W}[J^{(-)}, J^{(+)看不见}]]} = \int \mathcal{D}q_1 \mathcal{D}q_2 \langle q_1 | \bar{\rho}_1 | q_2 \rangle \langle x | \bar{K}^{J^{(+)}(t)}[\hat{J}^{(+)看不见}]] | q_2 \rangle^* \langle x | \bar{K}^{J^{(+)}(t)}[\hat{J}^{(+)看不见}]] | q_1 \rangle
$$

(12.4.12)

$$
= \int \mathcal{D}q_1 \mathcal{D}q_2 \rho_1(q_1, q_2) \int_B [d\phi_1] \int_B [d\phi_2]
$$

$$
\times \exp \left\{ \frac{i}{\hbar} \left( S^{'(+)\phi_1} - S^{'(+)\phi_2} \right) + i \int_{t_1}^{t_2} dt J^{(-)}(t) \phi^{(+)}(t) \right\}.
$$

(12.4.13)

Here $S^{'(+)\phi}$ represents the action of the system with external source $J^{(+)}$,

$$
S^{'(+)\phi} = \int_{t_1}^{t_2} dt \left\{ \frac{m}{2} \phi(t)^2 - \frac{m}{2} \omega^2 \phi(t)^2 - V(\phi(t)) + J^{(+)}(t) \phi(t) \right\}.
$$

(12.4.14)

The two path integrals $\int_B [d\phi_1]$ and $\int_B [d\phi_2]$ satisfy the boundary conditions $\phi_1(t_F) = \phi_2(t_F) = x$, $\phi_1(t_1) = q_1$, and $\phi_2(t_1) = q_2$. Here we have defined $\phi^{(+)}$, $\phi^{(-)}$ as $\phi^{(+)}(t) = (1/2)(\phi_1(t) + \phi_2(t)), \phi^{(-)}(t) = \phi_1(t) - \phi_2(t)$.

The Wigner representation of the initial distribution $\bar{\rho}_1(p, q)$ is defined as

$$
\rho_1(q_1, q_2) = \int dp dq \bar{\rho}_1(p, q) \delta \left( q - \frac{1}{2} (q_1 + q_2) \right) e^{i p \cdot (q_1 - q_2) / \hbar},
$$

(12.4.15)

and is known to become classical distribution function $\rho^{(c)}(p, q)$ in the classical limit. Now Eq. (12.4.15) is inserted into (12.4.13). If we use the phase space integral of (E.8), then we get

$$
e^{\bar{W}[J^{(-)}, J^{(+)看不见}]]} = \langle \int \mathcal{D}q_1 \mathcal{D}q_2 \delta \left( q - \frac{1}{2} (q_1 + q_2) \right) e^{i \phi \cdot (p + q_1 - q_2)} \int_B [d\phi_1] \int_B [d\phi_2]
$$

$$
\times \exp \left\{ \frac{i}{\hbar} \left( S^{'(+)\phi_1} - S^{'(+)\phi_2} \right) + i \int_{t_1}^{t_2} dt J^{(-)}(t) \phi^{(+)}(t) \right\} \rangle_{\bar{\rho}_1}.
$$

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\[ = \langle [d\phi^{(+)} d\phi^{(-)}] \delta(\phi^{(-)}(t_F)) \delta(q - \phi^{(+)}(t_i)) \right. \]
\[ \times \exp \left\{ \frac{i}{\hbar} \Phi_{\phi^{(+)} \phi^{(-)}}[\phi^{(+)}(t_F), \phi^{(-)}(t_i)] + i \int_{t_i}^{t_F} dt J^{(-)}(t) \phi^{(+)}(t) \right\} \rangle. \quad (12.4.16) \]

Here we have defined
\[ \Phi_{\phi^{(+)\phi^{(-)}}}[\phi^{(+)}, \phi^{(-)}] = S_{\phi^{(+)\phi^{(-)}}}[\phi_1] - S_{\phi^{(+)\phi^{(-)}}}[\phi_2], \quad (12.4.17) \]
\[ S_{\phi^{(+)\phi^{(-)}}}[\phi] = S_{\phi^{(+)\phi^{(-)}}} + p(\phi_i(t_i), \quad (i=1, 2) \quad (12.4.18) \]
and the following notation has been introduced,
\[ \int [d\phi^{(+)} d\phi^{(-)}] = \int d\phi^{(-)}(t_F) d\phi^{(+)}(t_i) \int d\phi^{(-)}(t_i) d\phi^{(+)}(t_F) \int_b [d\phi^{(+)}] \int_b [d\phi^{(-)}], \quad (12.4.19) \]

where in the last path integral, $\phi^{(\pm)}(t = t_i)$ and $\phi^{(\pm)}(t = t_F)$ are fixed and equal to the value $\phi^{(\pm)}(t_i)$ and $\phi^{(\pm)}(t_F)$ respectively.

We are in a position to take the limit $\hbar \to 0$. Then in the path integral representation (12.4.16) of $\widetilde{W}[J^{(-)}, J^{(+)\phi^{(-)}\phi^{(+)}}]$, the most dominant contribution comes from the path which gives the stationary phase of $\Phi_{\phi^{(+)\phi^{(-)}}}[\phi^{(+)}, \phi^{(-)}]$. We first rewrite $\Phi_{\phi^{(+)\phi^{(-)}}}[\phi^{(+)}, \phi^{(-)}]$ by using the partial integration remembering the conditions $\phi^{(\pm)}(t_F) = 0$ and $\phi^{(\pm)}(t_i) = q$,
\[ \Phi_{\phi^{(+)\phi^{(-)}}}[\phi^{(+)}, \phi^{(-)}] = \int_{t_i}^{t_F} dt m(\phi^{(+)}(t_F) + \phi^{(-)}(t_i) + p\phi^{(-)}(t_i)) \]
\[ = \int_{t_i}^{t_F} dt \{-\phi^{(-)}(t_F) m(\phi^{(+)}(t_F) + \phi^{(-)}(t_i) + p - m\phi^{(+)}(t_i)) \phi^{(-)}(t_i) \} \quad (12.4.20) \]
\[ = \int_{t_i}^{t_F} dt \{-\phi^{(-)}(t_F) m(\phi^{(+)}(t_F) + \phi^{(-)}(t_i) + m\phi^{(-)}(t_F) \phi^{(+)}(t_F) \]
\[ - m\phi^{(-)}(t_F) q + p\phi^{(-)}(t_i). \quad (12.4.21) \]

Thus the conditions satisfied by the stationary paths of $\phi^{(-)}(t)$ and $\phi^{(+)}(t)$ are obtained as
\[ 0 = \frac{\delta \Phi^{(+\phi^{(-)}}}{\delta \phi^{(-)}(t)} \]
\[ = -\Delta^{-1} \phi^{(+)}(t) - \frac{1}{2} V'(\phi_1) - \frac{1}{2} V'(\phi_2) + J^{(+\phi^{(-)}}(t) + \delta(t - t_i)(p - m\phi^{(+)}(t_i)) \}, \quad (12.4.22) \]
\[ 0 = \frac{\delta \Phi^{(+\phi^{(-)}}}{\delta \phi^{(+\phi^{(-)}}(t)} \]
\[ = -\Delta^{-1} \phi^{(-)}(t) - V'(\phi_1) + V'(\phi_2) + \delta(t - t_F)m\phi^{(-)}(t_F) \}. \quad (12.4.23) \]

Here $\Delta^{-1} = m(\delta t^2 + \omega^2)$. Equations (12.4.22) and (12.4.23) are satisfied if and only if the coefficients of $\delta(t - t_i)$ and $\delta(t - t_F)$ vanish. Therefore the classical limit produces the boundary conditions of $\phi^{(+)}, \phi^{(-)}$ as
\[ \dot{\phi}^{(+)}(t_f) = \frac{p}{m}, \quad \dot{\phi}^{(-)}(t_f) = 0. \]  
\[ (12.4.24) \]

From (12.4.22) \( \sim \) (12.4.24), we finally arrive at the result that the stationary paths \( \phi_1(t), \phi_2(t) \) are the solutions of classical equations of motion given by

\[ D^{-1}\phi_i(t) + V'(\phi_i(t)) = f^{(+)}(t), \quad (i=1, 2) \]  
\[ (12.4.25) \]

with boundary conditions,

\[ \phi^{(-)}(t_f) = 0, \quad \dot{\phi}^{(-)}(t_f) = 0, \]  
\[ (12.4.26) \]

\[ \phi^{(+)}(t_i) = q, \quad \dot{\phi}^{(+)}(t_i) = \frac{p}{m}. \]  
\[ (12.4.27) \]

By Eqs. (12.4.25) and (12.4.26), it follows that \( \phi_1(t) = \phi_2(t) \) for any \( t \). Therefore if we write as \( q_c(t, p, q, J^{(+)}) \) the solution of classical equation \( D^{-1}q(t) + V(q(t)) = f^{(+)}(t) \) with initial conditions \( q(t_0) = q_0, \dot{q}(t_0) = \frac{p}{m} \), then the stationary path becomes

\[ \phi_1(t) = \phi_2(t) = q_c(t, p, q, J^{(+)}). \]  
\[ (12.4.28) \]

We write in the following \( q_c(t, p, q) = q_c(t, p, q, J^{(+)} = 0) \).

The path integral in (12.4.16) can now be performed by using (12.4.28). We note here that

\[ \Phi_{\phi^{(+)}[\phi^{(+)}, \phi^{(-)}]}|_{\phi^{(-)} = 0} = 0. \]  
\[ (12.4.29) \]

The classical limit \( W_c[J^{(-)}, J^{(+)}] = \lim_{h \to 0} W[J^{(-)}, J^{(+)}] \) is finally given by (see Ref. 13 for more details),

\[ e^{iW_c[J^{(-)}, J^{(+)}]} = \int dp d\rho r_{\alpha}^{(-)}(p, q) \exp i \int_{t_i}^{t_f} dt f^{(-)}(t) q_c(t, p, q, J^{(+)}). \]  
\[ (12.4.30) \]

We have achieved our purpose of taking the limit \( h \to 0 \) of the quantum generating functional and have written it as the average over initial conditions of the classical trajectory.

Our \( W_c[J^{(-)}, J^{(+)}] \) is surely the classical statistical generating functional in the sense that the derivative of \( W_c[J^{(-)}, J^{(+)}] \) gives the classical average,

\[ \frac{\delta W_c[J^{(-)}, J^{(+)}]}{\delta f^{(-)}(t)} \bigg|_{f^{(-)} = 0} = \int dp d\rho r_{\alpha}^{(-)}(p, q) q_c(t, p, q). \]  
\[ (12.4.31) \]

The higher derivatives of \( W_c[J^{(-)}, J^{(+)}] \) produce the classical correlation functions of course which are the classical limits of the Green's functions of the quantum theory.

The above results can also be obtained by studying the structure of Feynman diagrams.\(^{14}\)

12.4.2. Classical limit of \( \Gamma[\phi_1, \phi_2] \)

The conventional definition of the effective action \( \Gamma[\phi_1, \phi_2] \) is through the Legendre transformation. However the classical limit of \( \Gamma[\phi_1, \phi_2] \) does not exist because the limit of \( W[J_1, J_2] \) is not finite. Thus we define \( \Gamma'[\phi^{(-)}, \phi^{(+)}] \) through the new generating functional \( \overline{W}[J^{(-)}, J^{(+)}] \) introduced in (12.4.8) and (12.4.11),
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\[
\Gamma[\phi^{(-)}, \phi^{(+)}) = W[J^{(-)}, J^{(+)}) - \int_{t_1}^{t_2} dt J^{(-)}(t) \frac{\delta W}{\delta J^{(-)}(t)} - \int_{t_1}^{t_2} dt J^{(+)}(t) \frac{\delta W}{\delta J^{(+)}}(t) ,
\]  
(12.4.32)

\[
\phi^{(-)}(t) = \frac{\delta W}{\delta J^{(+)}(t)} , \quad \phi^{(+)}(t) = \frac{\delta W}{\delta J^{(-)}(t)} .
\]  
(12.4.33)

The identities are

\[
\frac{\delta \Gamma}{\delta \phi^{(-)}(t)} = - J^{(+)}(t) , \quad \frac{\delta \Gamma}{\delta \phi^{(+)}}(t) = - J^{(-)}(t) .
\]  
(12.4.34)

Then the relation between \( \Gamma \) and \( \bar{\Gamma} \) turns out to be

\[
\Gamma[\phi_1, \phi_2] = \hbar \bar{\Gamma}[\phi^{(-)}, \phi^{(+)}) ,
\]  
(12.4.35)

\[
\phi_1(t) = \phi^{(+)}(t) + \frac{\hbar}{2} \phi^{(-)}(t) , \quad \phi_2(t) = \phi^{(+)}(t) - \frac{\hbar}{2} \phi^{(-)}(t) .
\]  
(12.4.36)

The time development of \( \phi^{(-)}(t) \) or \( \phi^{(+)}(t) \) is then governed by the equation of motion

\[
\frac{\delta \Gamma[\phi^{(-)}, \phi^{(+)})}{\delta \phi^{(-)}(t)} = 0 ,
\]  
(12.4.37)

\[
\frac{\delta \Gamma[\phi^{(-)}, \phi^{(+)})}{\delta \phi^{(+)}}(t) = 0 .
\]  
(12.4.38)

From (12.4.38) we get \( \phi^{(-)}(t) = 0 \), which is substituted into (12.4.37). Then there follows the equation of motion determining \( \phi^{(+)}(t) = \langle q(t) \rangle \) which is the physical average of \( \bar{q}(t) \):

\[
\frac{\delta \Gamma[\phi^{(-)}, \phi^{(+)})}{\delta \phi^{(-)}(t)} \bigg|_{\phi^{(-)}(t) = 0} = 0 .
\]  
(12.4.39)

The finite classical effective action \( \Gamma_{cl} \) is obtained through the replacement of \( \bar{W} \) appearing in (12.4.32) by \( W_{cl} \) given in (12.4.30).

The effective action which is simpler than (12.4.32) will be defined by setting \( J^{(+) = 0} \) in \( \bar{W}[J^{(-)}, J^{(+)}) \) from the start,

\[
\bar{W}[J] = \bar{W}[J^{(-)} = J, J^{(+) = 0} ,
\]  
(12.4.40)

\[
\bar{\Gamma}[\phi] = \bar{W}[J] - \int_{t_1}^{t_2} dt J(t) \frac{\delta \bar{W}[J]}{\delta J(t)} ,
\]  
(12.4.41)

\[
\phi(t) = \frac{\delta \bar{W}[J]}{\delta J(t)} .
\]  
(12.4.42)

The equation of motion is

\[
\frac{\delta \bar{\Gamma}[\phi]}{\delta \phi(t)} = 0 ,
\]  
(12.4.43)

which is identical to (12.4.39). We can take the limit \( \hbar \to 0 \) directly in this equation.

The equation of motion of the classical average \( \phi(t) = \langle q_{cl}(t, p, q) \rangle_{p, q} \) becomes
\[
\frac{\delta F_{\text{cl}}[\phi]}{\delta \phi(t)} = 0. \tag{12.4.44}
\]

We emphasize here again that in this form the equation of motion itself depends on initial conditions. Although \(\bar{F}[\phi]\) looks like a non-equilibrium generating functional of single variable, it does not "generate" the retarded Green's functions.

We end this subsection by the following observations. Notice that all the variables \(\{\bar{q}, \cdots, \bar{q}\}\) lose quantum fluctuations in the limit \(\hbar \to 0\) to become \(\bar{q} = q_{\text{cl}}\). However as \(q_{\text{cl}}\) it still microvariable, there exist classical statistical fluctuations in each \(q_i\) \((i = 1 \sim N)\) so that \(\langle q_{\text{cl}}(t)q_{\text{cl}}(s)\rangle_{p_{\text{cl}}} = \langle q_{\text{cl}}(t)\rangle_{p_{\text{cl}}} \cdot \langle q_{\text{cl}}(s)\rangle_{p_{\text{cl}}}\) for example. In diagrammatical sense, this means that the average \(\langle \cdot \rangle_{p_{\text{cl}}}\) plays the role of taking the "contraction" of two \(q_{\text{cl}}\)'s of external lines appearing in connected tree graphs \(\bar{G}_{\text{conn}}^{(n+1)}(\lambda, 0)\) of (F.16). This is usually called the initial correlation.

As will be explained in the next subsection, in contrast to the classical microvariables, the macrovariable \(\bar{X}\) (defined below) completely loses fluctuation in the limit \(N \to \infty\) and becomes a \(c\)-number denoted as \(\bar{X} = X\). However the microvariable, relative coordinates \(q'\) for example, are still quantum variables so that the numerical value of non-fluctuating macrovariable contains the factor \(\hbar\), which comes from the interaction between \(X\) and \(q'\).

Theory of generating functional of the macrovariable is developed in the next subsection. It will give us a clear image of the difference between quantum and classical variables or between micro- and macro-variables.

### 12.4.3. Macroscopic limit

We usually say that the macroscopic system can be treated classically. This statement is partly true but we have to make the explanation more precise. Our exact form of the statement is that the macrovariable of a macroscopic system becomes classical in the sense that it loses the fluctuation\(^{14}\) (more extensive study of macro-system will be performed in Chapter XIII). Consider a many particle system with dynamical variables \(q = (q_1, \cdots q_N)\). We will pick up below the macrovariable defined by the average over individual microvariables. The center of mass coordinate \(\bar{X} = \sum_{i=1}^{N} \bar{q}_i/N\) is an example. Let the Lagrangian of the system be \(L(q, \dot{q})\) \((\dot{q} \equiv dq/dt)\), which is an extensive quantity of order \(N\) and let us focus our attention on the following time evolution kernel for \(t_i \leq t \leq t_f\) in the path integral representation,

\[
\langle q^\prime| e^{-(i/\hbar)\hat{H}(t_f-t_i)}|q\rangle = \int [d^nq] \exp \left\{ \frac{i}{\hbar} S[q]\right\}, \tag{12.4.45}
\]

where \(S[q] = \int dt L(q, \dot{q})\) is the action. In the classical limit \(\hbar \to 0\), all the variables lose fluctuation since \(1/\hbar\) multiplies the whole action and each \(q_k\) obeys the deterministic Euler-Lagrange equation,

\[
0 = \frac{\delta S[q]}{\delta q_k(t)} = \frac{\partial L}{\partial q_k(t)} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_k(t)} \right). \tag{12.4.46}
\]
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The macroscopic limit $N \to \infty$ looks similar but has a crucial difference. To see this we first rewrite $S[q]$ in terms of the macrovariable $X$ and the remaining microscopic variable $q'$, relative coordinates for example. Then $S[q]$ has in general the form

$$S[q] = NS^{(1)}[X] + S^{(2)}[X, q'] + S^{(3)}[q'], \quad (12\cdot4\cdot47)$$

where $S^{(1)}[X]$ has always a factor $N$ in front since $S[q]$ is of extensive character. $S^{(2)}$ and $S^{(3)}$ involve the sum $\sum_{x}$ over the microvariable $q'$. We change the variable $q \to (X, q')$ with Jacobian $\det M = \exp \text{Tr} \ln M$, $M = \partial(q)/\partial(X, q')$. Since $\text{Tr}$ here involves $\sum_{x}$, $\det M$ is an exponential of the quantity of order $N$. Now we see clearly that only $X$ loses fluctuation and becomes a deterministic variable (whose value depends on $\hbar$) while $q'$ remains fluctuating. As will be explained in Chapter XIII the macrovariable becomes a classical number which specifies the Hilbert space spanned by the microvariables, which are still operators. We notice here that the integration over $q'$ affects the stationary value of $X$; the equation of motion of $X$ is dependent on the interaction between $X$ and $q'$.

Below we first introduce the definition of the macrovariable $X$ which is defined in the limit $N \to \infty$. However we sometimes call $X$ as the macrovariable when $N$ is a finite but large number.

The main purpose of this subsection is to derive the compact form of the macroscopic generating functional $W^{MC}$. The functional form of $W^{MC}$ is greatly simplified since the macrovariable loses its fluctuation as $N \to \infty$. A simple form of $\Gamma^{MC}$ is also derived by using the Legendre transformation. It is important to note that $W^{MC}$ and $\Gamma^{MC}$ contain the Planck constant $\hbar$ although the macrovariable is a deterministic quantity. This reflects the effect of the microscopic degrees of freedom which have been integrated over.

The compact expressions (12\cdot4\cdot66) and (12\cdot4\cdot69) below are the main results. Although it is not shown here, they can equally be derived by the methods other than that presented below, i.e. by the use of stationary phase or by the diagrammatic method of previous sections, see Ref. 14) for more details.

(i) Definition of macrovariable

The precise definition of macroscopic limit is given by quantized field theory since the particle statistics plays an essential role. This will be given in Chapter XIII but here we concentrate on $N$-particle system. As has been stated, the definition of macrovariable $X$ involves the average over macroscopic size of $q$. The most general expression is given by using general form of extensive quantity $Q$,

$$X = \lim_{N \to \infty} X^N, \quad X^N = \frac{1}{N} Q(q), \quad (12\cdot4\cdot48)$$

$$Q(q) = \sum_{n=1}^{\infty} \sum_{k_1, \ldots, k_n} Q^{(n)}_{k_1 k_2 \ldots k_n} q_{k_1} q_{k_2} \ldots q_{k_n}, \quad (12\cdot4\cdot49)$$

where the summation over $k$ extends from 1 to $N$. Coefficients $Q^{(n)}_{k_1 k_2 \ldots k_n}$ should satisfy the condition that when summed over $k_1, k_2, \ldots, k_n$ from 1 to $N$, then it is of order $N$,.
\[ \sum_{k_1,\ldots,k_N} Q_{k_1\cdots k_N}^{(n)} = O(N). \quad (12.4.50) \]

The right-hand side depends on \( n \) so that it is written as \( NQ_n \). A convenient way to judge whether a given function \( f(q) \) is an extensive quantity or not is to put \( q_k = C \) (constant which is independent of \( k \)) and see how \( f(q) \) behaves for large \( N \). In the case here \( Q(q) \) is required to behave as \( N \sum_{n=1}^{\infty} Q_n C^n \) which is \( O(N) \) if the sum over \( n \) converges. The macrovariable is the extensive quantity divided by \( N \). Since the Hamiltonian or the Lagrangian itself should have an extensive character, it is of the form \( (12.4.49) \).

In the above formula, the range over which the average is taken is \( N \), the whole extent of the system. But in a realistic application, we need the macrovariable averaged over the macroscopic size \( N_0 \) which is not the whole system. If we write \( N_0 = \alpha N \), this can be done by taking the limit \( N \to \infty \) while keeping \( \alpha \) fixed to be \( 0 < \alpha < 1 \). Although this is a more relevant case, we take whole \( N \) as the average size since it is simpler and the extension to the above case is straightforward.

(ii) Definition of \( W^{MC}[J^{(-)}, J^{(+)}] \)

Let us take \( \tilde{H} \) and \( \tilde{O} \) in (12.1.10) as follows: \( \tilde{H} = H_0 + V(\tilde{q}) \) as in (12.4.1), (12.4.2) and \( \tilde{O} = Q(\tilde{q}) \) of (12.4.49). Thus \( W[J_1, J_2] \) is written as follows,

\[ e^{i\langle H \rangle W[J_1, J_2]} = \text{Tr} \{ \tilde{R}^{J_1} \tilde{\rho} \tilde{R}^{J_2} \} , \quad (12.4.51) \]

\[ \tilde{R}^H = \text{Exp} \left[ -\frac{i}{\hbar} \int_{t_i}^{t_f} dt \{ \tilde{H} - J_i(t) Q(\tilde{q}) \} \right] . \quad (12.4.52) \]

In order to ensure the classical limit for finite \( N \), as was done in (12.4.8) and (12.4.9), we use \( \tilde{W}[J^{(-)}, J^{(+)}] \) defined by

\[ \tilde{W}[J^{(-)}, J^{(+)}] = \frac{1}{\hbar} W[J_1, J_2] \mid_{J_1, J_2 = J^{(+)} \pm (\hbar/2) J^{(-)}} , \quad (12.4.53) \]

where \( \tilde{W}[J^{(-)}, J^{(+)}] \) is the quantity of \( O(N) \).

Moreover it is necessary to rescale \( J^{(-)} \) to \( J^{(-)}/N \) in order to ensure the large \( N \) limit. Thus we define generating functional of macrovariable \( X \) as

\[ W^{MC}[J^{(-)}, J^{(+)}] = \lim_{N \to \infty} \tilde{W}[J^{(-)}/N, J^{(+)}] , \quad (12.4.54) \]

where \( W^{MC} \) is the macroscopic generating functional of \( O(1) \). Another way to get generating functional of \( O(1) \) is to divide \( \tilde{W}[J^{(-)}, J^{(+)}] \) by \( N \). We thus define \( W_1 \) as follows,

\[ W_1[J^{(-)}, J^{(+)}] = \lim_{N \to \infty} \frac{1}{N} \tilde{W}[J^{(-)}, J^{(+)}] . \quad (12.4.55) \]

\( W_1 \) has higher powers of \( J^{(-)} \) but \( W^{MC} \) contains only the term which is linear in \( J^{(-)} \). The first term of \( W_1 \) and \( W^{MC} \) is known to coincide with each other.\(^{10}\) We use, however, \( W^{MC} \) in the following. In the model calculation of Ref. 14, \( W_1 \) has also been used.

The necessary prescription is therefore just to replace \( J^{(-)} \) with \( \hbar J^{(-)}/N \). Now we
can write $W^{MC}[J^{(-)}, J^{(+)}]$ in the path integral representation as follows,

$$e^{i W^{MC}[J^{(-)}, J^{(+)}]} = \lim_{N \to \infty} \int \mathcal{D}^N \theta \, e^{i S[\phi_1, \phi_2] - \frac{i}{\hbar} \int_{t_i}^{t_f} dt J^{(-)}(t) \phi_1 - \frac{i}{\hbar} \int_{t_i}^{t_f} dt J^{(+)}(t) \phi_2} \left\langle \int_0^\infty dx \mathcal{K}^{(+) - (N/2N) J^{(+)}}_{N \phi_1} \left| \phi_1 \right\rangle \left\langle x \right| \mathcal{K}^{(-) - (N/2N) J^{(-)}}_{N \phi_2} \left| \phi_2 \right\rangle^* \right\rangle \right. \quad (12.4.56)$$

$$= \lim_{N \to \infty} \left[ \int \mathcal{D}^N \phi_1 d^N \phi_2 \right] \rho_i^N(\phi_1^t, \phi_2^t) e^{i \int S[\phi_1^t, \phi_2^t]} A_{J^{(-)}/N \phi_1^t}^{J^{(+)}/N \phi_2^t} \right\rangle \quad (12.4.57)$$

Here $\phi_{1,2}$ has $N$ components and $S[\phi]$ is the action of the system given by

$$S[\phi] = S_0[\phi] - \int_{t_i}^{t_f} dt V(\phi(t))$$

where $S_0$ is the free action (F.4) and $A_{J^{(-)}/N \phi_1^t}$ is the source term of the macrovariable defined as

$$A_{J^{(-)}/N \phi_1^t}^{J^{(+)}/N \phi_2^t}[\phi_1, \phi_2] \equiv \exp \left[ \frac{i}{\hbar} \int_{t_i}^{t_f} dt J^{(-)}(t) Q^{(-)}(\phi_1(t), \phi_2(t)) + i \int_{t_i}^{t_f} dt \frac{J^{(-)}(t)}{N} Q^{(+)}(\phi_1(t), \phi_2(t)) \right] \right. \quad (12.4.59)$$

We have introduced, using $Q(\vec{q})$ of (12.4.49),

$$Q^{(-)}(\phi_1, \phi_2) = Q(\phi_1) - Q(\phi_2) \quad (12.4.60)$$

$$Q^{(+)}(\phi_1, \phi_2) = \frac{1}{2} \left\{ Q(\phi_1) + Q(\phi_2) \right\} \quad (12.4.61)$$

The path integral $\int \mathcal{D}^N \phi_1 d^N \phi_2$ is performed for $t_i \leq t \leq t_f$ with the condition: $\phi_1(t_f) = \phi_2(t_f)$ with the same notation introduced in (F.5).

(iii) Compact form of $W^{MC}$ and $\Gamma^{MC}$

The disappearance of the fluctuation from macrovariable $\bar{X}$ is known from the well-known formula,

$$(W^{MC})_{0}(t, s) = \lim_{N \to \infty} \left\{ \frac{1}{2} \left\langle \bar{X}^N(t), \bar{X}^N(s) \right\rangle_{\rho_s} - \left\langle \bar{X}^N(t) \right\rangle_{\rho_s} \right\} \left\langle \bar{X}^N(t) \right\rangle_{\rho_s} \right\} \quad (12.4.62)$$

Here the following notations have been introduced,

$$(W^{MC}_{\alpha, \beta})_{0}(t, s) = \left. \frac{\delta^2 W^{MC}[J^{(-)}, J^{(+)}]}{\delta J^{(-)}(t) \delta J^{(+)}} \right|_{J^{(-)} = J^{(+)} = 0} \quad (\alpha, \beta = +, -) \quad (12.4.63)$$

If Eq. (12.4.62) is accepted, higher derivatives of $W^{MC}$ with respect to $J^{(-)}$ vanish so that we can show that $W^{MC}$ takes a very simple form in the large $N$ limit. In fact by taking the following conditions into consideration,

$$W^{MC}[J^{(-)}, J^{(+)}]_{J^{(-)} = 0} = 0$$

(12.4.64)
\[
\frac{\delta W^{MC}[J^{(-)}, J^{(+)}]}{\delta J^{(-)}(t)} \bigg|_{J^{(-)}=0} = X(t, J^{(+)}, \rho_i), \quad (12.4.65)
\]

we easily obtain \( W^{MC}[J^{(-)}, J^{(+)}] \) through the expansion by \( J^{(-)}(t) \) as

\[
W^{MC}[J^{(-)}, J^{(+)}] = W^{MC}[J^{(-)}, J^{(+)}] \bigg|_{J^{(-)}=0} + \int_{t_i}^{t_f} dt J^{(-)}(t) \left\{ \frac{\delta W^{MC}}{\delta J^{(-)}(t)} \bigg|_{J^{(-)}=0} \right\} + \ldots
\]

\[
= \int_{t_i}^{t_f} dt J^{(-)}(t) X(t, J^{(+)}, \rho_i). \quad (12.4.66)
\]

In the above formulas \( X(t, J^{(+)}, \rho_i) \) is the value of the macrovariable \( X(t) \) in the presence of \( J^{(+)} \). The equation corresponding to (12.4.66) for the classical case is (12.4.30). However \( W^{MC} \) has a simpler representation than \( W_0 \) because of the absence of the average over the initial distribution \( \bar{q}_{\phi}(\rho, q) \). This is true since \( X \) loses both quantum and thermal fluctuations.

The time development of the expectation value of an arbitrary physical observable is determined by the stationary condition of the effective action \( I'[X^{(-)}, X^{(+)}] \). In the case of the macrovariable \( X \), we first note the following relations,

\[
X^{(+)}(t) = \frac{\delta W^{MC}}{\delta J^{(+)}(t)} = X(t, J^{(+)}, \rho_i), \quad (12.4.67)
\]

\[
X^{(-)}(t) = \frac{\delta W^{MC}}{\delta J^{(-)}(t)} = \int_{t_i}^{t_f} ds J^{(-)}(s) \frac{\delta X(s, J^{(+)}(t), \rho_i)}{\delta J^{(+)}(t)} \equiv J^{(-)} \cdot A[J^{(+)}], \quad (12.4.68)
\]

where \( A[J^{(+)}] = (W^{MC}_r)[J^{(+)}] \) is easily seen to be the retarded Green's function of the macrovariables in the presence of \( J^{(+)} \). Note here that \( X^{(+)} \) or \( X^{(-)} \) is related to \( X_1 \), \( X_2 \) of (12.1.12) by \( X^{(+)} = (1/2)(X_1 + X_2), \) \( \hbar X^{(-)} = (X_1 - X_2) \).

The effective action \( I'^{MC}[X^{(-)}, X^{(+)}] \) is obtained by carrying out the Legendre transformation,

\[
I'^{MC}[X^{(-)}, X^{(+)}] = W^{MC}[J^{(-)}, J^{(+)}] - \int_{t_i}^{t_f} dt \{ J^{(-)}(t) X^{(+)}(t) + J^{(+)}(t) X^{(-)}(t) \}
\]

\[
= \int_{t_i}^{t_f} dt J^{(-)}(t) X(t, J^{(+)}, \rho_i) - \int_{t_i}^{t_f} dt \{ J^{(-)}(t) X(t, J^{(+)}, \rho_i) + J^{(+)}(t) X^{(-)}(t) \}
\]

\[
= - \int_{t_i}^{t_f} dt X^{(-)}(t) J^{(+)}(t, X^{(+)}, \rho_i). \quad (12.4.69)
\]

Here \( J^{(+)} \) is expressed in terms of \( X^{(+)} \) by inverting the relation (12.4.67). We emphasize the dual character of (12.4.66) and (12.4.69). Now the equation of motion of \( X(t) \) is given as

\[
0 = \frac{\delta I'^{MC}[X^{(-)}, X^{(+)}]}{\delta X^{(-)}(t)} \bigg|_{X^{(-)}=0} = - J^{(+)}(t, X, \rho_i), \quad (12.4.70)
\]

where we have used the fact that \( J^{(-)} = 0 \) corresponds to \( X^{(-)} = 0 \) by (12.4.68). Equation (12.4.70) corresponds to (12.1.16) written in terms of the variables \( X^{(a)} \). It can straightforwardly be obtained by inverting the relation (12.4.67) and by setting
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$J^{(+)} = 0$.

For the calculation of $W_{MC}[J^{(-)}, J^{(+)}]$ using an explicit model, see Ref. 14).

§ 12.5. Model calculation with initial equilibrium

The purpose of this section is to apply the Feynman rule taking the equilibrium distribution as an initial density matrix\textsuperscript{15,16} The diagrammatical rule becomes very concise in this case and this situation may exhaust almost all the experimental situations.

Necessary formula is derived in Appendix G for the quantum mechanical system. Here the rule is rewritten in field theoretical form and a simple field theoretical model is adopted which is a macroscopic system in a large volume $V$. This serves as a demonstration that our formalism can be applied, with modest changes of the rule, to a field theoretical system. Although the model is a simple one, the utility of inversion method in non-equilibrium is well exemplified. Thus we have two subjects in mind, (i) explicit application of Feynman rule to field theoretical model, (ii) explicit application of inversion method to non-equilibrium processes.

Before going into calculations, let us have a look at the present situation in the non-equilibrium theory. At present, there exist several formalisms of the field theoretical method at finite temperature\textsuperscript{1,2,7,17~19} In the situation where the initial state is prepared as an equilibrium distribution at some time $t_i$, there is a real time formulation in which $3 \times 3$ rather than $2 \times 2$ matrix form of the contour-ordered Green's functions is utilized. This has been given independently by Wagner\textsuperscript{20} and by Fukuda et al.\textsuperscript{15,16}

There is one thing that has to be noted. It is related to the interaction among particles in the initial state which is usually called the initial correlation. Concerning the problem of how to take the initial correlation into account in the non-equilibrium Green's function formalism or the Liouville operator method\textsuperscript{21} various attempts are present after the pioneering work of Fujita,\textsuperscript{22} in which he derived a generalized version of the Kadanoff-Baym equation by introducing initial correlation functions. Fujita's theory is based on the Kadanoff-Baym formalism\textsuperscript{18} which consists of the analytic continuation of the imaginary-time Green's function, and the discussion is somewhat complicated. Later Hall simplified the formalism by making use of the Schwinger-Keldysh theory in which only $2 \times 2$ matrix form of the contour-ordered Green's functions appear.\textsuperscript{23} The most remarkable difference between the theory due to Hall and Fukuda et al. and Wagner is that in the latter formalism it is allowed to treat the initial correlation just as same as the one defined at the later time while, in Hall's (and also Fujita's) theory, the initial correlation is artificially introduced. In addition, Hall's theory is known not to be suitable for discussing the long time phenomena compared to the relaxation time so that it does not describe in detail the relaxation of the system to the equilibrium state.

Here we emphasize the fact that the Hamiltonian describing the equilibrium state and the Hamiltonian that causes the time development of the system is essentially the same because we are studying one and the same system. The only difference is the absence or the presence of the external time-dependent parameters but among other
things the interaction of the particles or the fields making up the system is totally the same. Thus we have to treat the initial correlation and the time-dependent part of the Hamiltonian on an equal basis, as has been done in Refs. 15), 16) and 20). These results are utilized in the following model calculations.

12.5.1. The model

Now we specify the model. The field introduced is the Hermite bosonic field $\phi(x)$. It is assumed to have zero spin and to interact through the term $\phi^3$. Our model Hamiltonian is given by

$$H = H_0 + V', \quad (12.5.1)$$

$$H_0 = \frac{m}{2} \int d^3x \{ \dot{\phi}(x) + \phi(x) \phi^2(-\nabla^2) \phi(x) \}, \quad (12.5.2)$$

$$V' = g \int d^3x \phi(x)^3 - \int d^3xf(x, t)\phi(x), \quad (12.5.3)$$

where $\dot{\phi} \equiv (d/dt)\phi$ and $g$ represents the coupling strength. The time-dependent source $f(x, t)$ coupled linearly to $\phi$-field is introduced which brings the system into a non-equilibrium state. The mass parameters $m$ are inserted in order to make the comparison with the particle mechanics easy. The function $\omega(k^2) = \omega_k$ in Fourier space is the dispersion of the $\phi$ field. We assume the finite gap for $\omega_k$ otherwise the mode with infinitely long wave length may invalidate the existence of the thermodynamic limit where the volume of the system $V$ goes to infinity.\(^a\) (See § 13.4 for more details.) Thus it is required that

$$\omega_k > 0. \quad (12.5.4)$$

The free part $H_0$ can be diagonalized by the Fourier transform

$$\phi(x) = \frac{1}{\sqrt{V}} \sum_k e^{-ik \cdot x} \phi_k,$$

where $\mathbf{k} = (2\pi/L)(n_x, n_y, n_z)$ with $n_x, n_y, n_z = 0, \pm 1, \pm 2, \cdots$ and $L^3 = V$. Since the field is real, the real part of $\phi_k$ is even while the imaginary part is odd under $\mathbf{k} \leftrightarrow -\mathbf{k}$. Let us quantize the system. The canonical momentum $\hat{p}(x)$ is $m\dot{\phi}(x)$ and satisfies

$$[\hat{p}(x), \hat{p}(y)] = \frac{\hbar}{i} \delta(x-y) \quad (12.5.5)$$

or

$$[\hat{\phi}_k, \hat{\phi}_{-k}] = \frac{\hbar}{i} \delta_{k,-k}. \quad (12.5.6)$$

Suppose the external source $f(x, t)$ is absent in the interval $-\infty < t < t_1$ so the system is initially in the equilibrium with temperature given by $\beta = 1/T$. The onset of non-equilibrium process is denoted by the initial time $t = t_1$ and it is our purpose to follow the system after $t = t_1$.

In Appendix G, the path integral expression of $\mathcal{W}$ is given in the form of (G·22). Following the same procedure, it is easy to convince oneself that the expectation
value of any operator $\hat{O}(\phi)$ is written as

$$\langle \hat{O}(\phi) \rangle_t = \left( \exp \frac{S}{\hbar} \right) \exp \left[ -\frac{1}{\hbar} \int_{t_0}^{t} V^{(0)}(\phi(\tau)) d\tau \right] \left. \frac{i}{\hbar} \int_{t_0}^{t} \{ V^{(\phi_1(t))} - V^{(\phi_2(t))} \} dt \right] O(\phi(t)) \bigg|_{\text{conn}, \phi=0}. \quad (12.5.7)$$

Here the symbol $|_{\text{conn}}$ implies that only the diagrams that are connected with operator $\hat{O}$ have to be kept. We have used $O(\phi_1(t))$ for the operator $\hat{O}$ but $O(\phi_2(t))$ or $O(\phi^{(s)}(t))$ with $\phi^{(s)} = s\phi_1 + (1-s)\phi_2$ can equally be used. They all give the same results.

There are three kinds of independent fields $\phi(x, t), \phi_1(x, t), \phi_2(x, t)$ along the three contours and $V^{(\phi_1(t))}$, for example, is given explicitly by

$$g \int d^3 x \phi_1(x, t) - \int d^3 x f(x, t) \phi_1(x, t). \quad (12.5.8)$$

From (G.25)~(G.28) $S$ is expressed, by rewriting the formula in field theoretical notations as

$$S = \int d^3 x d^3 y S(x, y), \quad (12.5.9)$$

$$S(x, y) = i \int dtds \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(+)}(x, t)} \Delta(x - y, t - s) \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(-)}(y, s)} + f(y, s) \right) \right. \left. + \frac{1}{2} \int dtds \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(+)}(x, t)} \overline{\Delta}(x - y, t - s) \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(-)}(y, s)} \right. \left. + \int dt d\tau \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(+)}(x, t)} \overline{G}(x - y, t, \tau) \frac{\hbar}{i} \frac{\delta}{\delta \phi(y, \tau)} \right. \left. + \frac{1}{2} \int dt d\tau d\tau' \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(+)}(x, t)} \overline{G}(x - y, \tau, \tau') \frac{\hbar}{i} \frac{\delta}{\delta \phi(y, \tau')} \right). \quad (12.5.10)$$

Here we have set $j(-) = 0$ in (G.25)~(G.28) and have defined

$$\phi^{(+)} = \frac{\phi_1 + \phi_2}{2}, \quad \phi^{(-)} = \phi_1 - \phi_2. \quad (12.5.11)$$

The propagator $\Delta$, etc., are given in Fourier space as

$$\Delta(k, t - s) = \frac{1}{V} \sum_{\mathbf{k}} e^{i \mathbf{k} \cdot (x - y)} \Delta(k, t - s), \quad \text{etc.}, \quad (12.5.12)$$

$$\Delta(k, t - s) = \theta(t - s) \frac{\sin \omega_{\mathbf{k}}(t - s)}{m \omega_{\mathbf{k}}}, \quad (12.5.13)$$

$$\overline{\Delta}(k, t - s) = - \left( \coth \frac{\omega_{\mathbf{k}} \beta \hbar}{2} \right) \frac{\cos \omega_{\mathbf{k}}(t - s)}{2m \omega_{\mathbf{k}}}, \quad (12.5.14)$$
\[ G(k, \tau, \tau') = \theta(\tau' - \tau) \frac{\cosh \omega_h (\tau - \tau' + \frac{\beta \hbar}{2})}{2m\omega_h \sinh \omega_h \frac{\beta \hbar}{2}} + (\tau' \leftrightarrow \tau) \] (12.5.15)

and similarly for \( \bar{G} \) which depends explicitly on \( t_i \). The following properties of the above rules are crucial in the diagrammatic expansion. The \( \phi^{(\pm)} \)-field is connected only with \( \phi^{(\pm)} \) through \( A_s \) which is independent of \( \beta \). The remaining three propagators \( \bar{A}, \bar{G} \) and \( G \) represent the effects of the heat bath. The integration over \( t \) or \( s \) extends from \( t_i \) to \( t_f \) while \( \tau \) or \( \tau' \) ranges from \( \tau_i \) to \( \tau_f \). The final results turn out of course to depend only on the difference \( \tau_f - \tau_i = \beta \hbar \).

As the operator \( \hat{O}(\phi_1(t)) \) of (12.5.7) it is convenient to use \( \hat{O}(\phi^{(\pm)}(t)) \) and write also the potential as

\[ V^I(\phi_1(t)) - V^I(\phi_2(t)) \]

\[ = g \int d^3x \left\{ 3\phi^{(\pm)}(x, t)^2 \phi^{(\pm)}(x, t) + \frac{1}{4} \phi^{(-)}(x, t)^2 \right\} - \int d^3x f(x, t) \phi^{(-)}(x, t) . \] (12.5.16)

Since we have discussed all the necessary formulas of evaluating \( \langle \hat{O} \rangle_t \), we are going to actual evaluation using inversion method.

12.5.2. Dissipation through inversion method

A formal non-equilibrium inversion method is the following. Suppose the fictitious time-dependent source \( J(t) \) (we suppress \( x \) for simplicity) is coupled to the operator \( \hat{O} \) we are interested in and consider the Hamiltonian

\[ \hat{H}^I = \hat{H} - J(t) \hat{O} . \] (12.5.17)

We first calculate the expectation value of \( \hat{O} \) as a function of \( J \),

\[ \langle \hat{O} \rangle_t = F[J] . \] (12.5.18)

Invert (12.5.18) by solving it as a function of \( t \), in favour of \( J \) and set the fictitious source equal to zero,

\[ J(t) = F^{-1}[\langle \hat{O} \rangle_t] = 0 , \] (12.5.19)

where \( F^{-1} \) is the inverse function of \( F \). This is the equation of motion of \( \langle \hat{O} \rangle_t \). The correspondence between (12.5.19) and \( \Gamma[\phi_1, \phi_2] \) defined by the double Legendre transformation (12.1.11) is simply that \( \langle \hat{O} \rangle_t = \phi_1 = \phi_2 \). In fact \( J(t) \) in Eq. (12.5.19) equals to

\[ - \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_1(t)} \bigg|_{\phi_1 = \phi_2} \quad \text{or} \quad \frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_2(t)} \bigg|_{\phi_1 = \phi_2} . \]

Let us take the operator \( \hat{\phi}(x) \) as the simplest example of operator \( \hat{O} \). Since in our model \( J \) is present as a physical source, see (12.5.3), \( J \) is not a fictitious source and the first equality of (12.5.19) itself (without setting it to be zero) is the equation of motion of \( \langle \hat{\phi} \rangle_t \).
In Fig. 12.1, the diagrams up to the second order of $g$ are shown. The diagrams of Figs. 12.1(b) and (c) are independent of $J$ so that they are expected to add up to a constant which is independent of $t$. Indeed by an explicit calculation using (12.5.9) \( \sim (12.5.15) \) they give the equilibrium value $\langle \tilde{\phi}(x) \rangle_{eq}$ evaluated in the first order of $g$,

$$
\langle \tilde{\phi}(x) \rangle_{eq} = \frac{3\hbar}{m\omega_0^2} \sum_k \frac{\coth \frac{\omega_k \beta \hbar}{2}}{m \omega_k},
$$

(12.5.20)

where $\omega_0$ implies $\omega_{k=0}$. Since we are interested in the time evolution of $\langle \tilde{\phi}(x) \rangle_t$, the equilibrium value is subtracted below and we consider $\phi(x, t) \equiv \langle \tilde{\phi}(x) \rangle_t - \langle \tilde{\phi}(x) \rangle_{eq}$. The sum of the contributions from the diagrams Figs. 12.1(a) and (d) is given by

$$
\phi(x, t) = \int d^3y \int_{t_i}^t ds \Delta_h(x - y, t - s) f(y, s)

+ 36g^2\hbar \int d^3x' d^3yd^3y' \int_{t_1}^t dt' ds ds' \Delta_h(x - x', t - s) \tilde{A}(x' - y, s - s')

\times \Delta_h(x' - y, s - s') \Delta_h(y - y', s' - t') f(y', t').
$$

(12.5.21)

Here the inversion method in terms of $g$ is utilized. In this case it is simply accomplished up to order $g$ by inserting the lowest relation into the second terms on the right-hand side. We can of course use the inversion formulas (7.2.4) and (7.2.5) but the result is the same. Let us define the self-energy,

$$
\Sigma(x - y, t - s) = \tilde{A}(x - y, t - s) \Delta_h(x - y, t - s),
$$

then we get

$$
\phi(x, t) = \int d^3y \int ds \Delta_h(x - y, t - s) f(y, s)

+ 36g^2\hbar \int d^3x' d^3y \int_{t_i}^t dt' ds \Delta_h(x - x', t - t') \Sigma(x' - y, t' - s) \phi(y, s).
$$

(12.5.22)

This can be cast into the differential equation by using
\[ m\left( \frac{\partial^2}{\partial t^2} + \omega^2(-\nabla^2) \right) \Delta_\delta(x-y, t-s) = \delta^q(x-y) \delta(t-s). \]

In this way the equation of motion of Fourier component \( \phi_k(t) \) of \( \phi(x, t) \) is obtained up to \( g^2 \),

\[ m\left( \frac{\partial^2}{\partial t^2} + \omega_k^2 \right) \phi_k(t) - g^2 \int_{t_i}^t \sum_{k'} \Delta_k(t-s) \phi_{k'}(s) ds = J_k(t), \tag{12.5.23} \]

\[ \sum_{k'}(t-s) = 36 \hbar \frac{1}{V} \sum_{k'} J(k', t-s) \Delta_k(k-k', t-s). \tag{12.5.24} \]

Equation (12.5.23) is linear in \( \phi_k(t) \) but this is of course due to our approximation. For higher orders, non-linear terms appear.

In order to solve (12.5.22), the form of \( J(x, t) \) has to be fixed. For definiteness we take in the following two cases for the \( t \)-dependence of \( J \). In the first case \( t_i \) is taken to be \( -\infty \) which is suited for deriving the adiabatic equation of motion. We can study the correction term to the equilibrium process coming from the non-adiabatic effect. The second one is the case with \( t_i=0 \) and the behaviour of the system for \( t>0 \) is discussed. This case is more directly related to the real situation. With \( \epsilon>0 \), we thus consider

\begin{align*}
\text{Case I} & \quad t_i = -\infty, \quad J(x, t) = e^{\epsilon t} \bar{J}(x, t), \tag{12.5.25} \\
\text{Case II} & \quad t_i = 0, \quad J(x, t) = (1 - e^{-\epsilon t}) J(x). \tag{12.5.26}
\end{align*}

For Case I, \( \bar{J} \) is assumed to be slowly varying and to become finite when \( t \to -\infty \). When \( \bar{J} \) is independent of \( t \), both cases seem to be transformed each other by redefining the initial time. However the precise results of two cases are not the same and the applicability of the two for the practical problems are different of course.

(i) Case I

By using (12.5.25) in (12.5.21) and by assuming for the moment that \( \bar{J} \) is independent of \( t \), the lowest term is explicitly calculated in this case as

\[ \phi_k(t) = \int_{-\infty}^t \Delta_k(k, t-s) \bar{J} \epsilon e^{\epsilon s} ds = \frac{1}{m\omega_k} \frac{\omega_k}{\epsilon^2 + \omega_k^2} J_k(t). \tag{12.5.27} \]

\[ = \frac{1}{m\omega_k} \frac{\omega_k}{\epsilon^2 + \omega_k^2} J_k(t). \tag{12.5.28} \]

Note that for \( g=0 \) the minimum of the potential of the Hamiltonian of \( \phi \)-field (at the time \( t \)) is at \( J_k(t)/ \omega_k^2 \) whose absolute value is smaller than that of (12.5.28). Only for the adiabatic limit \( \epsilon=0 \), the system stays at the minimum which continuously changes with time. Otherwise it follows the minimum with some time delay.

Now the \( t \)-dependence of \( \bar{J} \) is recovered which is expanded around \( s=t \) as

\[ J_k(s) = e^{\epsilon s} \left( \bar{J}_k(t) + (s-t) \bar{J}_k(t) + \cdots \right), \tag{12.5.29} \]

and study the solution of (12.5.22) or (12.5.23). We take the limit \( \epsilon \to 0 \) after the calculation which leads to the correct adiabatic expansion and keep up to the first time derivative in the following. The lowest expression of (12.5.22) is
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\[
\phi_k(t) = \int_{-\infty}^{t} ds \Delta_{kn}(k, t-s) J_k(s) = \frac{J_k(t)}{m\omega_k} + \frac{\pi}{m\omega_k} \delta'(\omega_k) \int J_k(t) + \cdots. \tag{12.5.31}
\]

The second term of (12.5.31) vanishes due to (12.5.4). We insert the relation (12.5.31) into the second order term on the left-hand side of (12.5.23) and the adiabatic expansion (12.5.29) is made, which is again written in terms of $\phi_k(t)$. This process is the adiabatic inversion and the formulas (7.2.4) and (7.2.5) can alternatively be used regarding the expansion parameter $g$ there as the number of dots (time derivative) here. Both methods lead to the same result,

\[
m \dot{\phi}_k(t) + m\eta_k \phi_k(t) + (m\omega_k^2 + \rho_k) \phi_k(t) = J_k(t), \tag{12.5.32}
\]

\[
\rho_k = -\lim_{\epsilon \to 0} \int_{-\infty}^{0} \Sigma_k(-t)e^{\epsilon t} dt, \tag{12.5.33}
\]

\[
m\eta_k = -\lim_{\epsilon \to 0} \int_{-\infty}^{0} \Sigma_k(-t)te^{\epsilon t} dt. \tag{12.5.34}
\]

Here appeared two physical parameters $\rho_k$ and $\eta_k$ which we discuss in some detail. 1) $\rho_k$ represents the correction to the dispersion $\omega_k$. The following equilibrium relation holds:

\[
(m\omega_k^2 + \rho_k) \phi_k(t) - J_k(t) = \left. \frac{\delta F[\phi]}{\delta \phi_k} \right|_{\phi_k = \phi_k(t)}, \tag{12.5.35}
\]

where $F[\phi]$ is the equilibrium free energy as a function of $\phi$ with the source taking its value $J_k(t)$. In order to see this, let us calculate $F[\phi]$ following the definition of free energy through the Legendre transformation. Consider the Hamiltonian (12.5.1)~(12.5.3) and the equilibrium generating functional $W[j]$ defined by

\[
\exp(-\beta' W[j]) = \text{Texp} \left\{ -\beta' \left( \hat{H} - \int j(x) \phi(x) d^3 x \right) \right\}
\]

with $\beta'$ the temperature which is calculated later. The free energy $F[\phi]$ is defined by

\[\text{(a)}\]

\[\text{(b)}\]

\[\text{(c)}\]

Fig. 12.2. Diagrams for calculating the equilibrium generating functional $W[j]$. Each line represents the equilibrium propagator (11.4.15).
the Legendre transformation as

$$F[\phi] = W[j] - \int d^3x \, j(x) \frac{\delta W[j]}{\delta j(x)}, \quad (12.5.36)$$

$$\phi(x) = -\frac{\delta W[j]}{\delta j(x)}. \quad (12.5.37)$$

We have to calculate $W[j]$ and $F[\phi]$ up to order $g^2$. The diagrams to be studied are shown in Fig. 12.2, where only the source dependent graphs are considered. In Fig. 12.2, we have defined $\bar{J} = \bar{J}(x, t) = j(x, t) + j(x)$ and all the lines there represents the equilibrium propagator (12.5.15). The result of calculation is

$$W[j] = -\sum_k \frac{\bar{J}_k \bar{J}_k}{2 m \omega_k} (1 + C_k) \quad (12.5.38)$$

$$+ 3g^2 \sqrt{\frac{V}{m \omega_k}} \frac{1}{2} \sum_k \coth \frac{\omega_k \beta' \hbar}{2} \frac{1}{2 m \omega_k}, \quad (12.5.39)$$

where

$$C_k = \frac{9g^2 \hbar}{2 m \omega_k^2} \sqrt{\frac{V}{m}} \sum_{k'} \frac{1}{m^2 \omega_k \omega_{k'}} \left( \frac{\coth \frac{\omega_k \beta' \hbar}{2}}{\omega_k + \omega_{k'} + \omega_{k'-k}} - \frac{\coth \frac{\omega_k \beta' \hbar}{2}}{\omega_k - \omega_{k'-k}} \right). \quad (12.5.40)$$

$\phi_k$ has a $\bar{J}$-independent term by (12.5.37), which is subtracted from $\phi_k$. This is equivalent to calculate $F[\phi]$ by retaining only (12.5.38). Therefore

$$\phi_k = \frac{\bar{J}_k C_k}{m \omega_k^2}, \quad (12.5.41)$$

$$F[\phi] = \frac{1}{2} \sum_k \phi_k \frac{m \omega_k^2}{1 + C_k} \phi_{-k} - \sum_k J_k(t) \phi_{-k}$$

$$\simeq \frac{1}{2} \sum_k \phi_k m \omega_k^2 (1 - C_k) \phi_{-k} - \sum_k J_k(t) \phi_{-k}. \quad (12.5.42)$$

We have obtained $F[\phi]$ up to order $g^2$.

There is a relation $\rho_k = -m \omega_k^2 C_k$, which is straightforwardly proved by calculating (12.5.33) with (12.5.24). Then $\rho_k$ turns out to be equivalent to $-m \omega_k^2$ times (12.5.40) but $\beta'$ there is replaced by $\beta$. Up to the order we are considering, $\beta'$ can be set to $\beta$ since $\beta' - \beta$ is shown (see (12.5.63) below) to be of the order $g$ in the adiabatic limit. Recall that (12.5.40) is multiplied by $g^2$. Thus Eq. (12.5.35) is proved, which is however an example of the general theorem presented in § 12.6 below which is valid for any adiabatic processes.

2) The parameter $\eta_k$ represents the dissipative effect which is seen to be positive. The reason why Fig. 12.1(d) produces the dissipative term is that $\bar{A}$ represents the correlation of the particles in the heat bath. This fact can been seen by cutting $\bar{A}$ line. Then the loop in Fig. 12.1(d) becomes the scattering diagram of particle represented by external lines with that in the heat bath. $\eta_k$ is calculated as
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\[
\eta_h = \frac{4\hbar q^2}{V} \sum_k \frac{\coth \frac{\omega_k \beta \hbar}{2}}{2m^3 \omega_k \omega_{k-\nu}} \int_{-\infty}^{0} \sin(\omega_{k-\nu} t) \cos(\omega_k t) e^{st} dt
\]

\[
= \frac{4\hbar q^2}{m^3 V} \sum_k \frac{\pi}{2m^3 \omega_k \omega_{k-\nu}} \left( \coth \frac{\omega_k \beta \hbar}{2} \right) \left( \delta'(\omega_k + \omega_{k-\nu}) - \delta'(\omega_k - \omega_{k-\nu}) \right). \quad (12.5.43)
\]

In the above expressions, the first term in the curly bracket vanishes by (12.5.4) and the second term is the origin of dissipation. Here we note that \( \delta'(x) \) is an odd function and \( \coth x \) is a positive decreasing function of \( x > 0 \). Therefore (12.5.43) is positive. (This is seen by slightly regularizing \( \delta'(x) \) and replacing \( \coth(\omega_k \beta \hbar/2) \) by \( (1/2)(\coth(\omega_k \beta \hbar/2) - \coth(\omega_k - \omega_{k-\nu} \beta \hbar/2)) \). By using the full order expression, (12.5.48) below, the positivity of \( \eta \) can be proved quite generally. Incidentally \( \eta_h \) has a non-zero value in the classical limit since \( \hbar \coth(\omega_k \beta \hbar/2) \to 2/\beta \omega_k \) as \( \hbar \to 0 \).

Let us compare the mechanism of dissipation with that of Caldeira-Leggett (C-L).^{25} The expression (12.5.43) comes from the loop diagram and the finite \( \eta_h \) is obtained by the distribution of \( \omega_k \) which becomes continuous when \( V \to \infty \). The important point is that our mechanism holds even if (12.5.4) is imposed. In the model of Ref. 25), the coordinate \( \phi \) is linearly coupled with other \( \phi \) having the frequency \( \omega_i \). They assumed that \( \omega_i \) is distributed in the region including \( \omega_i = 0 \) and defined the distribution function

\[
\rho(\omega) = \sum_i \frac{\pi \delta(\omega - \omega_i)}{m \omega_i}. \quad (12.5.44)
\]

Their crucial assumption is \( \rho(\omega) \sim \eta \omega \) for small \( \omega \). In such a case \( \eta \) is given by

\[
\eta = \rho'(\omega)|_{\omega=0} = -\sum_i \int_{-\infty}^{0} \frac{\sin \omega_i t}{m \omega_i} e^{st} dt. \quad (12.5.45)
\]

We believe, however, that both the linear coupling and the assumed behavior of \( \rho(\omega) \) are not natural and will not be the general mechanisms realized in nature. Our mechanism however is universal in the sense that the dissipation originates from the non-linear interaction, i.e., scattering among particles, under the assumption (12.5.4), which gives zero for (12.5.45). Moreover the temperature dependence of \( \eta \) has to be introduced by hand in C-L while it is a calculable quantity in our method.

Here we compare the above results with the general form of time-dependent Ginzburg-Landau (TDGL) equation, which will be derived in general terms in the next section, see (12.6.21) below. In the case considered here, it takes the form

\[
D^2(\phi_h(t)) Y_h(t) \left[ \phi_h(t) \right] + \frac{\delta F[\phi_h(t)]}{\delta \phi_h(t)} = 0, \quad (12.5.46)
\]

where

\[
D(\phi_h(t)) = \frac{\delta^2 F}{\delta \phi_h(t) \delta \phi_h(t)}; \quad (12.5.47)
\]

\[
Y_h(t) = i \int_{-\infty}^{t} dt' \langle t' - t \rangle \left[ \phi_h(t'; t), \phi_h(t'; t) \right] \gamma_{eq}. \quad (12.5.48)
\]
We can prove quite generally that $Y_k(t) > 0$. In (12.5.48), $\langle \cdots \rangle_{eq}$ implies\(^6\) the equilibrium average (at $t$) of the “Heisenberg” operator $\tilde{\phi}(t'; t)$ where the source term $J_k(t)$ takes the constant value $J_k(t)$ independent of the integration variable $t'$. The equilibrium here is also the one with the fixed $J_k(t)$. Since $F[\phi]$ has been calculated in (12.5.42), what is left is the evaluation of $Y_k(t)$. This is again done by diagrams shown in Fig. 12.3. The diagram of Fig. 12.3(a) vanishes by (12.5.4) and Fig. 12.3(b) gives

$$Y_k(t) = g^2 \hbar \frac{1}{m^2 \omega_k^4} \frac{1}{V} \sum_{\nu} \frac{\pi \delta'(\omega_{\nu} - \omega_{k-\nu})}{m^2 \omega_{\nu} \omega_{k-\nu}} \times \left( \coth \frac{\omega_{\nu} \beta \hbar}{2} - \coth \frac{\omega_{k-\nu} \beta \hbar}{2} \right).$$

Here $\beta'$ is the equilibrium temperature at $t$, which is a function of $t$. But since $Y_k$ is already of order $g^2$, we can set $\beta' = \beta$. In the same way $D(\phi_k(t)) = m \omega_k^2$. Collecting these results and comparing with (12.5.43), (12.5.46) is seen to agree with (12.5.32) up to $\phi_k$.

(ii) **Case II**

We solve (12.5.23) by the Laplace transformation,

$$\tilde{\phi}_k(p) = \int_0^\infty dt e^{-pt} \phi_k(t), \quad (\text{Re} \ p > 0)$$

$$= \frac{\tilde{f}_k(p)}{m(p^2 + \omega_k^2) - g^2 \Sigma_k(p)},$$

The asymptotic behavior for $t \to \infty$ is determined by the zero of the denominator, which is written as $p = \pm i \omega_k + \delta_k$. Here $\delta_k$ is of the order $g^2$ and is given by

$$\delta_k = \frac{g^2 \Sigma_k(\pm i \omega_k)}{\pm 2 i \omega_k m} = - \delta_k^R + i \delta_k^I.$$  \hfill (12.5.51)

The real part of $\delta_k$ is calculated to be

$$\delta_k^R = \frac{9 g^2 \hbar \pi}{4 m^2 \omega_k} \times \frac{1}{V} \sum_{\nu} \coth \left( \frac{\omega_{\nu} \beta \hbar}{2} \right)$$

$$\times \left\{ \delta(\omega_{\nu} + \omega_{k-\nu} - \omega_k) - \delta(\omega_{\nu} + \omega_{k-\nu} + \omega_k) \right\}$$

$$+ \delta(\omega_{k-\nu} - \omega_{\nu} - \omega_k) - \delta(- \omega_{k-\nu} + \omega_{\nu} - \omega_k)$$

and the imaginary part $\delta_k^I$ has the same expression with $\delta$-function $\delta(\cdots)$ replaced by the principal part $\pm (1/\pi) P(1/(\cdots))$. $\Sigma_k(\pm i \omega_k)$ in (12.5.51), is defined to be $\lim_{p \to 0^+} \Sigma_k(\pm i \omega_k + \rho)$ since (12.5.49) requires $\text{Re} \rho > 0$. The positivity $\delta_k^R > 0$ can be
shown in the following way. In the curly bracket of (12.5.52), the first \( \delta \)-function gives positive value to \( \delta_k^R \) and the second vanishes due to (12.5.4). For the remaining two \( \delta \)-functions one can replace \( \coth(\omega_\nu \beta \hbar /2) \) by

\[
\{ \coth(\omega_\nu \beta \hbar /2) - \coth(\omega_{k-\nu} \beta \hbar /2) \} / 2.
\]

Then by the same argument used in (12.5.43) to prove \( \eta_k > 0 \), they are seen to be positive.

The above \( \delta_k^R \) is related to \( \eta_k \) of (12.5.43) by

\[
\eta_k = \lim_{\omega_k \to 0} \delta_k^R.
\]

The reason why we get different values for \( \eta_k \) and \( \delta_k^R \) if the limit \( \lim_{\omega_k \to 0} \) is not taken is due to the different choices of \( J \) in (12.5.25) and (12.5.26) and the expansion (12.5.29) for the case \( t_1 = -\infty \).

The solution \( J_k(t) \) is obtained by the inverse Laplace transformation. Using \( \tilde{J}_k(p) = (1/p - 1/(\epsilon + p)) J_k \), it is given, for the free case \( (\epsilon = 0) \), by

\[
\phi_k(t) = \frac{J_h}{m} \left\{ \frac{1}{\omega_k^2} e^{-\epsilon t} \frac{1}{\epsilon^2 + \omega_k^2} - \frac{e^{2 \omega_\epsilon t}}{\omega_k^2(\omega_k^2 + \epsilon^2)} \right\}.
\]

(12.5.53)

\( \phi_k(t) \) oscillates in the limit \( t \to \infty \) around the minimum value \( J_k/(m\omega_k^2) \) of the potential. For \( \epsilon \to 0 \) the amplitude of this oscillation becomes zero. Including the correction term of the order \( \epsilon^2 \), we obtain \( \phi_k(t) \) from (12.5.50),

\[
\phi_k(t) = \int_k \left\{ \frac{1}{m \omega_k^2} - \frac{g^2 \Sigma_k(0)}{\omega_k^2} \right\} e^{-\epsilon t} \frac{1}{m(\epsilon + \omega_k^2) - g^2 \Sigma_k(-\epsilon)}
\]

\[+ \exp(-\delta_k^R t) \times (\text{oscillating terms}). \]

(12.5.54)

The term proportional to \( \exp(-\delta_k^R t) \) comes from the pole at \( p = \pm i \omega_k + \delta_k \). As \( t \to \infty \), all the oscillating terms go away and the limiting value is given by

\[
\phi_k(\infty) = \frac{J_h}{m \omega_k^2 - g^2 \Sigma_k(0)}.
\]

(12.5.55)

This is equal to the adiabatic value as is seen by (12.5.32) and (12.5.33). The fact that \( \phi_k(\infty) \) is independent of \( \epsilon \) is due to the approximation we have made and if we include higher order of \( \epsilon \) it depends on how fast \( J_k(t) \) reaches a constant value. This is the case in general since internal energy of the system depends on the \( t \)-dependence of external parameter, i.e., the history of the process.

Although we have calculated only \( \langle \hat{\phi}_k \rangle \), any non-conserved operator is expected to tend to a constant value since the dissipative phenomenon comes from the loop diagrams which is universal for any operators.

(iii) Adiabatic temperature shift

A simple formula of the temperature shift due to adiabatic process exists\(^6\) and is derived as follows. Let us assume that the system is under equilibrium at \( t = -\infty \) and the Hamiltonian contains time-dependent parameter \( J(t) \) which varies adiabatically from \( J = 0 \) (at \( t = -\infty \)) to \( J \neq 0 \). The initial or final energy of the system is written as \( E \) or \( E' \) respectively where \( E' \) is a function of \( E \) and \( J \). Since the entropy is
conserved, we have

\[ S(E) = S'(E'(E, J)) \]

Therefore by differentiating with respect to \( E \), and by writing \( E' = E + \Delta E(E, J) \),

\[ \beta = \frac{\delta S}{\delta E} = \frac{\delta S'}{\delta E'} \frac{\delta E'}{\delta E} = \beta' \left( 1 + \frac{\partial \Delta E(E, J)}{\partial E} \right) \]

(12.5.56)

Therefore we get the formula

\[ \beta' - \beta = - \beta' \frac{\partial \Delta E}{\partial E} \]

(12.5.57)

The change in the temperature is caused by the dependence of the energy shift on the initial energy.

The energy difference \( \Delta E \) is obtained as follows. The expectation value of the Hamiltonian at time \( t \), \( \langle \hat{H}(t) \rangle \), is first calculated up to first order of \( g \). The Hamiltonian here contains of course the time-dependent parameter \( J(t) \) which is given in (12.5.25) and after diagrammatic evaluation we take the adiabatic limit \( \varepsilon \rightarrow 0 \). There are eight diagrams to be calculated (these can be straightforwardly written down) and the \( J \) dependent part of it is just \( \Delta E \) we are looking for. The result is\(^{16}\)

\[ \Delta E = \langle \hat{H}(t) \rangle_{ad} = - \sum_k \frac{J_k(t)J_{-k}(t)}{2m\omega_0^2} + \frac{3g\hbar \sqrt{V} J_0(t)}{2m\omega_0^2} \left( \frac{1}{V} \sum_k \coth \frac{\Omega_k \beta \hbar}{2} \right) \]

(12.5.58)

\[ = \int_0^{J(t)} X_k(t) dJ_k \]

(12.5.59)

\[ X_k(t) = \frac{J_{-k}(t)}{m\omega_0^2} + \delta_{k,0} 3g\hbar \sqrt{V} \frac{1}{2m\omega_0^2} \left( \frac{1}{V} \sum_k \coth \frac{\Omega_k \beta \hbar}{2} \right) \]

(12.5.60)

\[ = \delta W[j]/\delta j_k |_{j_k = 0} \]

(12.5.61)

Here \( W[j] \) is given in (12.5.38), (12.5.39) and we have used it up to order \( g \). \( X_k(t) \) is the adiabatic force exerted on the system and Eq. (12.5.59) represents the work done by the external source.

Now we can evaluate the temperature shift. The derivative \( \partial \Delta E / \partial E \) is evaluated as \( (\partial \Delta E / \partial \beta) (\partial \beta / \partial E) \) and \( \partial \beta / \partial E \) can be calculated by the lowest order relation as follows,

\[ \left( \frac{\partial \beta}{\partial E} \right)^{-1} = - \sum_k \left( \frac{\hbar^2 \omega_k^2}{4} \frac{1}{\sinh^2 \frac{\omega_k \beta \hbar}{2}} \right) \]

(12.5.62)

Therefore, by using (12.5.58) the adiabatic temperature shift is

\[ \beta' - \beta = - \frac{3g\hbar^2 \beta \sqrt{V} J_0}{2m\omega_0^2} \left( \frac{1}{V} \sum_k \frac{1}{2m\omega_0^2 \sinh^2 \frac{\omega_k \beta \hbar}{2}} \right) \times \left( \frac{\hbar^2 \omega_k^2}{4} \frac{1}{\sinh^2 \frac{\omega_k \beta \hbar}{2}} \right)^{-1} \]

(12.5.63)
The above result of temperature change starts from $O(g)$ and is also obtained by several different methods, see Ref. 16).

§ 12.6. Adiabatic inversion: TDGL equation

The inversion process in terms of adiabatic expansion has been discussed based on the perturbation in unharmonicity of the model Lagrangian. In this section, full order argument is given and the general form of time-dependent Ginzburg-Landau equation for any operator (other than Hamiltonian itself) is derived.\(^5,6\) For this purpose, Hamiltonian $\hat{H}(t)$ is assumed to contain time-dependent c-number parameters $\alpha_i(t)$ ($i=1\cdots N$) and is written as $\hat{H}(t)=\hat{H}(\alpha(t))$. Here we concentrate on the non-conserved operator.

Some of the parameters may appear in the Hamiltonian in the form $\alpha_i(t)\hat{O}_i(t)$ coupled to some operator $\hat{O}_i(t)$ but arguments below do not depend on the specific form of $\hat{H}(\alpha(t))$. Now the operator we are going to probe is the variables $\hat{X}_i(t)$ which is conjugate to $\alpha_i(t)$,

\[
\frac{d}{dt}\hat{X}_i(t)=\frac{\partial \hat{H}(\alpha(t))}{\partial \alpha_i(t)}.
\]  

In case $\alpha_i(t)$ couples linearly to $\hat{O}_i(t)$, we have $\hat{X}_i(t)=\hat{O}_i(t)$. In such a situation, we do not need explicit source term $J_i$ since $J_i$ is introduced as $J_i+\alpha_i$ and $J_i$ is eventually set to zero.

First, define the time evolution operator in the Schrödinger representation. In order to make the arguments general, we introduce extra fictitious sources $J_i(t)$ ($i=1\cdots M$) into Hamiltonian to probe the operator other than (12.6.1). They are Legendre transformed away afterwards. The parameters $\alpha_i(t)$ are on the other hand physical ones. In the following $(\alpha_i(t), J_i(t))$ is written as $\alpha_n(t)$ ($n=1\cdots N+M$) and the Hamiltonian is written as $\hat{H}(\alpha(t))$ as before. Using the time ordering operation, our time evolution operator is given by

\[
\hat{U}(t, t')=\text{Exp}\left\{-\frac{i}{\hbar} \int_{t'}^{t} ds \hat{H}(\alpha(s))\right\}.
\]  

Now at time $t$, the expectation value of any operator $\hat{X}_n(t)$ in Schrödinger representation is defined as

\[
\phi_n(t)=\langle \hat{X}_n(t) \rangle_t = \text{Tr}[\hat{\rho}_i \hat{U}(t, t_i)^\dagger\hat{X}_n(t) \hat{U}(t, t_i)]
\]

\[
= \left\langle \frac{\partial \hat{H}(\alpha(t))}{\partial \alpha_n(t)} \right\rangle_t,
\]  

where $\hat{\rho}_i$ is the initial equilibrium density matrix:

\[
\hat{\rho}_i=\frac{e^{-\beta \hat{H}_i}}{\text{Tr}e^{-\beta \hat{H}_i}},
\]

\[
\hat{H}_i=\hat{H}(t_i).
\]
Operator $\tilde{X}_n(t)$ in (12.6.3) can explicitly depend on $t$ which is called the kinematical time development. The dynamical time evolution, on the other hand, is the one caused by the Hamiltonian.

12.6.1. Adiabatic expansion

Now we concentrate on the adiabatic expansion of $\phi_n(t)$ assuming that the time variation of $a_n(t)$ is small. For this purpose we expand $a_n(t)$ according to the total number of dots (time derivatives). First few terms are given by; $a, \dot{a}, (\ddot{a}, (\ddot{a})^3), (\dddot{a}, \dddot{a}, (\dddot{a})^3)$, etc.

In the expression (12.6.3), $\tilde{U}(t, t_i)$ depends on $a(s)$ in the interval $t_i < s < t$. We expand $a(s)$ in $\tilde{U}(t, t_i)$ as follows,

$$a(s) = a(t) + \dot{a}(t)(s-t) + \cdots$$  \hspace{1cm} (12.6.6)

Of course, we can take other expansion scheme, but later we will see that the above choice turns out to be particularly suited for our purpose.

Keeping the term up to order $\dot{a}$, the expansion of $\tilde{H}(a(s))$ contained in $\tilde{U}(t, t_i)$ is given as follows,

$$\tilde{H}(s) = \tilde{H}(a(s)) = \tilde{H}(a(t)) + \frac{\partial \tilde{H}(a(t))}{\partial a_n(t)} \dot{a}_n(t)(s-t) + \cdots$$

$$= \tilde{H}(a(t)) + \tilde{H}_n(t) \dot{a}_n(t)(s-t) + \cdots.$$  \hspace{1cm} (12.6.7)

Then $\tilde{U}(t, t_i)$ becomes

$$\tilde{U}(t, t_i) = \prod_{i=1}^{L} \tilde{U}(t_i, t_{i-1}) = \prod_{i=1}^{L} \left( 1 - \frac{i}{\hbar} \Delta t \tilde{H}(t_i) \right)$$

$$= \prod_{i=1}^{L} \left( 1 - \frac{i}{\hbar} \Delta t \tilde{H}(a(t)) \right) + \sum_{k=1}^{L} \left[ \prod_{i=k+1}^{L} \left( 1 - \frac{i}{\hbar} \Delta t \tilde{H}(a(t)) \right) \right]$$

$$\times \left[ -\frac{i}{\hbar} \Delta t \dot{a}_n(t)(t_k - t) \tilde{X}_n(t) \right] \left[ \prod_{i=1}^{k-1} \left( 1 - \frac{i}{\hbar} \Delta t \tilde{H}(a(t)) \right) \right] + \cdots,$$  \hspace{1cm} (12.6.7)

where we have discretized the time interval $t - t_i$ into $L$ steps of size $\Delta t$. Let us introduce $\tilde{U}$ besides $\tilde{U}$ as

$$\tilde{U}(t_1, t_2) = \exp \left\{ -\frac{i}{\hbar} (t_1 - t_2) \tilde{H}(a(t)) \right\},$$  \hspace{1cm} (12.6.8)

which realizes the time evolution with parameters fixed to be $a(t)$. Thus we get

$$\tilde{U}(t, t_i) = \tilde{U}(t, t_i) - \frac{i}{\hbar} \int_{t_i}^{t} \tilde{U}(t, t') \tilde{a}_n(t')((t' - t) \tilde{X}_n(t)) \tilde{U}(t', t) + \cdots,$$  \hspace{1cm} (12.6.9)

where the relation $\tilde{U}(t', t_i) = \tilde{U}(t', t) \tilde{U}(t, t_i)$ has been used.

From (12.6.9), up to order $(\dot{a}(t))^3$, $(\dddot{a}(t))$, the following expression of $\phi_n(t)$ defined in (12.6.3) is thus obtained as
\[ \phi_n(t) = \text{Tr}\{ \hat{\rho}_1 \hat{U}(t, t_1)^\dagger \hat{X}_n(t) \hat{U}(t, t_1) \} + \sum_m \int_{t_1}^{t} \text{d}t' \frac{i}{\hbar} \hat{\alpha}_m(t') \times \text{Tr}\left\{ \hat{\rho}_1 \hat{U}(t, t_1)^\dagger [ \hat{U}(t, t') \left| (t' - t) \hat{X}_m(t') \right\rangle \left\langle \hat{U}(t', t) \right| \hat{X}_n(t) \right\} \hat{U}(t, t_1) \}. \]

(12.6.10)

Here \([A, B]\) represents the commutator. From now on we take \(t_1 = -\infty\) in order to discuss the adiabatic expansion. This is natural: in order to get finite increase of \(\phi\), an infinite time interval is required because the rate of the change in \(\alpha\) is very slow.

Let us discuss the operator \(\text{Tr}\{ \hat{\rho}_1 \hat{U}(t, t_1)^\dagger \cdots \hat{U}(t, t_1) \}\) appearing in the above formula. The time evolution operator \(\hat{U}(t, t_1)\) is the adiabatic limit of \(\hat{U}(t, t_1)\) in the sense that we have made all the derivatives of \(\alpha(t)\) go to zero (see (12.6.6)–(12.6.8)). The expectation value in the form \(\text{Tr}\{ \hat{\rho}_1 \hat{U}(t, t_1)^\dagger \hat{O} \hat{U}(t, t_1) \}\) = \(\text{Tr}\{ \hat{U}(t, t_1) \hat{\rho}_1 \hat{U}(t, t_1)^\dagger \hat{O} \}\) can be interpreted as a thermal equilibrium average at time \(t\), \(\text{Tr}\{ \hat{\rho}_{eq}(t) \hat{O} \}\). The state characterized by \(\hat{\rho}_{eq}(t)\) is obtained from \(\hat{\rho}_1\) by an adiabatic time evolution effected by \(\hat{U}\).

Now we study the same problem in more detail by rewriting (12.6.3) as

\[ \langle \hat{X}_n(t) \rangle_t = \text{Tr}\{ \hat{U}(t, t_1) \hat{\rho}_1 \hat{U}(t, t_1)^\dagger \hat{X}_n(t) \} \]

(12.6.11)

from the start and assume that we trace again the process of preceding adiabatic expansion of \(\hat{U}(t, t_1)\). Then we arrive at the same result (12.6.10) but in this case \(\hat{U}(t, t_1)\) appears in the combination \(\hat{U}(t, t_1) \hat{\rho}_1 \hat{U}(t, t_1)^\dagger\) which is the density matrix at time \(t\). In this form the state (represented by the density matrix) changes adiabatically which allows us to apply the adiabatic theorem to our result. Although this type of argument based on (12.6.11) is a simple repetition of (12.6.10) which is obtained in the Heisenberg representation (operator evolves in time), it is given in the Schrödinger picture. We recall here that the adiabatic theorem is usually formulated in the Schrödinger representation since it is a statement about the change of the levels of Hamiltonian. As is well known, the movement of each energy level can definitely be traced in the adiabatic limit. The picture becomes more transparent if we use the microcanonical ensemble with equal weight for each level in the energy interval \(E - \Delta E \sim E + \Delta E\). Note that the microcanonical distribution is equivalent to the canonical one, (12.6.4), for the macroscopic system and there is one to one correspondence between \(E\) of the microcanonical case and the temperature \(\beta^{-1}\) in the canonical distribution. Now after an adiabatic change the system is surely microcanonical again with the energy shifted from \(E\) to some \(E'\) and this determines new \(\beta'\).

Now employing the notation

\[ \langle \cdots \rangle_{eq,t} = \frac{\text{Tr}\{ e^{-\beta(\hat{H}(\alpha(t)))} \cdots \} }{\text{Tr} e^{-\beta(\hat{H}(\alpha(t)))} }, \]

we rewrite (12.6.10) as

\[ \phi_n(t) = \phi_{n,eq}(t) + \sum_m a_m(t) Y_{m,n}(\alpha(t)) + \cdots. \]

(12.6.12)

Here we have defined

\[ \phi_{n,eq}(t) = \langle \hat{X}_n(t) \rangle_{eq,t}, \]
\[ Y_{m,n}(t) = \int_{t_i}^{t} dt' (t' - t) \chi^\mu_{m,n}(t' - t, \alpha(t)), \quad (12 \cdot 6 \cdot 13) \]
\[ \chi^\mu_{m,n}(t' - t, \alpha(t)) = \frac{i}{\hbar} \langle [\tilde{X}_m(t'), \tilde{X}_n(t)] \rangle_{eq,t}, \quad (12 \cdot 6 \cdot 14) \]

where
\[ \tilde{X}(s) = \tilde{U}(s, t') \tilde{X}(t) \tilde{U}(s, t). \quad (12 \cdot 6 \cdot 15) \]

In (12 \cdot 6 \cdot 13), \( t \) is fixed in the course of time integration over \( t' \) and the average of \( \chi^\mu_{m,n} \) are taken by the equilibrium thermal state which is obtained by an infinitely slow change of \( \alpha(s) \) from \( s = t_i \) to \( t \). We arrived at this picture because we have chosen the expansion schemes (12 \cdot 6 \cdot 6) and (12 \cdot 6 \cdot 7).

In (12 \cdot 6 \cdot 12), the first term describes the adiabatic limit, that is, the equilibrium value while the second represents the leading non-equilibrium correction.

12.6.2. Equilibrium term

Now let us briefly discuss the equilibrium term, the first term on the right-hand side of (12 \cdot 6 \cdot 12). There are several ways of calculating equilibrium temperature \( \beta' \). The most straightforward way is to use the conservation of entropy in the adiabatic process, as given by (12 \cdot 5 \cdot 56). Once \( \beta' \) is fixed, it is easy to see that it can be written as a derivative of the potential \( ^{(5), 6} \)
\[ \phi_{n,eq}(t) = \left\langle \frac{\partial \tilde{H}(\alpha(t))}{\partial \phi_n(t)} \right\rangle_{eq,t} = \frac{\partial G(\alpha(t), T')}{\partial \alpha_n(t)}, \quad (12 \cdot 6 \cdot 16) \]

where \( G(\alpha(t), T') \) is the equilibrium Gibbs free energy at \( t \) with the temperature \( T' = 1/\beta' \), which also depends on \( t \),
\[ e^{-\beta G(\alpha(t), T')} = \text{Tr} e^{-\beta \tilde{H}(\alpha(t))}. \quad (12 \cdot 6 \cdot 17) \]

12.6.3. Inversion and TDGL

We are interested in the equation of motion of internal variable \( \phi_n(t) \) and solve (12 \cdot 6 \cdot 12) for \( \alpha_n(t) \). In order to perform this inversion, it is convenient to introduce the Legendre transform \( F(\phi_{n,eq}(t), T') \) of equilibrium potential \( G(\alpha(t), T') \) which is defined as
\[ F(\phi_{eq}(t), T') = G(\alpha(t), T') - \sum_n \alpha_n(t) \frac{\partial G(\alpha(t), T')}{\partial \alpha_n(t)}. \quad (12 \cdot 6 \cdot 18) \]

There is an identity,
\[ \frac{\partial G}{\partial \phi_{n,eq}(t)} = -\alpha_n(t). \quad (12 \cdot 6 \cdot 19) \]

The desired equation of \( \phi_n(t) \) is obtained using above \( F(\phi_{eq}(t), T') \). We thus write
\[ \alpha_n(t) = -\frac{\partial G(\phi(t), T')}{\partial \phi_n(t)} + \Delta \alpha_n, \quad (12 \cdot 6 \cdot 20) \]

and insert it into (12 \cdot 6 \cdot 12) to determine \( \Delta \alpha_n \) up to the lowest order of non-adiabaticity.
Alternatively we can apply directly the inversion formula \((7 \cdot 2 \cdot 4)\) and \((7 \cdot 2 \cdot 5)\) regarding the number of dots attached to variables as small expansion parameter \(g\). Both lead to the same result,\(^{5,6}\)

\[
\sum_{n'} D_{n,n'}(\phi(t)) \dot{\phi}_{n'}(t) + \frac{\partial F(\phi(t), T')}{\partial \phi_n(t)} + a_n(t) = 0 , \tag{12 \cdot 6 \cdot 21}
\]

where

\[
D_{n,n'}(\phi(t)) = \sum_{m,m'} F_{n,m}(\phi(t)) Y_{m',m}(\alpha(t)) F_{m',n'}(\phi(t)) ,
\]

\[
F_{n,m}(\phi(t)) = \frac{\partial^2 F(\phi(t), T')}{\partial \phi_n(t) \partial \phi_m(t)} . \tag{12 \cdot 6 \cdot 22}
\]

Note the order of indices \(m', m\) in \(Y_{m',m}\) and also that \(\alpha(t)\) in the argument of \(Y_{m',m}\) has to be expressed in terms of \(\phi(t)\). As the above arguments suggest, the functional form of \(F(\phi(t))\) is that of equilibrium free energy but \(\phi(t)\) itself takes the non-equilibrium value. This is precisely what we expect from the time-dependent Ginzburg-Landau (TDGL) equation.

However the conventional TDGL equation has the form, assuming \(a_n(t) = 0\),

\[
\dot{\phi}_n(t) = \sum_{m} K_{n,m} \frac{\partial F(\phi(t), T')}{\partial \phi_m(t)} , \tag{12 \cdot 6 \cdot 23}
\]

with \(K_{n,m}\) some constant matrix. But there is no reason why \(K_{n,m}\) is independent of \(\phi\) and exact treatment shown above indeed leads to \(K\) which is a function of \(\phi\).

The relaxation of \(\phi\) to the equilibrium value is studied by setting

\[
\phi_n(t) = \phi_{n,eq} + \Delta \phi_n(t) . \tag{12 \cdot 6 \cdot 24}
\]

Here we have assumed that \(\alpha_n(t) = 0\) in the original Lagrangian and \(\phi_{n,eq}\) is the stationary solution which minimizes the free energy \(F(\phi, T')\). The linearized equation

\[
\sum_{n'} D_{n,n'}(\phi_{eq}) \dot{\Delta} \phi_{n'}(t) + \sum_{n'} F_{n,n'}(\phi_{eq}) \Delta \phi_{n'}(t) = 0 \tag{12 \cdot 6 \cdot 25}
\]

has the solution of the form

\[
\Delta \phi_n(t) = e^{-\omega t} \Delta \phi_n(0) . \tag{12 \cdot 6 \cdot 26}
\]

The following properties of the eigenvalue \(\omega_i (i = 1 \sim N)\) can be proved:\(^6\)

(i) \(\text{Re} \omega_i \geq 0\) for any \(i\).

(ii) The number of real eigenvalues is \(2s - N\) while those with \(\text{Im} \omega_i \neq 0\) is \(2N - 2s\).

Here \(s\) is the number of operators with time reversal parity \(\epsilon_i^T = +1\) (or \(\epsilon_i^T = -1\) if it is larger than \(N/2\)).

These results lead to the Onsagar's reciprocity relation. For more about field theoretical discussion of TDGL, see Ref. 5) and the details about the non-adiabatic increase of the internal energy is found in Ref. 6).
References

9) As a textbook, see for example, C. Izykson and J. B. Zuber, Quantum Field Theory (McGraw-Hill, New York, 1980).
10) See, for example, A. L. Fetter and J. D. Walecka, Quantum Theory of Many-Particle System (McGraw-Hill, New York, 1971).
   G. Wentzel, Phys. Rev. 120 (1960), 1572.
   F. Mayne and I. Prigogine, Physica 22 (1956), 621.
Chapter XIII. Quantum Mechanics

The method of the Legendre transformation or on-shell expansion is quite useful also in quantum mechanical theory. The ground state, excited states and scattering process are our primary concerns all of which are determined in the scheme of on-shell expansion. Below we discuss several subjects of quantum mechanical system which can conveniently be studied by the technique of the Legendre transformation.

As has been stated in the Introduction, we will see that once the approximation is fixed at the level of generating functional, i.e., the effective action, no further approximation is allowed. This is so even if the Hamiltonian has no symmetry so that the approximation is not related to the violation of the symmetry as in the case of the discussion on excitation levels in superfluid system in Chapter XIV. This fact is illustrated in the calculation of energy levels.

After discussing the relation between stationary phase and the Legendre transformation and extending the effective action to the finite time interval case, we come to the investigation of the structure of the Hilbert space of macroscopic system. Here also the Legendre transformation is shown to be an important concept to elucidate the role of macrovariables. Using these results, we finally investigate and clarify the relation between the macrovariables and the theory of measurement.

§ 13.1. Energy levels by effective action

The formalism of the effective action \( \Gamma[\phi] \) is applied in this section to the quantum mechanical system to determine the energy eigenvalue of the excited levels.\(^1\) First, a formula is given which predicts the energy levels as a zero of ordinary function. Second, Bethe-Salpeter type equation is derived and it is shown that, in the ladder approximation, it gives the correct eigenvalue only when the self-energy type correction is included. Calculations show that the correct lowest order perturbative value is obtained if \( \Gamma[\phi] \) is kept up to lowest order and no further approximation is allowed. It follows that the usual ladder approximation where self-energy type graphs are neglected produces incorrect energy levels. These investigations show at the same time the essential difference between the case of local operator and that of non-local operator.

13.1.1. Energy levels by effective action — local source —

We consider one-dimensional quantum mechanical system described by the Lagrangian \( L(q(t), \dot{q}(t), t) \). The action is defined by

\[
I[q]=\int_{-\infty}^{\infty} dt L(q(t), \dot{q}(t), t), \tag{13.1.1}
\]

and the generating functional of the connected Green's function \( W[J] \) in the path integral form is also introduced as before by
\[ \exp(iW[J]) = \int[dq] \exp\left\{ iS[q] + i \int dt J(t) q(t)^N \right\}, \] (13.1.2)

where we have set \( \hbar = 1 \) and \( \int dq \) represents functional integral. \( J(t) \) is the artificially introduced source coupled to \( N \)-th power of \( q(t) \) with \( N \) some positive integer. We call \( J(t) \) local source since it couples to the product of \( q(t) \) referring to the same instant of time.

Now we define the effective action \( \Gamma \) through the Legendre transformation as usual,

\[ \Gamma[\phi] = W[J] - \int dt J(t) \phi(t), \] (13.1.3)

\[ \phi(t) = \frac{\delta W[J]}{\delta J(t)}. \] (13.1.4)

The well-known properties of the Legendre transformation lead to the following identities (see Appendix C),

\[ \frac{\delta^2 \Gamma[\phi]}{\delta \phi(t) \delta \phi(t')} = -\frac{\delta^2 W[J]}{\delta J(t') \delta J(t'')} = \delta(t - t''). \] (13.1.6)

To reproduce the original theory, we put \( J = 0 \) in (13.1.5) and get the equation of motion of \( \phi(t) \),

\[ \frac{\delta \Gamma[\phi]}{\delta \phi(t)} = 0. \] (13.1.7)

As in Chapter II, we assume that \( \phi = \phi^{(0)} \) and \( \phi = \phi^{(0)} + \Delta \phi \) are solutions to (13.1.7) and \( \Delta \phi \) is small. We get, up to 1st order in \( \Delta \phi \),

\[ \int dt' \left( \frac{\delta^2 \Gamma[\phi]}{\delta \phi(t) \delta \phi(t')} \right)_{t' = 0} \Delta \phi(t') = 0. \] (13.1.8)

In Fourier space this is written as

\[ K(\omega) \Delta \phi(\omega) = 0, \] (13.1.9)

where

\[ K(\omega) = -i \int dt \left( \frac{\delta^2 \Gamma[\phi]}{\delta \phi(t) \delta \phi(t')} \right)_{t' = 0} e^{i\omega(t - t')}, \]

\[ \Delta \phi(\omega) = \int dt \Delta \phi(t) e^{i\omega t} \] (13.1.10)

It can be checked that Eq. (13.1.9) determines the energy level of the system. In this sense we have called the same equation the mode determining equation (or the on-shell equation in the case of field theory), see Chapter II. Now Eq. (13.1.6) becomes diagonal in the Fourier representation,

\[ K(\omega) G(\omega) = 1. \] (13.1.11)
Since $G(\omega)$ is the Fourier transform of the second derivative of $W$, it has poles at the energy levels of the system. $K(\omega)$ has thus zeroes at the same points, and the converse is also true. Therefore if a zero point of $K(\omega)$ is found out, it is certainly the energy of the system.

Thus we arrived at the following procedure; the eigenvalues of the excitation energy is obtained by finding the zero of the ordinary analytic function $K(\omega)$,

$$K(\omega)=0. \quad (13\cdot 1\cdot 12)$$

Note that the pole cannot be found in a perturbative fashion but the zero can be. Note also that in the usual approach energy levels are found by solving the differential or integral equation or by looking for the eigenvalue of the energy matrix. The function $K(\omega)$ is calculable diagrammatically by expanding $K(\omega)$ in terms of the coupling constant contained in the Hamiltonian. This is explicitly done once the Hamiltonian $H$ is fixed. We have taken the simplest example of the Lagrangian,

$$L=L_0+L_1,$$

$$L_0=\frac{m}{2}\dot{q}(t)^2-\frac{m\omega_0^2}{2}q(t)^2, \quad L_1=-\lambda q(t)^4, \quad (13\cdot 1\cdot 13)$$

and have confirmed the validity of (13\cdot 1\cdot 12) perturbatively in $\lambda$, if $K(\omega)$ is calculated up to $n$-th order of unharmonicity $H_1$ by writing $H=H_0+H_1$, with $H_0$ the harmonic part, then the excited energy levels are correctly determined by (13\cdot 1\cdot 12) up to the same order.

### 13.1.2. Failure of ladder approximation — bilocal source —

Next we consider a system supplied with bilocal source term $\int dt dt' J(t, t') \times q(t)q(t')$ instead of the local term $\int dt J(t)q(t)^m$, namely

$$\exp[iW[J]]=\int[dq]\exp\left\{iS[q]+i\frac{1}{2}\int dt dt' J(t, t')q(t)q(t')\right\}. \quad (13\cdot 1\cdot 14)$$

By this choice of the source term the Bethe-Salpeter (BS) type wave equation\(^2\) emerges. In quantum mechanical case discussed here we are going to study the 2nd excited level, which corresponds to two-body BS equation. In this case, the second derivative of $W[J]$ evaluated at $J(t, t')=0$ gives the Green's function,

$$G(t_1, t_2; t'_1, t'_2)=-i\left(\frac{\delta^2 W[J]}{\delta J(t_1, t_2)\delta J(t'_1, t'_2)}\right)_0$$

$$=\langle 0|T \bar{q}(t_1) \bar{q}(t_2) \bar{q}(t'_1) \bar{q}(t'_2)|0\rangle$$

$$-\langle 0|T \bar{q}(t_1) \bar{q}(t_2)|0\rangle \langle 0|T \bar{q}(t'_1) \bar{q}(t'_2)|0\rangle$$

$$=\langle 0|T \bar{q}(t_1) \bar{q}(t_2) \bar{q}(t'_1) \bar{q}(t'_2)|0\rangle. \quad (13\cdot 1\cdot 15)$$

The functional derivative rule

$$\delta J(t_1, t_2)/\delta J(t'_1, t'_2)=\delta(t_1-t'_1)\delta(t_2-t'_2)+\delta(t_1-t'_2)\delta(t_2-t'_1)$$

is used in this subsection, assuming that $J(t, t')$ is symmetric with respect to $t$ and $t'$;
\[ J(t, t') = J(t', t) \]

Fourier transforming this expression after inserting complete set, we obtain \( G \) as a function of total energy \( E \) and relative energy \( \omega_n, \omega \),

\[
G(E; \omega, \omega') = \int dt dt' G(t_1, t_2; t_1', t_2') e^{iE t + i\omega t - i\omega' t'}
\]

\[
= i \sum_{n=1}^{\infty} \left( \frac{g_n(\omega) \bar{g}_n(\omega')}{E - \omega_n + i\epsilon} - \frac{\bar{g}_n(\omega) g_n(\omega')}{E + \omega_n - i\epsilon} \right) + \text{(regular part)} ,
\]  

(13.1.16)

where

\[
T = \frac{1}{2} (t_1 + t_2 - t_1' - t_2') , \quad t = t_1 - t_2 , \quad t' = t_1' - t_2' ,
\]  

(13.1.17)

\[
g_n(\omega) = \int dt g_n(|t|) e^{i\omega t} , \quad \bar{g}_n(\omega) = \int dt \bar{g}_n(|t|) e^{-i\omega t} ,
\]  

(13.1.18)

\[
g_n(|t|) = \langle 0 | T \bar{q}(t_1) q(t_2) | n \rangle e^{-i\omega_n (t_1 + t_2)/2} ,
\]

\[
\bar{g}_n(|t|) = \langle n | T \bar{q}(t_1) q(t_2) | 0 \rangle e^{-i\omega_n (t_1 + t_2)/2} .
\]  

(13.1.19)

Recall that the right-hand sides of (13.1.19) are functions of \(|t|\). Let us define the effective action,

\[
\phi(t, t') = \frac{\delta W[J]}{\delta J(t, t')} ,
\]  

(13.1.20)

\[
\Gamma(\phi) = W[J] - \frac{1}{2} \int dt dt' J(t, t') \phi(t, t') .
\]  

(13.1.21)

Hereafter, we use the matrix notation by regarding \( t, t' \) as single subscript of vector \( J \) or of matrix \( G \), etc. Of course the notation of the product of functionals follows the conventional matrix definition,

\[
(AB)(t_1, t_2; t_1', t_2') = \int dt dt' A(t_1, t_2; t_1', t_2') B(t_1', t_2; t_1, t_2') .
\]

Again by the properties of the Legendre transformation, we have

\[
\frac{\delta \Gamma(\phi)}{\delta \phi} = - J ,
\]  

(13.1.22)

\[\frac{1}{2} \frac{\delta^2 W[J]}{\delta J} \frac{\delta^2 \Gamma(\phi)}{\delta \phi \delta \phi} = -(1 + \bar{1}) ,
\]  

(13.1.23)

where \( 1 \) and \( \bar{1} \) denote two kinds of unit matrix, respectively, defined by

\[
1(t_1, t_2; t_1', t_2') = \delta(t_1 - t_1') \delta(t_2 - t_2') ,
\]

\[
\bar{1}(t_1, t_2; t_1', t_2') = \delta(t_1 - t_1') \delta(t_1' - t_2) .
\]  

(13.1.24)

In the Fourier representation, Eq. (13.1.23) becomes

\[
\frac{1}{2} GK = (2\pi)^2 (1 + \bar{1}) ,
\]  

(13.1.25)

where
\[ K(E; \omega, \omega') = -i \int dT dt dt' \left( \frac{\delta^2 \Gamma[\phi]}{\delta \phi(t_1, t_2) \delta \phi(t'_1, t'_2)} \right)_0 e^{iET + i\omega t - i\omega' t'} , \tag{13.1.26} \]

and the definition of \( G \) is given in (13.1.16). In (13.1.25), \( G(E; \omega, \omega') \) and \( K(E; \omega, \omega') \) are regarded as matrices with \( \omega \) and \( \omega' \) specifying rows and columns, but \( E \) is a parameter common to \( G \) and \( K \), and

\[ 1(\omega, \omega') \equiv \delta(\omega - \omega') , \quad \overline{1}(\omega, \omega') \equiv \delta(\omega + \omega') . \]

As in the preceding section, we define \( \phi^{(0)} \) by setting \( J = 0 \) in (13.1.20), which is the solution of equation of motion \( \delta \Gamma/\delta \phi = 0 \). Let us look for another solution of \( \delta \Gamma/\delta \phi = 0 \) in the form \( \phi = \phi^{(0)} + \Delta \phi \). Then we obtain, see (2.1.4a),

\[ \int d\omega' K(E; \omega, \omega') \Delta \phi(\omega') = 0 . \tag{13.1.27} \]

This is the Bethe-Salpeter equation in our problem and the eigenvector \( \Delta \phi \) corresponds to the B-S amplitude,

\[ \Delta \phi(\omega) \propto g_n(\omega) . \tag{13.1.28} \]

(i) **Free case**

We adopt the Lagrangian \( L_0 \) of (13.1.13). Then the effective action is known to be given by the following expression, see Appendix C,

\[ \Gamma[\phi] = -\frac{i}{2} \text{Tr} \ln \phi + \frac{i}{2} \text{Tr} \Delta^{-1}_F \phi , \tag{13.1.29} \]

where \( \text{Tr} \) and \( \ln \) must be taken in the matrix sense, i.e. we regard \( \omega \) and \( \omega' \) (\( t_1, t_2 \) and \( t'_1, t'_2 \)) as the indices of rows and columns, respectively. The equation of motion of \( \phi \) is

\[ 0 = \frac{\delta \Gamma[\phi]}{\delta \phi} = -i(\phi^{-1} - \Delta^{-1}_F) . \tag{13.1.30} \]

We put the solution \( \phi^{(0)} \) of the above equation into \( K \) of (13.1.26),

\[ \phi^{(0)} = \Delta_F , \tag{13.1.31} \]

\[ K = \Delta^{-1}_F \Delta^{-1}_F (1 + \overline{1}) \]

\[ = -2\pi m^2 F_0 \left( \frac{E}{2} + \omega \right) F_0 \left( \frac{E}{2} - \omega \right) \left( \delta(\omega - \omega') + \delta(\omega + \omega') \right) , \tag{13.1.32} \]

where \( F_0(\pm) \) is the inverse of the free propagator,

\[ F_0 \left( \frac{E}{2} \pm \omega \right) \equiv \omega^2 - \left( \frac{E}{2} \pm \omega \right)^2 - i\epsilon . \tag{13.1.33} \]

Hehe \(-i\epsilon \) is written explicitly. From (13.1.32) and (13.1.33) it is easy to see that eigenvalue equation (13.1.27) has the following solution,

\[ \Delta \phi(\omega) \propto \delta(\omega) , \tag{13.1.34} \]
\[ E = 2\omega_0. \quad (13.1.35) \]

The result (13.1.35) corresponds to the energy level of the 2nd excited state of harmonic oscillator. The reason we have got only the level of the 2nd excited state is that the matrix element of (13.1.19) vanishes in the free case except \( n = 2 \). Result (13.1.34) can also be checked by using (13.1.28) and by evaluating explicitly (13.1.18) and (13.1.19). We have thus seen that our eigenvalue equation (13.1.27) has the solution (13.1.34) and (13.1.35).

(ii) Perturbation

Next we consider the interaction Lagrangian \( L_I \) of (13.1.13). The effective action is given by (Appendix C),

\[ \Gamma[\phi] = -\frac{i}{2} \text{Tr} \ln \phi + \frac{i}{2} \text{Tr} \Delta_F^{-1} \phi - i\gamma[\phi], \quad (13.1.36) \]

where \( \gamma[\phi] \) stands for the sum of all the two-particle irreducible vacuum graphs whose internal lines are replaced by \( \phi \). Up to 1st order in \( \lambda \), \( \gamma[\phi] \) is given by the diagram looking like "8",

\[ \gamma[\phi] = -3i\lambda \int d\tau \phi(\tau, \tau)^2. \quad (13.1.37) \]

The equation of motion is

\[ 0 = -\frac{\delta \Gamma[\phi]}{\delta \phi(t, t')} \]

\[ = -i\{\phi^{-1}(t, t') - \Delta_F^{-1}(t, t') - 12i\lambda \phi(t, t) \delta(t - t')\}. \quad (13.1.38) \]

The solution, up to order \( \lambda \), is then given by

\[ \phi^{(0)}(t, t') = \Delta_F(t - t') - 12i\lambda \Delta_F(0) \int d\tau \Delta_F(t - \tau) \Delta_F(\tau - t'), \quad (13.1.39) \]

and we get

\[ K = \phi^{(0)-1}(1 + \bar{\lambda}) - \frac{\delta^2 \gamma[\phi]}{\delta \phi \delta \phi} \]

\[ = -2\pi m^2 F\left(\frac{E}{2} + \omega\right) F\left(\frac{E}{2} - \omega\right) (\delta(\omega - \omega') + \delta(\omega + \omega')) + 24i\lambda, \quad (13.1.40) \]

where

\[ F\left(\frac{E}{2} \pm \omega\right) = F_0\left(\frac{E}{2} \pm \omega\right) + 12g, \quad g = \frac{\lambda}{2m^2 \omega_0}. \quad (13.1.41) \]

\( F \) is the Fourier transformation of the inverse of the modified propagator \( \phi^{(0)} \) which contains the self-energy correction given by \( \delta \gamma[\phi] / \delta \phi \). Then Eq. (13.1.27) becomes

\[ F\left(\frac{E}{2} \pm \omega\right) F\left(\frac{E}{2} \pm \omega\right) \Delta \phi(\omega) = \frac{6i\lambda}{\pi m^2} \int d\omega' \Delta \phi(\omega'), \quad (13.1.42) \]

where we have assumed \( \Delta \phi(\omega) \) to be an even function since odd functions are trivial
solutions of (13.1.27). The solution of (13.1.42) is, apart from constant factor, the following,

\[ \Delta \phi(\omega) = \frac{6i\lambda}{\pi m^2} \frac{1}{F(E/2+\omega)F(E/2-\omega)}. \]  

(13.1.43)

The condition that Eq. (13.1.42) has a nonzero solution is

\[ 1 = \frac{6i\lambda}{\pi m^2} \int d\omega \frac{1}{F(E/2+\omega)F(E/2-\omega)}. \]  

(13.1.44)

This equation determines the energy of the 2nd excited state \( E \). Setting \( E = 2\omega_0 + E^{(1)} \), where \( E^{(1)} \) is the level shift of order \( \lambda \) (or \( g \)), and comparing the leading order of both sides of Eq. (13.1.44), we obtain the correct value,

\[ E^{(1)} = \frac{9\lambda}{m^2 \omega_0^2}. \]  

(13.1.45)

(iii) Incorrectness of ladder B-S equation

Here we note the following fact. If we remove the 2nd order part \((12g)^2\) contained in \( F(E/2+\omega)F(E/2-\omega) \) of (13.1.42) (because it is higher order in \( g \)), the result is altered to be \( 3\lambda/m^2 \omega_0^3 \), which is of course incorrect. In the usual "ladder" approximation, the self-energy part corresponding to \((12g)^2\) is neglected. But it is not allowed.

The reason why we cannot neglect the 2nd order term when we calculate 1st order energy value is that \( F_0(E/2 \pm \omega) \) given in (13.1.41) are in fact order \( \lambda \) near the solution \( E = 2\omega_0 + O(\lambda) \). Indeed, evaluating the \( \omega \)-integration in (13.1.44) by the contour which encloses the upper half-plane, the contribution from the two poles of the integrand at

\[ \pm \omega = \frac{E}{2} + \omega_0 + O(\lambda) = O(\lambda) \]  

(13.1.46)

turns out to be \( O(1/\lambda) \) because the distance between these poles is \( O(\lambda) \). (This cancels the prefactor \( \lambda \) in (13.1.44).) The contributions from others are \( O(1) \) at the same value of \( E \). So that \( F_0 \) in (13.1.41) is in fact order \( \lambda \). Therefore the seeming order of each term contained in \( F \) is not to be relied upon, so that the terms which are apparently higher order might contribute to the energy values of lower order.

Then the following question arises; is it enough to keep the terms of \( F \) up to 1st order in \( \lambda \) if we want to calculate the energy level up to 1st order? In the case of 1st order of the energy in \( \lambda \), it can be proved that the higher terms do not contribute to the result. This is seen as follows. If a seemingly higher-order term contained in \( F \) becomes order \( \lambda \) at the solution \( E = 2\omega_0 + O(\lambda) \), \( \omega = O(\lambda) \), it must have simple or multiple pole there. Otherwise it is indeed higher order in \( \lambda \). However, since \( F \) is the inverse of the full propagator, it has the form \( F_0 + \Sigma \) where \( \Sigma \) is the self-energy which is one-particle irreducible with external legs amputated. Thus \( F \) does not have any poles near the solution. Therefore \( F \) has no contribution which is effectively of order \( \lambda \) except for free term and 1st order term. Thus our treatment in which all the higher order terms have been neglected is justified since we are inter-
ested in the energy level up to order $\lambda$.

The above argument can be applied for higher-order calculation of the energy levels and once the 1st order energy is correctly obtained, naive perturbative treatment works for higher-order corrections.

13.1.3. Field theory

It is easy to convince oneself that the same conclusion holds for field theoretical case. Indeed we have confirmed the incorrectness of neglecting self-energy in the ladder approximation using a field theoretical model Hamiltonian.

In field theory, the Bethe-Salpeter equation in the usual ladder approximation neglects the self-energy correction. In such an approximation, it is known that the abnormal solution\(^{(4,5)}\) exists which has no non-relativistic counter part and that most of the solutions have negative norm.\(^{(6)}\) These phenomena might be the diseases of the ladder approximation. What we have shown above is that the eigenvalue itself, which is the most fundamental quantity to be calculated, is not reproduced correctly in the ladder approximation. The self-energy correction, which is included in a natural way if we start from the approximation to the effective action, recovers the correct value. Whether the inclusion of the self-energy also solves the other two diseases is an interesting problem. In this respect Higashijima has made an interesting observation using a model,\(^{(7)}\) where several pathological features have been shown to disappear when one includes self-energy corrections.

§ 13.2. Stationary phase and Legendre transformation

The relation between the stationary phase appearing in various integral formulas and the Legendre transformation is well known and it supplies a convenient calculational tool. We discuss such a relation in this section and in the following sections, the utility of the stationary phase is exemplified with some examples. The subject is discussed in this section by taking thermodynamic examples because the mathematical manipulation is easier than the quantum mechanical case. Translation of the following formulas into the zero temperature quantum mechanics will then be straightforward.

(1) Potentials of equilibrium thermodynamics

We start from the definition of entropy $S$ as a function of energy $E$,

$$ e^{S} = \text{Tr} \delta (\hat{H} - E). \tag{13\cdot2\cdot1} $$

Here $\hat{H}$ is the Hamiltonian of the system and the Boltzman constant has been set to unity. Now an integral representation of $\delta$-function is inserted as

$$ e^{S} = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dJ \text{Tr} e^{-J(\hat{H} - E)} = \frac{1}{2\pi i} \int dJ e^{JE - W(J)}, \tag{13\cdot2\cdot2} $$

where

$$ \text{Tr} e^{-\hat{H}} = e^{-W(J)}. \tag{13\cdot2\cdot3} $$

If the system is of macroscopic size of volume $V$, then we expect that $E$ and $W(J)$ is
of order $V$ and the above integral is dominated by the stationary point denoted by $J = \beta$. This $\beta$ is assumed to be real positive and plays the role of inverse temperature, which is defined by

$$\frac{\partial}{\partial J}(JE - W(J))\bigg|_{\beta} = 0. \quad (13.2.4)$$

Thus $E$ is given by $E = \partial W(\beta)/\partial \beta$ from which we get the relation $\beta = \beta(E)$. Thus, for large $V$, $S(E)$ and $W(\beta)$ are the Legendre transforms of each other,

$$S(E) = -W(\beta) + \beta \frac{\partial W(\beta)}{\partial \beta}. \quad (13.2.5)$$

Now define $F$ by $W(\beta) = \beta F(\beta)$, then

$$E = F + \beta \frac{\partial F}{\partial \beta}, \quad (13.2.6)$$

therefore from (13.2.5),

$$S(E) = \beta(E - F) = \beta^2 \frac{\partial F}{\partial \beta} = -\frac{\partial F}{\partial T},$$

where $T = \beta^{-1}$ is the temperature. The relation (13.2.6) itself can be regarded as a Legendre transformation between $E$ as a function of $S$ and $F$ as a function of $T$,

$$E(S) = F(T) - T \frac{\partial F(T)}{T}. \quad (13.2.7)$$

Through identities of the Legendre transformations (Appendix A), various thermodynamic relations such as $\partial E/\partial S = T$ are obtained.

(2) Expectation value in equilibrium

Let us take again a macroscopic system and consider the microcanonical expectation value of some operator $\hat{O}$,

$$\langle \hat{O} \rangle_k = \frac{\text{Tr} \delta(\hat{H} - E) \hat{O}}{\text{Tr} \delta(\hat{H} - E)} = \frac{\int dJe^{J\hat{H}} e^{-W(J)} \hat{O}}{\int dJe^{J(\hat{H} - E)} e^{-W(J)}} = \frac{\int dJe^{J\hat{H}} e^{-W(J)} \hat{O}}{\int dJe^{J\hat{H}} e^{-W(J)}}. \quad (13.2.8)$$

Here in the numerator, we have used the fact that for fixed $J$,

$$\text{Tr} e^{-\hat{H}} \hat{O} = \frac{\text{Tr} e^{-\hat{H}} \hat{O}}{\text{Tr} e^{-\hat{H}}} \times \text{Tr} e^{-\hat{H}} = \langle \hat{O} \rangle_k e^{-W(J)}.$$

Note that the numerator has been factorized into two disconnected factors, the one is the vacuum type graph which is summed into $e^{-W(J)}$ and the other factor is written as $\langle \hat{O} \rangle_k$, which is the sum of the graphs connected to the operator $\hat{O}$. The point is that $J$ integration of both numerator and denominator of (13.2.8) are dominated by the same stationary value of $W(J)$ at $J = \beta$ and get

$$\langle \hat{O} \rangle_J = \frac{\text{Tr} e^{-\beta \hat{H}} \hat{O}}{\text{Tr} e^{-\beta \hat{H}}} = \langle \hat{O} \rangle_k. \quad (13.2.9)$$
The above arguments show that microcanonical and canonical distribution are equivalent for macroscopic system, i.e., if the stationary point dominates.

(3) \(\delta\)-function formalism and Legendre transformation

There is a formalism which is closely related to the definition of free energy by the Legendre transformation. It consists in inserting \(\delta\)-function into the path-integral representation of free energy,

\[
e^{-\beta F(\beta)} = \text{Tr} e^{-\beta \hat{H}} = \int dq \langle q | e^{-\beta \hat{H}} | q \rangle = \int_{\beta} [dq] \exp \left\{ - \int_0^\beta d\tau L(\dot{q}(\tau), q(\tau)) \right\}.
\]  \hspace{1cm} (13.2.10)

Here \(\int_{\beta} [dq]\) implies the path-integration with the boundary condition \(q(0) = q(\beta)\). We have written all the coordinates of the macroscopic system by \(q\) and \(L\) is the imaginary time Lagrangian defined by

\[
L(\dot{q}(\tau), q(\tau)) = H(p(\tau), q(\tau)) - p(\tau) \frac{\partial H}{\partial p(\tau)}, \quad \dot{q}(\tau) = -\frac{\partial H}{\partial p(\tau)}.
\]  \hspace{1cm} (13.2.11)

Let us assume that \(O\) is a function of the coordinate \(q\) and insert

\[
1 = \prod_{\tau = 0}^\beta \int d\varphi(\tau) \delta \left( O(q(\tau)) - \varphi(\tau) \right)
\]

\[
= \prod_{\tau = 0}^\beta \int d\varphi(\tau) \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} df(\tau) e^{f(\tau)(O(q(\tau)) - \varphi(\tau))}
\]

into (13.2.10). Here suitable discretization of the interval \(0 < \tau < \beta\) has been assumed. Performing the path-integration over \(q\), we get

\[
e^{-\beta F(\beta)} = \prod_{\tau = 0}^\beta \int d\varphi(\tau) \frac{1}{2\pi i} \int df(\tau) \exp \left\{ W[J] - \int_0^\beta d\tau f(\tau) \varphi(\tau) \right\},
\]

\[
e^{W[J]} = \int_{\beta} [dq] \exp \left[ - \int_0^\beta d\tau \{ L + J(\tau) O(q(\tau)) \} \right].
\]  \hspace{1cm} (13.2.12)

Now we assume that the system is of macroscopic size and the Hamiltonian satisfies the condition that our system has a well-defined thermodynamic limit. We further assume that the operator \(O(q)\) is an extensive variable. Then both \(W[J]\) and \(\varphi(\tau)\) are proportional to the volume of the system and in the limit of large volume, the integral over \(J\) in (13.2.12) is dominated by the stationary point,

\[
e^{-\beta F(\beta)} = \prod_{\tau = 0}^\beta \frac{1}{2\pi i} \int d\varphi(\tau) e^{\Gamma[\varphi]},
\]  \hspace{1cm} (13.2.13)

where we have introduced

\[
\Gamma[\varphi] = W[J_c] - \int_0^\beta d\tau J_c(\tau) \varphi(\tau).
\]  \hspace{1cm} (13.2.14)

The stationary point \(J_c\) is defined by the solution of
\[ \frac{\delta W[J]}{\delta J(\tau)} - \varphi(\tau) = 0. \quad (13\cdot2\cdot15) \]

Note that \( I[\varphi] \) is just the Legendre transformation of \( W[J] \) and plays the role of Helmholtz free energy and hence is an extensive quantity. The final integration over \( \varphi \) in (13\cdot2\cdot13) is again dominated by the stationary point and the requirement of stationarity is just \( J = 0 \),

\[ \frac{\delta I[\varphi]}{\delta \varphi(\tau)} = -J(\tau) = 0. \quad (13\cdot2\cdot16) \]

Thus in the macroscopic limit

\[ e^{-\beta F(\beta)} = e^{\Gamma[\varphi^{(0)}]} = e^{W[J = 0]}, \quad (13\cdot2\cdot17) \]

where \( \varphi^{(0)} \) is the solution to (13\cdot2\cdot16). In the above argument \( \tau \) dependent source \( J(\tau) \) is not necessary if we are interested only in equilibrium quantities.

(5) Comparison between \( \delta \)-function formalism and Legendre transformation

Here we take a quantum mechanical system and study the differences between \( \delta \)-function formalism and the Legendre transforms. For any states \( |I\rangle \) and \( |F\rangle \), let us consider

\[ K = \langle F | e^{-i\theta(t^b - t^a)} | I \rangle = \int_B [dq] \exp \left\{ i \int_{t^a}^{t^b} dt \cdot L \right\}. \quad (13\cdot2\cdot18) \]

(i) \( \delta \)-function method

We insert

\[ 1 = \prod_{t^a}^{t^b} \int d\varphi(t) \delta \left( O(q(t)) - \varphi(t) \right) \]

into (13\cdot2\cdot18) and perform the path-integration over \( q \). The result has the form

\[ K = \prod_{t^a}^{t^b} \int d\varphi(t) e^{\Gamma[\varphi]} . \quad (13\cdot2\cdot19) \]

(ii) Legendre transform

Our original way of defining \( I[\varphi] \) was through the Legendre transformation,

\[ K_I = \int_B [dq] \exp \left\{ i \int_{t^a}^{t^b} dt \cdot [L + J(t)O(q(t))] \right\} = e^{W[J]}, \]

\[ I_2[\varphi] = W[J] - \int dt f(t) \frac{\delta W[J]}{\delta J(t)}. \]

The differences between (i) and (ii) are the following.

The presence of integration over \( \varphi \) implies that \( \varphi \) is the operator in (i) but it is \( c \)-number in (ii). Therefore \( I_1[\varphi] \) is the quantum action of the variable \( \varphi \) whereas in (ii) \( I_2[\varphi] \) is a \( c \)-number action whose stationary equation \( \delta I_2/\delta \varphi(t) = 0 \) determines the expectation value of operator \( \hat{O} \). The stationary equation for \( I_1 \) has no particular physical meaning except for the case that the stationary point of \( \varphi \) integration
dominates. On the other hand, for \( I_2 \) only the stationary solution has a physical significance, otherwise \( J \) does not vanish and we are looking at a theory different from the original one for which \( J = 0 \).

The spectrum in \( \phi \) channel can be studied as follows. In (i) we make an adiabatic expansion of \( I_1 \) in time variable,

\[
I_1[\phi] = -\int dt V(\phi(t)) + \int dt Z(\phi(t)) \dot{\phi}(t)^2 + \cdots. \tag{13.2.21}
\]

Taking first two terms of this expansion, for example, quantum theory of \( \phi \) channel, including excitation spectrum and so forth, can be developed.

In the formalism (ii), however, general on-shell expansion scheme does this job, as explained in Chapter II. Although \( \phi \) is a c-number variable, \( I_2[\phi] \) keeps fluctuating properties of the operator \( \hat{\mathcal{O}} \) in its functional form, which allows us to reconstruct the Hilbert space.

As has been stated, \( I_1[\phi] \) and \( I_2[\phi] \) are equal when the system is macroscopic and the operator \( \hat{\mathcal{O}} \) is an extensive quantity.

§ 13.3. Effective action of finite time interval

In quantum theory, we are usually interested in time evolution of the system which is governed by the time dependence of wave function. Once the initial wave function is fixed, it is calculated by solving the Schrödinger equation. Our attitude here is, instead, to study the expectation value of some operator we are interested in at any instant of time. The method of effective action enables us to know the expectation values of physical quantities without the knowledge of time-dependence of the wave function itself. When one wants to apply the effective action formalism, one has necessarily to incorporate the initial condition of the state. Thus we are led to effective action which depends on initial time \( t_i \) and initial state. Below we discuss these problems.

13.3.1. Effective action of single variable

The first definition of the effective action in the case considered is through the time evolution formula of the wave function,

\[
\psi(q, t) = \langle q | \psi, t \rangle = \int dq' K(q, t; q', t_i) \psi(q', t_i), \tag{13.3.1}
\]

\[
K(q, t; q', t_i) = \langle q | \hat{K}_i | q' \rangle. \tag{13.3.2}
\]

Here \( \hat{K}_i \) has been defined in (12.1.4). Effective action in finite time interval is given by first introducing the functional \( W_b[J] \) which contains the information of both boundaries at \( t = t_i, t_f \):

\[
e^{(i\hbar)W_b[J]} = K_f(q, t_f; q', t_i), \tag{13.3.3}
\]

where \( K_f \) is defined as in (13.3.2) and (12.1.4) with the replacement

\[
\hat{H}(t') \to \hat{H}(t') + J(t') \hat{\mathcal{O}}. \tag{13.3.4}
\]

\[
The operator $\hat{O}$ is the one we are going to probe. Effective action $\Gamma_\delta$ is given as
\begin{equation}
\Gamma_\delta[\varphi] = W_\delta[J] - \int_{t_\ell}^{t_\ell'} dt' J(t') \frac{\delta W_\delta[J]}{\delta J(t')} ,
\end{equation}
(13·3·5)
\begin{equation}
\varphi(t) = \frac{\delta W_\delta[J]}{\delta J(t)} . \quad (t_\ell \leq t \leq t_\ell')
\end{equation}
(13·3·6)

However the above definition of effective action does not satisfy the condition that $\varphi(t)$ is the expectation value of the operator $\hat{O}$ at $t$. The reason is that in (13·3·2) the time flows in one direction from $t_\ell$ to $t_\ell'$ whereas the expectation value requires the form $K^* \hat{O}K$ and the kernel $K^*$ represents the backward time evolution.

There are cases, however, where the solution to
\begin{equation}
\frac{\delta \Gamma_\delta[\varphi]}{\delta \varphi(t)} = 0
\end{equation}
(13·3·7)
corresponds to the expectation value $\langle \hat{O} \rangle$ at time $t$. This happens when the stationary phase dominates the path integral or when the Hamiltonian contains at most bilinear term of $q$ and $p$. This is easily seen for the case of dominance of the stationary phase since the stationary trajectory coincides with the expectation value itself.

In order to study the bilinear case, let us take a simple example. Consider thus the Hamiltonian
\begin{equation}
H_f(t) = \frac{1}{2m} p^2 + \frac{m\omega^2}{2} q^2 - J(t) q .
\end{equation}
(13·3·8)

We define $W$ by
\begin{equation}
e^{i W_{\delta[J]}} = \int_\delta [dq] \exp\left\{ i \int_{t_\ell}^{t_\ell'} dt' L(t') \right\} ,
\end{equation}
(13·3·9)
where the boundary conditions $q(t_\ell) = q'$, $q(t_\ell') = q$ have to be satisfied of course. The Lagrangian $L(t)$ is given by
\begin{equation}
L(t) = \frac{m}{2} \dot{q}^2 - \frac{m\omega^2}{2} q^2 + J(t) q .
\end{equation}
(13·3·10)

Using the result of Appendix E, see (E·18), the kernel $K_f$ corresponding to the above $L(t)$ is expressed as
\begin{align}
K_f(q, t_\ell' ; q', t_\ell) &= N \exp\{A\} , \\
\{A\} &= a(q^2 + q'^2) + bqq' + \int_{t_\ell}^{t_\ell'} dt \{v_1(t)q + v_2(t)q'\} J(t) \\
&\quad - \frac{1}{2} \int_{t_\ell}^{t_\ell'} dt \int_{t_\ell'}^{t_\ell'} ds J(t) G(t, s) J(s) .
\end{align}
(13·3·11)

Thus $W_\delta$ is given by
\begin{equation}
i W_\delta[J] = A + \ln N ,
\end{equation}
(13·3·12)
and $\Gamma_b$ has the expression
\[
\begin{align*}
\text{i} \Gamma_b[\varphi] &= a(q^2 + q'^2) + bqq' \\
&\quad - \frac{1}{2} \int_{t_1}^{t_2} dt \int_{t_1}^{t_2} ds \{i \varphi(t) - v_1(t)q - v_2(t)q'\} G^{-1}(t, s) \\
&\quad \times \{i \varphi(s) - v_1(s)q - v_2(s)q'\}, \\
&= \frac{q \sin \omega(t - t_1) + q' \sin \omega(t_2 - t)}{\sin \omega T},
\end{align*}
\]
(13.3.13)
where $G^{-1}$ is the inverse function of $G$. Now the equation of motion (13.3.7) has the solution
\[
\varphi(t) = \frac{1}{i} (v_1(t)q + v_2(t)q') = \frac{q \sin \omega(t - t_1) + q' \sin \omega(t_2 - t)}{\sin \omega T},
\]
(13.3.14)
where $T = t_2 - t_1$. This coincides with the expectation value of quantum operator $\tilde{q}$ at $t$ (and also with the classical trajectory), but as stated above it is a special property of our bilinear Hamiltonian. For general Hamiltonian the stationary solution of the above defined $\Gamma_b$ is not the expectation value of any operator. (Higher derivatives of $\Gamma_b$ have the meaning of time ordered Green's functions at finite time interval which will be useful objects in itself.)

13.3.2. Effective action of double variables

Construction of effective action whose stationary solution really corresponds to the expectation value of operator requires double variables as its arguments. The reason is that the expectation value involves complex conjugation of the wave function which evolves backward in time. The wave function $\Psi$ and $\Psi^*$ cannot be described by single time evolution kernel.

Let us consider the operator $\tilde{K}_1$ of (12.1.4) and the Schrödinger state $|\Psi, t\rangle$ at $t$. Then the expectation value of an operator $\tilde{O}$ at $t$ is given by using $|\Psi, t_i\rangle$ as
\[
\langle \Psi, t|\tilde{O}|\Psi, t\rangle = \langle \Psi, t_1|\tilde{K}_1^* \tilde{O} \tilde{K}_1|\Psi, t_1\rangle
\]
(13.3.15)
\[
= \text{Tr} (\tilde{\rho}_1 \tilde{K}_1^* \tilde{O} \tilde{K}_1).
\]
(13.3.16)
Here we have introduced density matrix which represents the pure state in this case,
\[
\tilde{\rho}_1 = |\Psi, t_1\rangle \langle \Psi, t_1|.
\]
(13.3.17)
It is possible to rewrite (13.3.15) as a derivative of something if two kinds of sources $J_1, J_2$ are introduced. The situation is the same as in Chapter XII. As in (12.1.9) and (12.1.10), we define $\mathcal{W}[J_1, J_2]$ and $\tilde{K}_1^{[J_2]}$. Note here that in (12.1.10) $t_2$ is arbitrary as long as it is greater than $t$. Now the effective action $\Gamma'[\varphi_1, \varphi_2]$ is defined by (12.1.11) and (12.1.12). By taking the coordinate representation, (12.1.9) can be written as
\[
e^{(\text{i}/\hbar)\mathcal{W}[J_1, J_2]} = \int dq \int dq' \langle q|\tilde{\rho}_1|q\rangle \langle q'|\tilde{K}_1^{[J_2]}|q\rangle
\]
(13.3.18)
\[
= \int dq \int dq' \langle q|\tilde{\rho}_1|q\rangle \kappa[J_1, q, q'].
\]
(13.3.19)
Diagrammatical evaluation of $\kappa[J_1, q, q']$ has been discussed in § 12.4 and Appendixes
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E, F where we have shown that $q$ and $q'$ appear as external lines of diagrams. Once the initial wave function $\Psi(q, t_i) = \langle q | \Psi, t_i \rangle$ is given, $W[J_1, J_2]$ is calculable by using

$$\langle q | \tilde{\rho}_1 | q' \rangle = \Psi(q, t_i) \Psi^*(q', t_i).$$  \hfill (13.3.20)

For the reference of the discussions in the next subsection, the formula of $\kappa[J_1; q, q']$ is given below by using (G.13), (G.14) and (G.15) for the case of the Hamiltonian,

$$H = \frac{1}{2m} p^2 + \frac{m\omega^2}{2} q^2 + V(q),$$  \hfill (13.3.21)

$$\kappa[J_1; q, q'] = V_{op} \times \langle q | K_0^{J_1} K_0^{J_1} | q \rangle,$$  \hfill (13.3.22)

$$V_{op} = \exp\left\{ - \frac{i}{\hbar} \int_{t_i}^{t_f} dt V\left( \frac{\hbar}{i} \frac{\delta}{\delta J_1(t)} \right) + \frac{i}{\hbar} \int_{t_i}^{t_f} dt V\left( - \frac{\hbar}{i} \frac{\delta}{\delta J_2(t)} \right) \right\},$$  \hfill (13.3.23)

$$\langle q | K_0^{J_1} K_0^{J_1} | q \rangle = \delta(q^{(-)} - \int_{t_i}^{t_f} dt \Delta_s(t - t_1) J^{(-)}(t))$$

$$\times \exp\left[ \frac{i}{\hbar} \int_{t_i}^{t_f} dt \int^{t_f}_{t_i} d\tau J^{(-)}(t) \left\{ q^{(+)} \omega(t - t_i) \right. \right.$$

$$\left. + \int_{t_i}^{t_f} \Delta_s(t - s) J^{(+)}(s) ds \right\},$$  \hfill (13.3.24)

$$\Delta_s(t - s) = \theta(t - s) \frac{\sin \omega(t - s)}{m\omega}. \hfill (13.3.25)$$

Here we have defined

$$q^{(+)} = \frac{1}{2}(q + q'), \quad q^{(-)} = q - q'.$$

For the detailed study of the Feynman rule of finite time interval, see Appendixes E, F and G.

We emphasize that the formalism of effective action with double arguments is applicable not only for non-equilibrium thermodynamics as in Chapter XII but it can equally be used for pure quantum mechanics. The only difference is that the density matrix takes the form of pure, instead of mixed, state in the case of quantum mechanics.

§ 13.4. Hilbert space of macroscopic system

One of the most interesting subjects which can be discussed by the use of the Legendre transformation or by closely related technique of stationary phase is to determine the Hilbert space structure of macroscopic systems.\(^8,9\) This clarifies the relation between microscopic quantum mechanical description and the phenomenon of our ordinary life. The subject has been discussed in § 12.4.3 in connection with the non-equilibrium theory but here we discuss the subject as a quantum mechanical problem. We follow the functional method of Ref. 9).

As an application of stationary phase and the Legendre transformation, let us consider the quantum mechanical structure of macroscopic system by focusing our
attention on the path integral expression of the Feynman kernel. Before studying the Hilbert space structure, we have to clarify how the wave function of a macroscopic system looks like.

13.4.1. Wave function of $N$-particle system

As a simple example, consider a system of $N$ harmonic oscillators described by the Lagrangian or the Hamiltonian as

$$L = \frac{m}{2} \sum_{i=1}^{N} \dot{q}_i^2 - \frac{m \omega^2}{2} \sum_{i=1}^{N} q_i^2,$$

$$H = \frac{1}{2m} \sum_{i=1}^{N} p_i^2 + \frac{m \omega^2}{2} \sum_{i=1}^{N} q_i^2. \quad (13\cdot4\cdot1)$$

The wave function and total energy are given by

$$\phi(q) = \prod_{i=1}^{N} \phi(q_i),$$

$$\phi(q_i) = N_n H_n(\sqrt{m \omega} q_i) \exp\left(-\frac{m \omega}{2} q_i^2\right),$$

$$E = \sum_{i=1}^{N} E_i, \quad E_i = \omega\left(n_i + \frac{1}{2}\right). \quad (13\cdot4\cdot3)$$

Here $q$ signifies $(q_1, q_2 \cdots q_N)$ and $n_i$ takes the non-negative integer, $H_n$ is the Hermite polynomial, with $N_n$ being the normalization constant. Now the wave function can be written as

$$\phi(q) = M_n(q) e^{F[q]},$$

$$M_n(q) = \prod_{i=1}^{N} N_n H_n(\sqrt{m \omega} q_i), \quad F[q] = -\frac{m \omega}{2} \sum_{i=1}^{N} q_i^2. \quad (13\cdot4\cdot4)$$

We have used $n$ to denote $(n_1, n_2 \cdots n_N)$. The energy is written as

$$E = \frac{\omega}{2} N + \frac{\omega}{2} \sum_{i=1}^{N} n_i. \quad (13\cdot4\cdot5)$$

Let us see the differences between $F[q]$ and $M_n[q]$. $F$ is clearly an extensive quantity since it is written as a sum over $i$ from 1 to $N$. We now give a convenient way of judging whether a given quantity is extensive or not.

**Extensive variable** A function of $q_i$ is extensive if it is proportional to $N$ when $q_i$ is set to a constant independent of $i$.

The function $F$ and Lagrangian $L$ or Hamiltonian $H$ are all extensive quantities of course. Recall that $F$ represents zero point motion which is common to all modes and corresponds to the first term of $E$ of $(13\cdot4\cdot5)$. Now $M_n[q]$ contains information about excitation, which can be either extensive or intensive depending on $n_i$. We rewrite $M_n(q)$ as

$$M_n[q] = \exp \sum_{i=1}^{N} [\ln N_{n_i} + \ln H_n(\sqrt{m \omega} q_i)]. \quad (13\cdot4\cdot6)$$
Since the first term in the exponential is a constant, let us focus on the second term. Because \( H_{n=0} = 1 \), the sum over \( i \) is actually a finite sum if the number of \( n_i \) which is different from zero is finite. In such a case \( M_n(q) \) is intensive, there appears no factor of \( N \) if we set \( q_i = \text{const} \). This means that for finite excitation energy, \( M_n(q) \) is an intensive quantity. The important fact is, however, that for all the wave functions of finite excitation energy, \( e^{F(q)} \) is a common factor.

On the other hand, consider the case where \( n_i = n_0 \) for all \( n_i \). Then the second term in the exponential of (13.4.6) becomes \( N \ln H_n(\sqrt{m\omega} q) \) if we set \( q_i = q \), showing that it is extensive. In this case the energy is macroscopically, i.e., of order \( N \), different from that of the ground state, \( E = \omega((1/2) + n_0)N \). The wave function is now,

\[
\phi(q) = \exp \left\{ N \ln N_0 + \sum_{i=1}^{N} \left[ \ln H_n(\sqrt{m\omega} q_i) - \frac{m\omega}{2} q_i^2 \right] \right\} = \exp (F[q] + \Delta F[q]) .
\] (13.4.7)

Here both \( F \) and \( \Delta F \) are extensive quantities of order \( N \).

For more general case where \( n_i \) is not independent of \( i \), we write, by setting \( q_i = q \),

\[
\sum_{i=1}^{N} \ln H_n(\sqrt{m\omega} q) = N \cdot \frac{1}{N} \sum_{i=1}^{N} \ln H_n(\sqrt{m\omega} q).
\] (13.4.8)

When the average operation \( (1/N) \sum_{i=1}^{N} \) brings us a finite function \( f(q) \) of \( q \), in the limit \( N \to \infty \), then we are left with an extensive quantity \( Nf(q) \) in (13.4.8). In this case the wave function \( \phi(q) \) acquires in the exponential an extensive term \( \Delta F \) besides \( F \) and this corresponds to the energy of macroscopic excitation,

\[
E = \omega \left( \frac{1}{2} + \bar{n} \right) , \quad \bar{n} = \frac{1}{N} \sum_{i=1}^{N} n_i .
\] (13.4.9)

To summarize, the wave function of macroscopically excited state has the form (13.4.4) with

\[
M_n[q] = M_n[q] \exp(\Delta F[q]) , \quad \Delta F[q] = O(N) .
\] (13.4.10)

Here \( M_n[q] \) describes the microscopic details of the state and is the quantity of \( O(1) \).

Now we consider the inverse problem; imagine the following wave function besides (13.4.10),

\[
M_n[q] = M_n[q] \exp(\Delta F[q]) .
\] (13.4.11)

The question is whether two states (13.4.10) and (13.4.11) have different macroscopic energies if \( \Delta F \) and \( \Delta F' \) differ from each other by \( O(N) \). The answer is no. For example, consider the case where \( n_i = n_0 + 1 \) for \( i = 1 \sim (N/2) \), and \( n_i = n_0 - 1 \) for \( i = (N/2) + 1 \sim N \). The energy of such a state is the same as the one with \( n_i = n_0 \) for all \( i \) but the wave function becomes, after setting \( q_i = q \) for all \( i \),
\[
\phi(q) = \exp \left( \frac{N}{2} \left( \ln N_{n+1} + \ln N_{n-1} \right) + \frac{N}{2} \left[ \ln H_{n+1}(\sqrt{m\omega} q) + \ln H_{n-1}(\sqrt{m\omega} q) \right] - \frac{N m\omega}{2} q^2 \right). 
\] (13.4.12)

The wave function (13.4.12) differs from (13.4.7) by \(O(N)\) in the exponential which implies that two macroscopically different states have the same macroscopic energy. The fact that two states are indeed macroscopically different can be seen by considering, for example, the value of

\[
\tilde{H} = \sum_{i=1}^{N} \left( \frac{p_i^2}{2m} + \frac{m\omega^2}{2} q_i^2 \right). 
\] (13.4.13)

The difference in \(\tilde{H}\) for two states is \(O(N)\). We call the situation \textit{macroscopic degeneracy} if two macroscopically different states correspond to the same macroscopic energy. Here we define:

\textbf{Macrovariable} it is an extensive variable divided by \(N\).

It is denoted by \(X\) in the following. Using these terminologies, we summarize above findings as follows.

The wave function of the energy eigenstate of a macroscopic system has the form

\[
\phi(q) = M_{\phi}(q) \exp(F(q)).
\]

Here \(F\) is \(O(N)\) and for two \(F\)'s which are different by \(O(N)\), we have two macroscopically different states where some macrovariable \(X_i\) takes different values. In the above example \(X_i = \tilde{H}\).

The above statement has been proved for non-interacting \(N\)-particle system. The interacting system has to be studied next. For that purpose we have to be careful about the fact that for the system with identical particles the macroscopic limit, i.e., the thermodynamic limit, is crucially affected by statistics. In order to investigate these points, we take below a second quantized field theoretical system. The conclusion obtained above turns out to be correct in this case also and we get the wave function written as

\[(\text{intensive quantity}) \times \exp(\text{extensive quantity}).\]

13.4.2. \textit{Second quantized system}

Including the correct description of spin and statistics, any macroscopic system can best be described by a second quantized field theory so here we take a field theoretical model of macroscopic system. The quantization volume \(V\) of the field theory plays the role of \(N\) and we assume \(V\) to be large but finite for the moment.

Both bosonic and fermionic system can equally be discussed but the discussions become clear if we take a specific example. As a model of the macroscopic system, we adopt the following Lagrangian \(L\) described by Hermite bosonic field \(\phi(x)\) defined in a large volume \(V\):

\[
L = \int_0^V d^3 x \left( \frac{m}{2} \phi^2(x) - \frac{m}{2} \phi(x) \frac{\omega}{\sqrt{-\nabla^2}} \phi(x) \right) - V' [\phi] \equiv L_0 + L'. 
\] (13.4.14)

Here \(m > 0\) is some parameter and \(\dot{\phi} \equiv d\phi/dt\). The function \(\omega(-\nabla^2)\) represents the
dispersion of $\phi(x)$. The Lagrangian should fulfill the following two conditions for the theory to exist in the limit $V \to \infty$:

(a) The dispersion relation $\omega(k^2) = \omega_k$ in Fourier space does not vanish for any $k$ and has a finite gap separated from zero. We assume $\omega_k > 0$ in the following.

(b) The interaction is of short range type. This is stated more precisely as follows. $V'[\phi]$ can be written in general as

$$V'[\phi] = \sum_{n=1}^{\infty} \int dx_1 \cdots \int dx_n v^{(n)}(x_1, x_2, \ldots, x_n) \phi(x_1) \phi(x_2) \cdots \phi(x_n). \quad (13.4.15)$$

Then our assumptions on the $v^{(n)}$s are that they are functions of the difference $x_i - x_j$ and they vanish sufficiently fast as the distance of any of the pair $|x_i - x_j|$ goes to infinity. A typical example is $\exp(-\rho |x_i - x_j|)$ with $\rho > 0$. The local interaction, $\int d^3 x \phi'(x)$ for instance, is of course an allowed one.

The Hamiltonian in Fourier space is written as

$$H = \sum_{k, \sigma} \left( \frac{1}{4m} \Pi_k^{\sigma^2} + m\omega_k^2 \phi_k^{\sigma^2} \right) + V'[\phi_k]$$

$$\equiv H_0 + H', \quad (13.4.16)$$

where we have defined $\phi(x) = (1/\sqrt{V}) \sum_k e^{i k \cdot x} \phi_k$. If we write $\phi_k$ as a sum of real and imaginary part, $\phi_k = \phi_k^R + i \phi_k^I$, then $\phi_k^R = \phi_k^R$, $\phi_k^I = -\phi_k^I$. The notation $\phi_k^R = (\phi_k^R, \phi_k^I)$ has been introduced and the symbol $\sum_k$ implies the summation over half $k$-space and $\sigma$ signifies the real or the imaginary part. The conjugate momentum $\Pi_k^\sigma = 2m \phi_k^\sigma$ satisfies the quantization condition

$$[\Pi_k^\sigma, \phi_k^\sigma] = \frac{1}{i} \delta^{\sigma^\sigma^\sigma} \delta_{kk^\prime}. \quad (13.4.17)$$

The $\phi$-representation is adopted in the following where $\phi_k$ is diagonal,

$$\hat{\phi}_k \phi = \phi_k \phi. \quad (13.4.18)$$

Here $\phi$ denotes the set of eigenvalues $\phi \equiv \{\phi_k\}$.

13.4.3. Eigenfunctional of Hamiltonian

Now we study the form of the wave function of the eigenstate of the Hamiltonian. Let us start from the free field case and then proceed to include the interaction.

(i) Free field case

The situation is similar to harmonic $N$-particle system, since $H_0$ is the sum of the independent harmonic oscillators. We need a set of integers $m_k^\sigma$ for each mode $(k, \sigma)$ in order to specify the whole set of the eigenfunction of $H_0$. By writing $m = \{m_k^\sigma\}$ ($m_k^\sigma = 0, 1, 2, \ldots$), the wave function and the energy eigenvalue is given as

$$\langle \phi | m \rangle = \langle \{\phi_k^\sigma\} | \{m_k^\sigma\} \rangle$$

$$= \prod_{k, \sigma} N_{m_k^\sigma} H_{m_k^\sigma} (\sqrt{2m\omega_k^2} \phi_k^\sigma) \exp(-m\omega_k \phi_k^{\sigma^2}). \quad (13.4.19)$$
Here $\Pi'$ means the product over half $k$-space and the energy eigenvalue is
\[ E = \sum_k \epsilon (\mathbf{p} + (1/2)) \omega_k. \]

Since
\[ \sum_k m \omega_k \phi_k^2 = -\frac{m}{2} \int d^3x \phi(x) \omega(-\nabla^2) \phi(x) = O(V), \tag{13.4.20} \]
it is an extensive variable which is of the order of the system size $V$. Note that in deriving this conclusion we have used the above condition (a) on $\omega_k$. (A precise definition of the extensive quantity is given below.) Therefore the wave function with the finite excitation energy is given by the sum of the term $(\phi_1^* \phi_2^* \cdots \phi_N^*) \times e^{F[\phi]}$ where $F[\phi]$ is the functional of $\phi$ which is of the order of $V$ and since $H_n(x)$ is the polynomial of order $n$, $l$ as a finite integer. Thus
\[ \langle \phi | m \rangle = (\text{polynomial in } \phi_k^*) \times e^{F[\phi]}, \tag{13.4.21} \]
where $F[\phi]$ is $O(V)$. Remember that $F[\phi]$ is common to all the states of the finite excitation energy.

Now let us define the extensive and intensive variables in field theoretical case.

**extensive variable** In the expression
\[ I[\phi] = \sum_{n=1}^{\infty} \int dx_1 \cdots \int dx_n G^{(n)}(x_1, x_2, \cdots x_n) \phi(x_1) \phi(x_2) \cdots \phi(x_n), \tag{13.4.22} \]
if the function $G^{(n)}$ enjoys the same properties imposed on $v^{(n)}$ in (13.4.15), we call $I[\phi]$ the extensive variable. In this case, $I[\phi]$ is explicitly proportional to $V$ if we set $\phi(x)$ to be independent of $x$. As in the case of $N$-particle system, this is a convenient way of judging whether a given functional of $\phi$ is an extensive quantity or not. In (13.4.22), some of $\phi(x_i)$'s can be replaced by $\Pi(x_i)$'s (the conjugate momentum).

**intensive variable** There are two kinds of intensive variables,

(a) Class I—macrovariable

The variables obtained by dividing the extensive variable through $V$ belong to this class. They involve averaged information of the global region $V$ and are denoted by $X[\phi]$ in the following and we call them macrovariables writing it as
\[ X[\phi] = I[\phi]/V. \tag{13.4.23} \]
In the macroscopic limit $V \rightarrow \infty$, they lose fluctuations as we shall see. We can say that in the experiment the macrovariables are the only variables that are observed. The simplest example of the macrovariable is the centre of mass coordinate. For finite $V$, the macrovariable fluctuates and the quantum diffusion is present but it is extremely small for a realistic macrosystem and is undetectable by the usual method.

(b) Class II—microvariable

The variables which are originally contained in the Hamiltonian, $\phi(x)$ and $\Pi(x)$, belong to this class. The combination $\int d^3y \phi(x) C(x - y) \phi(y)$ with suitable function $C(x)$ is also called the microvariable. They contain the microscopic local informa-
tion but they fluctuate even in the macroscopic limit.

(ii) Interacting system

Our final purpose is to show that the same property of the wave function holds even in the presence of the interaction as long as it is short ranged. For this purpose we use the adiabatic theorem in the form of Gell-Mann and Low.10) Up to now it is not known whether or not we can use the adiabatic theorem for a macroscopic system but in the following we assume its validity by taking the adiabatic limit before the limit of infinite volume.

First the eigenstate \(|m\rangle\) of free Hamiltonian \(H_0\) with the eigenvalue \(E_m^0\) is prepared at \(t = -\infty\). The interaction is then assumed to be turned on adiabatically from \(t = -\infty\) to \(t = 0\). The Hamiltonian at time \(t\) is thus

\[
H(t) = H_0 + e^{-at}H'. \quad (a > 0)
\]

We take the limit \(a \to 0\) in the end and then it is known that the state started from \(|m\rangle\) remains an eigenstate of \(H(t)\) for any \(t\). Mathematical expression of this fact is as follows. If we define \(|m\rangle\) at \(t = 0\) by

\[
|m\rangle = \lim_{\epsilon \to 0} \frac{U_a(0, -\infty)|m\rangle}{\langle m|U_a(0, -\infty)|m\rangle},
\]

then, for \(H = H_0 + H'\) we get\(^{9,10}\)

\[
H|m\rangle = E|m\rangle, \quad E = E_m^0 + \Delta E.
\]

For our purpose we do not need the formula for the energy shift \(\Delta E\). The time evolution operator \(U_a\) is defined in the interaction representation as

\[
U_a(t', t) = \exp(iH_0 t') \exp \left(-i \int_t^{t'} dt'' H(t'')\right) \exp(-iH_0 t).
\]

Let us now concentrate on the wave function \(\langle \phi|m\rangle\). For that purpose the constant factor in the denominator of (13.4.25) is neglected since it gives an infinite constant which cancels the \(\phi\)-independent infinities in the numerator. In what follows we set \(t' = 0\) but \(t\) and \(a\) are taken to be finite and take the limit \(t \to -\infty, a \to 0\) afterwards. Then

\[
\langle \phi|m\rangle \sim \langle \phi|U_a(0, t)|m\rangle
\]

\[
= \int [d\phi'] \langle \phi| \exp \left(-i \int_t^0 dt'' H(t'')\right) \phi' \rangle \langle \phi'|m\rangle e^{-iE_m^0 t}
\]

\[
= Ke^{-iE_m^0 t}.
\]

We have written the completeness property as \(\int [d\phi]|\phi\rangle \langle \phi'| = 1\) with \([d\phi] = \prod_{\alpha, \sigma} d\phi \xi\). By diagrammatic expansion in terms of interaction \(H'\), it can be shown\(^9\) that \(K\) is written in the form

\[
K = M_\alpha[\phi, t] e^{F_\alpha[\phi, t]}, \quad F_\alpha[\phi, t] = O(V),
\]

where \(M\) is a finite microscopic functional. The essential ingredient used here is the
following theorem; the sum of diagrams is represented as \( \exp(G_c) \) where \( G_c \) is the sum of connected diagrams. The connected diagrams are indeed \( O(V) \) if the conditions (a) and (b) of § 13.4.2 are satisfied.

Before we obtain the wave function of the eigenstate of the energy, we have to divide \( K \) by \( e^{i\omega t_0} \langle m | U_a(0, t) | m \rangle \) and take the limit \( t \to -\infty, \ a \to 0 \). This limit is known to exist as long as \( V \) is finite and since the factor which divides \( K \) is a constant independent of \( \phi \), the functional form given in (13.4.29) is preserved in this limit.

Thus we finally arrived at the conclusion that the wave function has the same structure as in the free case:

\[
\langle \phi | m \rangle = M[\phi] e^{F[\phi]}, \quad F[\phi] = O(V),
\]

(13.4.30)

where \( M[\phi] \) is essentially the polynomial of \( \phi \) which is finite as \( V \to \infty \); a microscopic variable. For the ground state, \( M[\phi] = 1 \). As in the free field case, \( F[\phi] \) is common to all the excited states of the finite excitation energy and the macroscopically excited states are given by the form

\[
M^\prime[\phi] e^{F[\phi] + \Delta F[\phi]},
\]

(13.4.31)

where both \( F[\phi] \) and \( \Delta F[\phi] \) are extensive quantities and \( M^\prime[\phi] \) is some microscopic functional. These results are the same as in harmonic \( N \)-particle case.

13.4.4. Structure of Hilbert space

We are in a position to investigate how the Hilbert space of our macroscopic system looks like if \( V \) is brought to infinity. Let us consider first the norm of the ground state \( |0\rangle \). Since the wave function is real, we concentrate on

\[
D^{(0)} = \int [d\phi] \langle \phi | 0 \rangle^2 = \int [d\phi] e^{2F[\phi]} = 1.
\]

In order to see the contribution to \( D^{(0)} \) from a fixed value of the macrovariable \( X[\phi] \), we insert an identity and rewrite \( D^{(0)} \) in an obvious way,

\[
D^{(0)} = \int [d\phi] \int dX \delta(X - X[\phi]) e^{2F[\phi]}
\]

\[
= \frac{V}{2\pi i} \int [d\phi] \int_{-\infty}^{\infty} df \int dX \exp(2F[\phi] - VJX[\phi] + VJX).
\]

There is a theorem about the result of the \( \phi \)-integration:

**Theorem** Let \( L[\phi, J_i] \) be an extensive variable which is the functional of the fields \( \phi(x), J_i(x) \) \((i = 1 \sim N)\). The most general form is

\[
L = \sum_{n,m} \int dx_1 \cdots \int dx_{n+m} \bar{G}^{[n,m]}(x_1, x_2, \cdots, x_{n+m}) \phi(x_1) \cdots \phi(x_n) J_{i_1}(x_{n+1}) \cdots J_{i_m}(x_{n+m}),
\]

where \( \bar{G}^{[n,m]} \) satisfies the necessary conditions for \( L \) to be an extensive variable as stated above (some of the \( \phi(x_i)'s \) can be the \( H(x_i)'s \)). Then we get

\[
\int [d\phi] \exp L[\phi, J_i] = \exp F[J_i],
\]

(13.4.32)
where $F[J_i]$ itself is an extensive variable given by

$$F[J_i] = \sum \int dx_1 \cdots \int dx_n E^{(n)}_{i_1} \cdots (x_1 \cdots x_n) J_{i_1}(x_1) \cdots J_n(x_n)$$  \hspace{1cm} (13.4.33)

with $E^{(n)}$ having the same property as $G^{(n,m)}$.

**Proof**  The term involving $G^{(2,0)}(x_1 - x_2)$ is regarded as the free Lagrangian (or the action) of $\phi$ and the diagrammatic expansion is made by considering all other terms as the interaction. These diagrams are constructed by the propagator $G^{(2,0)}$ and the vertices specified by the interaction. We assume here that the $\phi$-integral leading to each expression of the diagram converges. The sum of the diagrams is represented as the exponential of the sum of the connected Green's functions with external lines $J_i(x)$. They are extensive variables because of the connected property. \hspace{1cm} (QED)

Now we apply the above theorem to $D^{(0)}$ by regarding $2F[\phi] - VJX[\phi]$ as $L[\phi, J]$. Since $J$ is independent of $x$ in this case, we conclude

$$\int [d\phi] \exp (2F[\phi] - VJX[\phi]) = \exp (-VW(J)),$$

$$D^{(0)} = \frac{V}{2\pi} \int dJ \int dX \exp (-VW(J) + VJX).$$  \hspace{1cm} (13.4.34)

We note that $W(0) = 0$ because of the normalization condition. Here the Legendre transformation appears in the limit $V \to \infty$. First we perform the $J$-integration where the stationary point $J = J^0(X)$ dominates in the limit $V \to \infty$. Expanding $W[J]$ around $J^0$ up to $(J - J^0)^2$ we get the result,

$$D^{(0)} = \frac{V}{2\pi} \int dX \sqrt{-\frac{2\pi}{VW''(J^0(X))}} \exp (-VT(x)),$$

$$\Gamma(X) = W(J^0(X)) - J^0(X)X.$$  \hspace{1cm} (13.4.35)

Here $J^0(X)$ is the solution of

$$-W'(J) + X = 0.$$

The function $\Gamma(X)$, is the Legendre transform of $W(J)$, the "effective action" in this case, and satisfies

$$\frac{\partial \Gamma(X)}{\partial X} = -J^0(X), \quad \Gamma''(X)W''(J) = -1.$$  \hspace{1cm} (13.4.36)

The remaining $X$-integration is again dominated by the stationary point $X = X^0$ which is a solution to

$$0 = \frac{\partial \Gamma(X)}{\partial X} = -J^0(X).$$  \hspace{1cm} (13.4.37)

Expanding again $\Gamma(X)$ around $X = X^0$ up to the second order of $X - X^0$,

$$D^{(0)} = \frac{V}{2\pi} \int dX \sqrt{-\frac{2\pi}{VW''(J^0)}} \exp \left\{ -V \left( \Gamma(X^0) + \frac{1}{2} \Gamma''(X^0)(X - X^0)^2 \right) \right\}.$$
\[ \frac{V}{2\pi} \int dX \sqrt{\frac{2\pi}{-VW''(J^0)}} \sqrt{\frac{VT''(X_0)}{2\pi}} \delta(X - X_0) e^{-VT(X_0)} \]

\[ = \int dX \delta(X - X_0). \quad (13.4.38) \]

Here we have used (13.4.36) and \( \Gamma(X_0) = W(0) = 0 \). Equation (13.4.38) says that the macrovariable \( X[\phi] \) is fixed to be \( X_0 \) and it has no fluctuation in the ground state. The above derivation shows that we have more general formula,

\[ \int [d\phi] \delta(X - X[\phi])\langle \phi|0\rangle^2 = \delta(X - X_0). \quad (13.4.39) \]

We proceed to slightly more general expression,

\[ D^{(n)} = \int [d\phi] \langle \phi|0\rangle^2 \phi(x_1)\phi(x_2)\cdots\phi(x_n). \]

As before we divide and multiply \( D^{(n)} \) by the factor (13.4.34). \( D^{(n)} \) then becomes

\[ D^{(n)} = \frac{V}{2\pi} \int dX \int dJ \exp \{-V(W(J) - JX)) \times \left[ \int [d\phi] \exp \left\{ 2F[\phi] - VJX[\phi] \right\} \phi(x_1)\cdots\phi(x_n) \exp \{VW(J)\} \right]. \quad (13.4.40) \]

The expression in the square bracket of (13.4.40) corresponds to the nothing but the \( n \)-point Green's function \( H_n(x_1,x_2\cdots x_n; J) \) of the theory whose "action" is \( 2F[\phi] - VJX[\phi] \), where the vacuum type graphs are deleted. This is a microscopic quantity and is finite in the limit \( V \to \infty \). Therefore as \( V \to \infty \)

\[ D^{(n)} = \int dX dJ \exp \{-V(W(J) - JX)) \} H_n(x_1,x_2\cdots x_n; J) \]

\[ \cong \int dX \delta(X - X_0) H_n(x_1,x_2\cdots x_n; J^0(X)) \]

\[ = H_n(x_1,x_2\cdots x_n; J = 0). \quad (13.4.41) \]

We emphasize here that \( X_0 \) is the same value appeared in the vacuum case (13.4.38). The formula similar to (13.4.39) also holds in this case. The most general case is

\[ D^{(n,0)} = \int [d\phi] \phi(x_1)\cdots\phi(x_n)\Pi(x_{n+1})\cdots\Pi(x_{n+i})\langle \phi|0\rangle^2. \quad (13.4.42) \]

Here \( \Pi(x) = (1/i)\delta/\delta\phi(x) \) is the canonical momentum, which can be written as a (non-local) sum of \( H_n \) given above and hence is finite as \( V \to \infty \). We get the following formula for this quantity,

\[ D^{(n,0)} = \int [d\phi] \delta(X - X[\phi])\phi(x_1)\cdots\phi(x_{n+i})\langle \phi|0\rangle^2 \]

\[ = \delta(X - X_0) P^{(n,0)}(x_1,x_2\cdots x_{n+i}; J = 0). \quad (13.4.43) \]

where \( X_0 \) is the same as in (13.4.38) and \( P^{(n,0)}(x_1, x_2\cdots) \) is the Green's function which can be written as a (non-local) sum of \( H_n \) given above and hence is finite as \( V \to \infty \).
Since the Hilbert space is constructed by applying arbitrary power of $\phi(x)$ or $\Pi(x)$ to the ground state and since Eq. (13.4.43) holds for any $n$ or $l$, we conclude that as $V \to \infty$ the macrovariable takes a fluctuationless value (c-number) in a Hilbert space.

The last statement corresponds to the fact that the c-number cannot be transformed by any operator transformation. Stated in another way, to different values of the macrovariable corresponds a different Hilbert space.

Note that the macrovariable takes the continuous c-number value so that we are led to the notion of the set of continuous Hilbert space. In this sense Araki’s continuous Hilbert space of macroscopic system\(^{11}\) is realized by the continuous value of the macrovariable. Each Hilbert space is of course constructed by microvariables which fluctuate even in the macroscopic limit and hence are operators.

The above results can be checked by taking the explicit expression (13.4.30) or (13.4.31) as the wave function. Consider

$$\int [d\phi] dX \delta(X - X[\phi]) M[\phi]^{2} e^{2\Psi[\phi]}.$$ 

By the same procedure as above, the $X$-integration is seen to be dominated by the stationary point which is independent of $M[\phi]$ because $M[\phi]$ is a microscopic function. The macrovariable $X[\phi]$ becomes fluctuationless and takes the same value $X_{0}$ as (13.4.38) for any excited level with the finite excitation energy. For the state (13.4.31), $X[\phi]$ takes fluctuationless value other than $X_{0}$ in general. Thus the states having the exponentials which are macroscopically different belong to different Hilbert spaces.

In order to see the above statement more closely, let us take two macroscopically different states $|\phi\rangle_{i}$ ($i=1, 2$),

$$\langle \phi | \phi \rangle_{i} = e^{2\Psi[\phi]} M[\phi]. \quad (13.4.44)$$

Here $F_{i}[\phi]$ and $F_{2}[\phi]$ are macroscopically different and $X[\phi]$ takes the deterministic values $X_{1}$ and $X_{2}$ for $F_{1}$ and $F_{2}$ respectively. We study the matrix element

$$\int [d\phi]_{1} \langle \phi | \phi \rangle \phi(x_{1}) \cdots \Pi(x_{n+1}) \cdots \langle \phi | \phi \rangle_{2}.$$ 

(13.4.45)

As is obvious from the above arguments, if we insert $1 = \int dX \delta(X - X[\phi])$, $X$-integration is dominated by the stationary point which is independent of the presence of the microscopic factor $M_{i}[\phi]$ and $\phi(x_{1}) \cdots \Pi(x_{n+1}) \cdots$. In order to make the arguments clear we omit these factors. Let us consider the following constrained inner product,

$$\int [d\phi] \delta(X - X[\phi])_{1} \langle \phi | \phi \rangle \langle \phi | \phi \rangle_{2}$$

$$= \int [d\phi] \delta(X - X[\phi]) \exp(F_{1}[\phi] + F_{2}[\phi])$$

$$\leq \left\{ \int [d\phi] \delta(X - X[\phi]) \exp 2F_{1}[\phi] \times \int [d\phi] \delta(X - X[\phi]) \exp 2F_{2}[\phi] \right\}^{1/2}$$

$$\longrightarrow \{ \delta(X - X_{1}) \delta(X - X_{2}) \}^{1/2}, \quad (V \to \infty) \quad (13.4.46)$$
where we have used the Schwarz type inequality and (13·4·39). The same factor appearing in (13·4·46) serves as the bound on the matrix element (13·4·45) even if we include the factor $M_{\tilde{\Pi}}(\phi)$ or $\phi(x_1)\cdots\tilde{\Pi}(x_{n+1})\cdots$. Thus we get further statement, matrix elements of any polynomial of $\phi$ or $\tilde{\Pi}$ between two macroscopically different states vanish in the limit $V=\infty$.

One of the consequences of this statement is that the operator which has the non-vanishing matrix elements between macroscopically different states is typically of the form

$$e^{\Delta F[\phi]},$$  \hspace{1cm} (13·4·47)

where $\Delta F[\phi]$ is an extensive variable (here $\Delta F$ may depend on $\tilde{\Pi}$ also). This operator connects the two states of the wave function $e^{\tilde{\Pi}[\phi]}$ satisfying $F_1-F_2=\Delta F$.

The expression (13·4·47) can in general be regarded as an operator which causes a macroscopic change to macroscopic system in a finite time interval. In order to understand this statement we have to discuss the time evolution.

Before studying the time evolution, we state here the definition of the pure and the mixed state for the macroscopic system in our terminology:

**Pure state**······ a state in a single Hilbert space and hence the macrovariable takes only one value.

**Mixed state**······ a state which lies in several Hilbert spaces and is expressed by an incoherent sum of the pure state. Therefore the value of the macrovariable extends over some interval.

Since the macrovariable takes a continuous c-number value, the more realistic definition of the pure state is that the region of the value $X$ of $X[\phi]$ is arbitrary small; $X_0-\delta<X<X_0+\delta$ with $\delta/X_0\ll1$.

13.4.5. **Time evolution**

The next task is to show that the structure of the wave function shown in (13·4·30) is preserved during the time evolution: if the wave function is a sum of the terms given by (13·4·30) at $t=0$ then it has the same form for any $t$.

Let us take one of the terms and write it as $\langle\phi|\phi\rangle$. We discuss its time evolution,

$$\langle\phi|\phi\rangle_t=\int[d\phi']K(\phi, \phi', t-0)\langle\phi'|\phi\rangle,$$  \hspace{1cm} (13·4·48)

where

$$K(\phi, \phi'; t-0)=\langle\phi|\exp\left\{-i\int_0^tH(t')dt'\right\}|\phi'\rangle.$$  \hspace{1cm} (13·4·49)

We have generalized our discussions to the case of the time-dependent Hamiltonian. $H(t)$ is assumed to satisfy the condition for the extensive variable given in § 13.4.3 (see the definition (13·4·22)) and is written as $H(t)=H_0+H^I(t)$. In this case the wave function (13·4·30) is not an eigenstate of the Hamiltonian but is regarded as an arbitrarily prepared macroscopic wave function. Through this generalization we can study a more realistic case: from $t=-\infty$ to $t=0$, the system is in the eigenstate
of the Hamiltonian which is independent of the time and for \( t \geq 0 \) it becomes time dependent through the change of the external parameter which is included in \( H'(t) \).

The proof proceeds just as in the case of adiabatic theorem above. We have to keep the dependence of \( U_{a}(t', t) \) in (13.4.27) on \( t, t' \) and expand in powers of \( H'(t) \). Then \( \langle \phi | \phi \rangle_{t} \) can be seen to have the form,

\[
\langle \phi | \phi \rangle_{t} \approx M_{t}[\phi] e^{F_{t}[\phi]} , \quad F_{t}[\phi] = O(V) .
\]  

Here \( M_{t}[\phi] \) is the \( t \)-dependent microscopic functional of \( \phi_{Y} \) and \( F_{t}[\phi] \) specifies the \( t \)-dependent stationary trajectory of macrovariable \( X[\phi] \).

Let us study the time evolution of the macrovariable. We simply repeat the same arguments of § 13.4.3 by using \( \langle \phi | \phi \rangle_{t} \) in place of \( |m\rangle \). The only difference is that \( \langle \phi | \phi \rangle_{t} \) is not a real function so that \( \langle \phi | m \rangle^{2} \) is replaced by \( |\langle \phi | \phi \rangle|^{2} \) which has again the form (13.4.30) with \( M[\phi] \) and especially \( F[\phi] \) dependent on \( t \). Therefore \( X[\phi] \) takes a \( t \)-dependent deterministic value which is fixed by the \( t \)-dependent stationary point of the function \( \Gamma_{t}[X] \). This is the "effective action" (13.4.35) at time \( t \).

The generalization of (13.4.46) is now straightforward. Take two wave functions \( \langle \phi | \phi \rangle_{X_{i}} \) (\( i = 1, 2 \)) at time \( t \) with are complex in general, then

\[
\left| \int [d\phi] \delta(X - X[\phi])_{X_{i}, \langle \phi | \phi \rangle_{\phi} X_{i}} \right|^{2} \\
\leq \int [d\phi] \delta(X - X[\phi]) \langle \phi | \phi \rangle_{X_{i}}^{2} \times \int [d\phi] \delta(X - X[\phi]) \langle \phi | \phi \rangle_{X_{i}}^{2} \\
\rightarrow \delta(X - X_{1}) \delta(X - X_{2}) \quad (V \rightarrow \infty) \quad (13.4.51)
\]

The matrix element of any microscopic variable \( M[\phi] \), or \( \phi(x_{1}) \cdots \phi(x_{n}) \Pi(x_{n+1}) \cdots \Pi(x_{n+1}) \) in particular, has a similar bound; its absolute square is bounded by \( \delta(X - X_{1}) \delta(X - X_{2}) \) multiplied by some finite quantity.

There is another way of obtaining the equation of motion. In fact the time dependence can also be studied by deriving the equation of motion for \( X[\phi] \) for any time \( t \geq 0 \). The most general and convenient tool is the double path effective action \( \Gamma[X_{1}, X_{2}] \) as has been introduced in Chapter XII and § 13.3.2. The equation of motion of \( \langle X[\phi] \rangle_{t} = X(t) \) is obtained by solving

\[
0 = \frac{\delta \Gamma[X_{1}, X_{2}]}{\delta X_{1}(t)} \bigg|_{X_{1}(t) = X_{2}(t) = X(t)} . \quad (13.4.52)
\]

The functional form of this equation depends on the initial state in general. Equation (13.4.52) is a deterministic one for macrovariable \( X \).

§ 13.5. Measurement theory in terms of macrovariables

By the use of the results of the preceding sections, a theory of measurement\(^{12,13}\) can be developed. We take \( V \) to be large but finite throughout the discussions. Our arguments are general enough and applicable to most of the macrosystem but the discussions become transparent if we take a specific model. We therefore use the Lagrangian (13.4.14) or the Hamiltonian (13.4.16) to describe the detector system.
and assume that the measured quantity is some macrovariable $X[\phi]$, the needle position for example.

Besides $\phi(x)$, the microscopic degree of freedom is required describing the object which is to be measured. We denote it as $\sigma$. This can be the coordinate $r$ of the object and/or the spin degrees of freedom, etc. Let us assume that we are going to measure the operator $\hat{O}$ of the object and expand the wave function $\psi(\sigma)$ of the object before the measurement as

$$\psi(\sigma) = \sum_n C_n \psi_n(\sigma),$$

where $\hat{O}\psi_n(\sigma) = \lambda_n \psi(\sigma)$. Suffix $n$ discriminates the microscopic difference of various states having different values of $\lambda_n$. The wave function of macroscopic detector system is also introduced as $\Psi[\phi]$. The total Hamiltonian or the Lagrangian of the whole system, object plus detector, is given by (13.4.14), which describes the detector system, plus the Hamiltonian of the object and also the one which represents the interaction of the object with the detector.

The measurement is performed by detecting the change of the macrovariable before and after the measuring process. It consists in mapping a microscopic difference of the object to the macroscopic difference of the detector system; in our terminology difference in the macrovariable $X[\phi]$. This is called the amplification which is the essential part of the measurement. There are several cases\(^{10,11}\) of amplification mechanism depending on how the energy is supplied. It may be supplied by the object itself which is in a highly energetic state or by arranging the detector system in a macroscopic high energy unstable state whose energy is released by a microscopic trigger caused by the interaction with the object. Another possibility is to change the external parameter by applying the electric field for instance, thereby supplying the macroscopic energy to the system.

Now consider the measuring process. The wave function of the macroscopic system has the form (13.4.30) and in terms of the macrovariable $X[\phi]$ it has a sharp peak centered at some $X_0$ with the width of the order $1/\sqrt{V}$. Due to the quantum diffusion the width spreads out with the time but the time required for the appreciable spreading is extremely large and it cannot be detected for the macroscopic body. This explains the deterministic character of the ordinary macroscopic system.

Let us use the suffix $X$ for the wave function to denote the centre value of $X[\phi]$. The process of the measurement can be described as follows. Note here that as long as $V$ is large but finite, everything can be calculated by the Schrödinger equation. The time development of the total system is described by

$$\psi(\sigma) \Psi[\phi]_{x_0} = \sum_n C_n \psi_n(\sigma) \Psi[\phi]_{x_0} \quad t = t_0 \quad (13.5.1)$$

$$\rightarrow U(t, t_0) \sum_n C_n \psi_n(\sigma) \Psi[\phi]_{x_0} \quad (t_0 \rightarrow t)$$

$$= \sum_n C_n U(t, t_0) \psi_n(\sigma) \Psi[\phi]_{x_0}$$

$$= \sum_n C_n \Psi^{(n)}(\sigma, \phi, t)_{x_0}, \quad t = t. \quad (13.5.2)$$
Here $U(t, t_0)$ is the time evolution operator of whole system, object plus detector, and $t_0$ is the time before the interaction of the object with the detector and $t$ is the time after the measurement.

The measurement is accomplished if $X_n \neq X_{n'}$ for $n \neq n'$. The amplification device of the observational tool is such that it maps the microscopically different states $\psi_n$, $\psi_{n'}$ of the object into different states of the detector characterized by $X_n \neq X_{n'}$. Stated in a stationary phase argument, we have one stationary point in (13.5.1) but in (13.5.2) it separates into multiple stationary trajectories depending on the index $n$. Thus measuring process corresponds to branching of a stationary trajectory.

This corresponds to the many world picture of Everett III but “many world” is replaced in our case by “many stationary trajectories”. In contrast to Ref. 14, the reduction does not occur in our theory and the linear combination (13.5.2) remains as it is after the measurement. This is of course due to the fact that we have assumed only the Schrödinger equation plus the limit $V \to \infty$. The situation is illustrated in Fig. 13.1 schematically.

Complicated quantum mechanical processes are going on in the shaded region of the figure where branching of stationary phase takes place. But once the model is fixed, it is calculable in principle as a function of time.

The interference terms vanish for the state with different values of $X_n$ by the mechanism explained just after (13.4.45). Thus after measurement, the interference goes away in the sense of (13.4.46) where matrix elements of any polynomial of $\phi(x)$ or $\Pi(x)$ vanish in the limit $V \to \infty$. This is a necessary condition of measurement.

References

2) E. E. Salpeter and H. A. Bethe, Phys. Rev. 84 (1951), 1232.


10) M. Gell-Mann and F. E. Low, Phys. Rev. 84 (1951), 350.


14) H. Everett III, Rev. Mod. Phys. 29 (1957), 454.
Chapter XIV. Superfluid $^4$He

The theory of $^4$He superfluidity is a nice subject to apply the Legendre transformation, which enables us to take the order parameter $\langle \hat{\phi}(x) \rangle$, the expectation value of the $^4$He field operator, as an independent variable. After discussing the condensation $\langle \hat{\phi}(x) \rangle$ or $\langle \hat{\phi}^+(x) \rangle$, we come to the problem of pairing in $^4$He, where the absence of the gap in the excitation spectrum is shown by investigating the structure of the on-shell equation.

The main subject of the present chapter is to derive the whole set of phenomenological equations of the two fluid model (without dissipation) starting from the microscopic Hamiltonian. In this process we neglect the effect of pairing and consider only $\langle \hat{\phi}(x) \rangle$ and $\langle \hat{\phi}^+(x) \rangle$.

Here again the Legendre transformation turns out to be extremely useful. Recall that the condensation brings about the singular contribution to various Green's functions. This singular term appears due to the presence of $\langle \hat{\phi}^{(1)}(x) \rangle$ and it plays an essential role in the superfluid phenomenon. But the generating functional $\Gamma$, defined through the Legendre transform, enjoys the property of 1PI in a diagrammatical language so that $\Gamma$ itself has no singular part. If we use $\Gamma$, the singular part appears separately in various equations and we can easily recognize it. Here the terminology 1PI implies that, as explained repeatedly, $\Gamma$ does not contain the graphs which are separated into two disconnected parts when any one of the propagator lines of the $\hat{\phi}$-field is cut. Thus we conclude that $\Gamma$ or the derivative of it is regular in the limit of the zero energy momentum, except for possible infrared logarithmic divergences (due to the gapless character of the phonon excitation spectrum). This is crucial if one wants to study the hydrodynamic limit where one evaluates Green's functions in the long wave length limit. As for the infrared divergences, although not stated explicitly, we assume "fictitious gap" introduced by Gavoret-Nozieres\(^1\) in the course of calculation and it is removed in the end. However, it has been shown by Nepomnyashchii-Nepomnyashchii\(^2\) that the infrared divergences do not invalidate the relations which hold in the limit of zero energy momentum for a specific type of Green's function. The same may well be the case in our hydrodynamic relations derived below. Indeed we have checked all our hydrodynamic equations up to 1-loop level.

In the course of derivation, we rely heavily on the zero energy momentum limit of various kinds of Ward-Takahashi (W-T) identities which relate different kinds of Green's functions involving the mass current and energy momentum tensor. When W-T relations are written using $\Gamma$, it is assumed that they are not singular in the above sense. Then, W-T identities enable us to write the microscopic Green's functions in terms of the macroscopic physical quantities. Under these reservations, fundamental equations of the two fluid model can be derived. In this study the dissipative terms are not discussed, leaving it as a future investigation.

The required set of equations of the two fluid model which are to be derived below are summarized below,
\begin{align*}
\langle \bar{n} \rangle &= n_s + n_n, \\
\langle \bar{j}^i \rangle &= n_s v_s^i + n_n v_n^i, \\
\langle \bar{T}^i_\ell \rangle &= -m(n_s v_s^i + n_n v_n^i), \\
\langle \bar{T}^i_{\bar{\ell}} \rangle &= mn_n v_{\bar{\ell}i} + mn_n v_{n\bar{\ell}i} - \delta_{\ell\bar{\ell}} P, \\
\langle \bar{\mathcal{E}} \rangle &= \bar{E}^{(0)}(v_s - v_n) + v_n^i mn_n (v_s^i - v_n^i) + \frac{1}{2} m v_n^2 n, \\
\langle \bar{j}^i_{\bar{\ell}} \rangle &= \left( \bar{\mu} + \frac{1}{2} m v_s^2 \right) (n_s v_s^i + n_n v_n^i) + T_s v_n^i + mn_n v_n^i \{ v_n \cdot (v_n - v_s) \}, \\
P &= -\mathcal{E}^{(0)} + T_s + \bar{\mu} n + mn_n (v_n - v_s)^2, \\
m \frac{\partial v_s^i}{\partial t} + \mathcal{P} \left( \frac{1}{2} m v_s^2 + \bar{\mu} \right) &= 0.
\end{align*}

These relations are of course supplemented by the conservation laws for mass, momentum, energy and/or entropy. The notations we adopt in this work are summarized in Table 14.1, where the comparison with those used in the textbook by Landau-Lifshitz\textsuperscript{3} is made. As shown in Table 14.1, we use in the following both the superscript and suffix. For example, the velocity is written as \( v = v^i = -v_i \).

The same problem has been discussed by Hohenberg and Martin\textsuperscript{4} and by Bogolyubov et al.\textsuperscript{5} For one-loop study, see Glassgold et al.\textsuperscript{6} In order to study the spontaneous symmetry breaking in general terms, it is usually done to introduce the notion of \( \eta \)-ensemble\textsuperscript{4} or quasi-average,\textsuperscript{5} which is replaced by the Legendre transformation in our approach. We believe that our method is more transparent and suited for the actual calculations since we deal solely with the expectation values which are \( c \)-numbers and are directly related to the observed quantities.

\begin{table}[h]
\centering
\caption{Comparison between the symbols used in this chapter and those in Ref. 3.}
\begin{tabular}{|c|c|c|}
\hline
variables & this article & Landau-Lifshitz \\
\hline
superfluid velocity & \( v_s^i = -v_{si} \) & \( v_{si} \) \\
normal fluid velocity & \( v_n^i = -v_{ni} \) & \( v_{ni} \) \\
total density & \( \rho \) & \( \rho \) \\
superfluid density & \( \rho_s \) & \( \rho_s \) \\
normal part density & \( \rho_n \) & \( \rho_n \) \\
mass flow & \( j_i \) & \( j_i \) \\
momentum density & \( T^0 \) & \( -j_i \) \\
momentum flow & \( T_{\bar{\ell}i} \) & \( -\Pi_{\bar{\ell}i} \) \\
energy density & \( \mathcal{E} = T^0_\ell + \mu n \) & \( E \) \\
energy flow & \( j_{\bar{\ell}i} = T^0_\ell + \mu j_i \) & \( Q_{\bar{\ell}} \) \\
chemical potential & \( \bar{\mu} \) & \( m\mu \) \\
entropy density & \( s \) & \( \rho s \) \\
pressure & \( P \) & \( \rho \) \\
energy density in the frame \( v_s = 0 \) & \( \mathcal{E}_s^{(0)} \) & \( E_0 \) \\
energy density in the frame \( v_n = 0 \) & \( \mathcal{E}_n^{(0)} \) & \( \ldots \) \\
\hline
\end{tabular}
\end{table}
§ 14.1. Condensation $\langle \hat{\phi} \rangle$ and $\langle \hat{\phi}' \rangle$

The complex (i.e., non-Hermite) field operator $\hat{\phi}(x)$ of $^4$He is expected to have a non-vanishing expectation value below the critical temperature $T_c$ of the Bose condensation. The model Hamiltonian is the same as in (12.3.47),

$$\tilde{H} = \int d^3x \hat{\phi}^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \hat{\phi}(x)$$
$$+ \frac{1}{2} \int d^3x d^3y \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(y) U_0(x-y) \hat{\phi}(y) \hat{\phi}(x),$$
$$U_0(x-y) = U_0(y-x), \quad [\hat{\phi}(t, x), \hat{\phi}^\dagger(t, y)] = \delta^3(x-y). \quad (14.1.1)$$

For simplicity the local form for the repulsive potential, $U_0(x-y) = U_0 \delta^3(x-y)$, is assumed in the following and we use $x = (t, x)$. The Heisenberg operator $\hat{\phi}^{(i)}(x)$ is introduced here and we define the condensation $\phi^i(x) \equiv \langle \hat{\phi}^{(i)}(x) \rangle$ and introduce the notations which are slightly different from (12.3.48),

$$\phi^i \equiv (\hat{\phi}, \hat{\phi}), \quad \phi^i \equiv (\hat{\phi}, \hat{\phi}^\dagger), \quad \phi^i = (\phi, \phi), \quad \phi^i = (\phi, \phi^i). \quad (i=1, 2) \quad (14.1.2)$$

(Compared with § 12.3.2, we have interchanged the indices $i$ and $\alpha$ for the notional conveniences in this chapter. The suffix $i$ has nothing to do with the suffix $\alpha$ or $\beta$ introduced in a moment which discriminates the branch of the contour time paths.)

In order to discuss the condensation $\langle \hat{\phi}^{(i)}(x) \rangle$, let us consider $\tilde{H}_f$,

$$\tilde{H}_f = \tilde{H} - \int d^3x \{ J(x) \hat{\phi}^\dagger(x) + J^\dagger(x) \hat{\phi}(x) \}. \quad (14.1.3)$$

Now we have to generalize the probes to $J$, $J^\dagger$ as in (12.3.49) in order to define the non-equilibrium generating functional,

$$\tilde{H}_J(t) = \tilde{H} - \int dx \{ J(x) \hat{\phi}^\dagger(x) + J^\dagger(x) \hat{\phi}(x) \}. \quad (14.1.4)$$

Here $\alpha=1, 2, 3$ and we introduce the notion of the complex contour $C_\alpha$ of the time integration in order to write various formulas in a compact way. For this purpose we first assume that the initial state is in the equilibrium of the temperature $T = (k_B \beta)^{-1}$, with $k_B$ the Boltzman constant. The contour path generalizes the double path formalism due to Schwinger, Keldysh, Chou et al., to the three time paths including the imaginary time path. See for this purpose Niemi and Semenoff, Wagner, Fukuda et al. and also § 12.2.2 where the connection between the three path formalism and the equilibrium free energy has been discussed. The contour time integral, for example, $\int dt$ extends over the contour $C_\alpha$ which runs as $C_1 \rightarrow C_2 \rightarrow C_3$ (see Fig. 14.1).

![Fig. 14.1. Contour time path $C_\alpha, \alpha=1, 2, 3.$](image-url)
Each path is defined to be $C_1$: $t_i \to t_f$ and $C_2$: $t_f \to t_i$ (return path) $C_3$: $t_l \to t_i - i\beta \hbar$ (imaginary time path). The contour time ordering operator $T_c$ orders the time sequence according to its location on the contour. Furthermore the following notation is used

$$J(x) = J_a(x) \quad \text{if } t \text{ is on } C_a \quad (a = 1, 2, 3) \quad (14.1.5)$$

With these notations and assuming the equilibrium initial distribution, we can write

$$\exp \frac{i}{\hbar} W[J_1, J_2, J_3] = \exp \frac{i}{\hbar} W[J] = \text{Tr} T_c \exp \left( -\frac{i}{\hbar} \int_c dt \tilde{H}_\delta(t) \right), \quad (14.1.6)$$

where $\tilde{H}_\delta(t)$ is equal to $\tilde{H}_{3\delta}(t)$ given in (14.1.4) if $t$ is on $C_\delta$. The contour $\delta$ function is introduced as

$$\int_c dt \delta_c(t - t') f(t) = f(t'). \quad (14.1.7)$$

Similarly the contour $\theta$ function and the contour functional differentiation are defined

$$\theta_c(t - t') = \int_c^{t'} dt'' \delta_c(t'' - t'), \quad (14.1.8)$$

$$\frac{\delta f(t)}{\delta f(t')} = \delta_c(t - t'). \quad (14.1.9)$$

As for the Legendre transformed $\Gamma$ of (12.2.9), the formula of the loop expansion has been established by several authors\textsuperscript{14,16} (see Appendix C) but these works are limited to the zero temperature case or to the equilibrium systems. The non-equilibrium case where the imaginary time path is absent has been discussed by Chou et al.\textsuperscript{10} We use in the following the contour time path defined above in case the imaginary time path is needed. It turns out that the use of contour integral makes it easy to generalize the known results to the non-equilibrium case. See Appendix J for the calculational technique of $\Gamma$ in loop expansion.

Now we study the stationary solution for $\phi_a'(x)$ defined in (12.2.10) which is the starting task of our program. The solution discussed is a static homogeneous one which is independent of $x$ and hence independent of $a$ $(a = 1, 2, 3)$; $\phi_a'(x) = \phi'$. In § 12.2.2, it has been shown that in such a case the non-equilibrium generating functional and the equilibrium free energy are related by (12.2.15). By this relationship the usual free energy $\mathcal{O}[\phi', \phi]$, up to one-loop level for example, is given by the $C_3$ part of $\langle J \cdot 2 \rangle$ and $\langle J \cdot 8 \rangle$. The evaluation of the trace-log appearing in $\Gamma_{1 \text{-loop}}$ is easily done in Fourier space. We give below the result of calculations up to one-loop as an illustration. Numerically it is well-known that such a weak coupling expression is not good, however our purpose is not the numerical one but is to see that the solution of the condensation does exist which will surely be confirmed by loop expansion. The result is

$$\mathcal{O}[\phi', \phi] = -\frac{i}{\hbar \beta} (\Gamma_{\text{tree}} + \Gamma_{1 \text{-loop}})$$
\[ V = \left. -n_0 \mu + \frac{1}{2} n_0^2 U_0 - \frac{d^3 k}{(2\pi)^3} \left\{ \frac{1}{2} \left( \frac{E_k}{2} - \mu + 2n_0 U_0 \right) - \frac{1}{\beta} \ln \sinh \left( \frac{\beta E_k}{2} \right) \right\} \right] . \tag{14\cdot1\cdot10} \]

Here, \( V \) is the volume of the system and we have defined
\[ E_k = \sqrt{\left( \frac{\epsilon_k^0 - \mu + 2n_0 U_0}{2} \right)^2 - \left( n_0 U_0 \right)^2}, \quad n_0 = \phi^\dagger \phi, \quad \epsilon_k^0 = \frac{\hbar^2 k^2}{2m}. \tag{14\cdot1\cdot11} \]

The stationary value of \( n_0 = n_0^{(0)} = \phi^\dagger \phi^{(0)} \) is determined by the following equation:
\[ 0 = \frac{\partial \Omega}{\partial \phi^\dagger} = -\phi^{(0)} \left( \mu - n_0^{(0)} U_0 + U_0 \int \frac{d^3 k}{(2\pi)^3} \left\{ \frac{1}{2} \frac{\epsilon_k^0 - \mu + \frac{3}{2} n_0^{(0)} U_0}{E_k} \coth \frac{\beta E_k}{2} \right\} \right), \tag{14\cdot1\cdot12} \]

where \( n_0 \) contained in \( E_k \) is replaced by the stationary solution \( n_0^{(0)} \). From the above results, the known results of one-loop are reproduced. The average particle number is
\[ n = \frac{1}{V} \frac{\partial \Omega}{\partial \mu} = \frac{i}{\beta \hbar V} \frac{\partial \Gamma}{\partial \mu} = n_0^{(0)} - U_0 \int \frac{d^3 k}{(2\pi)^3} \left\{ \frac{1}{2} \frac{\epsilon_k^0 - \mu + 2n_0^{(0)} U_0}{E_k} \coth \frac{\beta E_k}{2} \right\} . \tag{14\cdot1\cdot13} \]

If the solution is non-trivial, (14\cdot1\cdot12) becomes
\[ \mu = n_0^{(0)} U_0 - U_0 \int \frac{d^3 k}{(2\pi)^3} \left( 1 - \frac{\epsilon_k^0 - \mu + \frac{3}{2} n_0^{(0)} U_0}{E_k} \coth \frac{\beta E_k}{2} \right). \tag{14\cdot1\cdot14} \]

These results agree with those obtained by several authors.\(^{6,7,16}\) The critical temperature \( T_c \) is determined by setting \( n_0^{(0)} = 0 \) in (14\cdot1\cdot13) and (14\cdot1\cdot14). Then, by writing \( \beta_c = (k_B T_c)^{-1} \),
\[ n = \frac{1}{(2\pi)^3} \frac{1}{e^{\beta_c (\epsilon_k^0 - \mu)} - 1}, \quad \mu = 2 U_0 \int \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta_c (\epsilon_k^0 - \mu)} - 1} = 2n U_0, \tag{14\cdot1\cdot15} \]

where we have used the fact that the \( x^{-1} \coth x \) is an even function of \( x \). On the other hand, for the trivial solution of (14\cdot1\cdot12), the following equation follows from (14\cdot1\cdot13)
\[ n = \int \frac{d^3 k}{(2\pi)^3} \frac{1}{e^{\beta_c (\epsilon_k^0 - \mu)} - 1}. \tag{14\cdot1\cdot16} \]

This equation holds for any \( \beta \) above the critical temperature, which coincides with the result of ideal gas. This implies that the above \( T_c \) the interaction does not affect the stationary solution of \( \Gamma \) is one-loop approximation. As is well-known we have to take more diagrams into account in order to see the effect of interaction on \( T_c \) or more detailed potential other than the local contact interaction has to be considered.
The above result has a severe difficulty. Indeed the consistency equation for \( \mu \), the second relation of (14.1.15), has no real solution for \( \beta_c \). Since \( \mu=2nU_0>0 \) in the presence of interaction, the integral diverges or, if it is analytically regularized, \( \beta_c \) becomes necessarily complex. If we want to keep \( \beta_c \) to be real, then another parameter such as \( n \) or \( \mu \) becomes complex. As noted above, this is related to the fact that, within the approximation adopted, the effect of interaction is not sufficiently taken into account by one-loop calculation.

The problem then is how to avoid the difficulty. One possibility is to include higher loop contributions but one can easily convince oneself that this does not work. The reason is that the propagator \( D \) used in higher loop diagrams is the same one which appears in one-loop term \( T \ln D^{-1} \). Since the difficulty is related to the zero of \( D^{-1} \), higher loops make things even worse. We have somehow to sum up an infinite number of loop diagrams but this is not a wise strategy.

Here we take the number density as another independent variable and add a new source term \( -\int d^3x \phi^*(x)K_\omega(x)\phi(x) \) to \( H_{\sigma}(t) \) in (14.1.4) and proceed to two-loop diagrams. Then we perform the double Legendre transformation from \( (f^i, K) \) to \( (\phi^i, \phi^* \phi) \) where \( \phi^* \phi \) is the connected part of \( \langle \phi^*(x)\phi(x) \rangle \). This enables us to get self-consistent determination of the number density. In case \( K(x) \) is independent of \( x \), \( K \) plays the same role as \( \mu \) but it is more convenient to introduce both \( \mu \) and \( K \) and set \( K=0 \) as a stationary condition. Here we write down only the result of two-loop approximation,

\[
\Gamma[\phi, \phi^* \phi, \mu] = \beta \hbar V \left[ n_0 \mu - \frac{1}{2} n_0^2 U_0 + U_0 (\hbar \phi^* \phi)^2 \right. \\
\left. + \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{2} \left( \epsilon^0 - \mu + 2nU_0 \right) - \frac{1}{\beta} \ln 2 \sinh \frac{\beta E_k}{2} \right\} \right],
\]

where \( n \) is the number density which is a function of \( \mu \) and is given by

\[
n = \frac{\partial \Gamma}{\partial \mu} = n_0 + \hbar \phi^* \phi, \quad \hbar \phi^* \phi(x) = \langle \phi^*(x) \phi(x) \rangle_{\text{conn}},
\]

\[
E_k = \sqrt{\left( \epsilon^0 - \mu + 2nU_0 \right)^2 - (n_0 U_0)^2}.
\]

In this approximation, we see that the stationary condition, the average particle number and non-trivial solution is gotten by replacing \( n_0^{(0)} \) by \( n \) in (14.1.12) \( \sim (14.1.14) \), and we have only to put \( \mu - 2nU_0 \) in place of \( \mu \) appearing inside the \( \hbar \) integral of (14.1.15) and (14.1.16). In this way we can avoid the difficulties stated above.

Below we add the source \( K(x) \) whenever it is essential but in other cases it is not introduced for simplicity.

\section*{§ 14.2. Pairing in superfluid \(^4\)He}

Now the above formalism is applied to construct the pairing theory of superfluid \(^4\)He. The reason why this subject is inserted here is that there has been controversy,\(^{17}-^{24}\) concerning the absence or the presence of the gap in the phonon excitation
Chapter XIV. Superfluid 4He

spectrum after the pairing occurs. The problem can be answered in our formalism in a transparent way.

In order to discuss this problem, we introduce the symmetry breaking source terms as probes of \( \langle \hat{\phi} \rangle \), \( \langle \hat{\phi}^\dagger \rangle \) and \( \langle \hat{\phi} \hat{\phi} \rangle \), \( \langle \hat{\phi}^\dagger \hat{\phi}^\dagger \rangle \). These are chosen to be order parameters and we thus consider the following Hamiltonian:

\[
\hat{H}_{J, K}(t) = \hat{H} - \int d^3x (J(x) \hat{\phi}^\dagger(x) + J(x) \hat{\phi}(x))
- \int d^3x \left( K(x) \hat{\phi}^\dagger(x) \hat{\phi}^\dagger(x) + K(x) \hat{\phi}(x) \hat{\phi}(x) + K_a(x) \hat{\phi}^\dagger(x) \hat{\phi}(x) \right).
\] (14.21)

Here \( \hat{H} \) is the Hamiltonian (14.1.1) and for convenience the probe \( K_a(x) \) has also been introduced which couples to the number density.

The non-equilibrium generating functional is defined next assuming the equilibrium distribution at initial time,

\[
\exp \frac{i}{\hbar} W[J^i, K^i] = \text{Tr} \left( \rho_{J^i, K^i} U_{J^i, K^i}(\infty, t_i) U_{J^i, K^i}(\infty, t_i) \right),
\]

\[
U_{J^i, K^i}(t, t_i) = \text{Te}^{\frac{i}{\hbar} \int_{t_i}^t dt' \hat{H}_{J^i, K^i}(t')} \), \quad (a=1, 2)
\]

\[
\rho_{J^i, K^i} = \text{Tr} \exp \left( -\int_0^{\infty} d\tau \hat{H}_{J^i, K^i}(\tau) \right).
\] (14.22)

Here the suffix \( a=1, 2 \) represents the real time path. We call them path 1 and path 2 and the superscript \( i \) indicates the component of the following vectors (note the change in the notations compared with § 12.3.2),

\[
\begin{pmatrix} J^1 \\ J^2 \end{pmatrix} = \begin{pmatrix} J \\ J \end{pmatrix}, \quad \begin{pmatrix} K^1 \\ K^2 \\ K^3 \end{pmatrix} = \begin{pmatrix} K \\ K \\ K_a \end{pmatrix}, \quad \begin{pmatrix} \hat{\phi}^\dagger \\ \hat{\phi}^\dagger \end{pmatrix} = \begin{pmatrix} \hat{\phi}^\dagger \\ \hat{\phi}^\dagger \end{pmatrix}, \quad \begin{pmatrix} \hat{\phi} \bar{\phi} \\ \hat{\phi} \bar{\phi} \end{pmatrix} = \begin{pmatrix} \hat{\phi}^\dagger \hat{\phi} \\ \hat{\phi}^\dagger \hat{\phi} \end{pmatrix}.
\] (14.23)

For third path, \( a=3 \), the imaginary time \( \tau \) has been introduced for \( \rho_{\tau} \) with \( t = t_i - i \tau \) and the symbol \( T \) or \( T_{\tau} \) implies the time or \( \tau \)-ordering of the operator appearing to the right of it. Note that we have introduced, besides \( J^i, J^i, K^i \) and \( K_a^i \), the source terms \( J^i, K^i, K_a^i \) for the path 3.

Let us define order parameters \( \phi \) and \( \Phi \),

\[
\frac{\delta W}{\delta J_a^i(x)} = (-)^{a+1} \phi_a^i(x), \quad \frac{\delta W}{\delta J_a^i(\tau, x)} = \frac{\hbar}{i} \phi_a^i(\tau, x),
\]

\[
\frac{\delta W}{\delta K_a^i(x)} \equiv (-)^{a+1} \Psi_a^i(x) = (-)^{a+1} (\phi_a^i(x) \phi_a^i(x) + \hbar \Phi_a^i(x)),
\]

\[
\frac{\delta W}{\delta K_a^i(\tau, x)} = \frac{\hbar}{2i} \Psi_a^i(\tau, x) = \frac{\hbar}{2i} (\phi_a^i(\tau, x) \phi_a^i(\tau, x) + \hbar \Phi_a^i(x)),
\]

\[
\frac{\delta W}{\delta K_a^i(\tau, x)} = (-)^{a+1} \Psi_a^i(x) = (-)^{a+1} (\phi_a^i(x) \phi_a^i(x) + \hbar \Phi_a^i(x)),
\]

\[
\frac{\delta W}{\delta K_a^i(\tau, x)} \equiv (-)^{a+1} \Psi_a^i(x) = (-)^{a+1} (\phi_a^i(x) \phi_a^i(x) + \hbar \Phi_a^i(x)).
\]
\[
\frac{\delta W}{\delta K_3^\alpha(r, x)} = (-)^{\alpha + 1} \Psi_3^\alpha(r, x) = \frac{\hbar}{i} \left( \phi_3^\alpha(r, x) \phi_3^\beta(r, x) + \hbar \Phi_3^\alpha(r, x) \right).
\]

In the above equations \( \alpha = 1, 2 \) and \( i = 1, 2 \) and \( \hbar \Phi_3^\alpha(x) \) is the connected part of the pairing parameter \( \Psi_3^\alpha(x) \). Now the Legendre transformation is performed and the second generating functional \( \Gamma \) is introduced

\[
\Gamma[\phi^i, \Phi^i] = W[J^i, K^i] - \int_t^\infty d^4x \sum_{i=1,2} J_i^i(x) \phi_i^i(x) + \int_t^\infty d^4x \sum_{i=1,2} J_3^i(x) \phi_3^i(x)
- \frac{\hbar}{i} \int_0^{\hbar} d\tau d^3x \sum_{i=1,2} J_i^i(\tau, x) \phi_i^i(\tau, x)
- \int_t^\infty d^4x \sum_{i=1,2} K_i^i(x) \Psi_i^i(x) + \int_t^\infty d^4x \sum_{i=1,2,3} K_3^i(x) \Psi_3^i(x)
- \frac{\hbar}{i} \int_0^{\hbar} d\tau d^3x \sum_{i=1,2,3} K_3^i(\tau, x) \Psi_3^i(\tau, x).
\]

When we define \( \Gamma[\phi_3^i, \Phi_3^i] \), Eq. (14.2.4) has to be solved and \( J \) or \( K \) is expressed in terms of \( \phi \) and \( \Phi \).

In the two-loop approximation, we use the inversion formulas and it can be shown that the pairing solution does exist and it agrees with the results obtained in Refs. 17) ~24). Now let us come to the problem of the presence or the absence of the gap in the excitation spectrum. We show in full order that the gap does not exist.\(^{25}\)

Starting point is the fact that \( \Gamma \) is invariant under the phase transformation,

\[
\phi(x) \rightarrow e^{i\theta} \phi(x), \quad \phi^*(x) \rightarrow e^{-i\theta} \phi^*(x),
\]

\[
\Phi(x) \rightarrow e^{i\theta} \Phi(x), \quad \Phi^*(x) \rightarrow e^{-i\theta} \Phi^*(x).
\]

We have written \( \Phi_3^\alpha \) as \( \Phi^\alpha \). Thus the following identity is obtained,

\[
0 = \frac{\delta \Gamma[\phi_3^i, \Phi_3^i]}{\delta \theta} = \sum_{\alpha=1,2,3, i} \int d^4y \left( \frac{\delta \Gamma}{\delta \phi_3^\alpha(y)} \frac{\delta \phi_3^\alpha(y)}{\delta \theta} + \frac{\delta \Gamma}{\delta \Phi_3^\alpha(y)} \frac{\delta \Phi_3^\alpha(y)}{\delta \theta} \right).
\]

All the indices have been written here: \( \alpha \) for the three paths and \( i \) for the components. For the infinitesimal \( \theta(=\delta \theta) \), we have

\[
\delta \phi_3^\alpha(x) = (-i\delta \theta \phi_3^\alpha(x), i\delta \theta \phi_3^\alpha(x)),
\]

\[
\delta \Phi_3^\alpha(x) = (-i2\delta \theta \Phi_3^\alpha(x), i2\delta \theta \Phi_3^\alpha(x), 0).
\]

In this way it is obtained that

\[
0 = \sum_{\alpha=1,2,3} \int d^4y \left( \frac{\delta \Gamma}{\delta \phi_3^\alpha(y)} \phi_3^\alpha(y) - \frac{\delta \Gamma}{\delta \Phi_3^\alpha(y)} \Phi_3^\alpha(y) \right)
+ 2 - \frac{\delta \Gamma}{\delta \Phi_3^\alpha(y)} \Phi_3^\alpha(y) - 2 \frac{\delta \Gamma}{\delta \Phi_3^\alpha(y)} \Phi_3^\alpha(y). \tag{14.2.10}
\]

Let us differentiate (14.2.10) with respect to \( \phi_i^i \) or \( \Phi_i^i \). After taking the derivative by \( \phi_i(x) \), for example, we get
\[ 0 = \sum_{\alpha=1,3} \int d^4y \left( \frac{\delta^2 \Gamma}{\delta \phi_\alpha(x) \delta \phi_\alpha(y)} \phi_\alpha(y) - \frac{\delta^2 \Gamma}{\delta \phi_\alpha(x) \delta \phi^*_\alpha(y)} \phi^*_\alpha(y) ight) + 2 \frac{\delta^2 \Gamma}{\delta \phi_\alpha(x) \delta \phi_\alpha(y)} \phi_\alpha(y) - 2 \frac{\delta^2 \Gamma}{\delta \phi_\alpha(x) \delta \phi^*_\alpha(y)} \phi^*_\alpha(y) + \frac{\delta \Gamma}{\delta \phi_\alpha(x)} . \]

(14.2.11)

Now (14.2.11) is evaluated at the constant stationary solution \( \phi^\alpha(x) = \phi^\alpha(0), \phi^\alpha_i(x) = \phi^{\alpha(0)} \). Then owing to the space-time homogeneity

\[ (\Gamma^{\alpha\beta}(x,y))_0 = (\Gamma^{\alpha\beta}(x-y))_0 , \]

so that \( y \)-integration in (14.2.10) projects out the \( k = 0 \) mode of the Fourier component,

\[ \int d^4y (\Gamma^{\alpha\beta}_k(x,y))_0 = (\Gamma^{\alpha\beta}(k=0))_0 . \]

Here the index \( A \) or \( B \) implies the components of the vector \( \phi^A = (\phi^*, \phi, \phi^*, \Phi, \Phi^* \) When we take \( t_i = -\infty \), then \( \alpha = 3 \) in the sum of (14.2.11) does not contribute and in \( \alpha \)-space the sum over \( \alpha = 1, 2 \) remains. Thus we get the form \( \Gamma^{\alpha\beta}_1 + \Gamma^{\alpha\beta}_2 = \Gamma^{\alpha\beta}_0 \) which is the inverse of the retarded function \( W^{\alpha\beta}_1 + W^{\alpha\beta}_2 \), see (12.3.12). We differentiate (14.2.10) by \( \phi^i(x), \phi_i(x), \phi_i^*(x), \Phi_n(x) \) then they can be written in the matrix form,

\[
\begin{pmatrix}
\Gamma^{\alpha\beta}(\omega=0, k=0)
\end{pmatrix}_0 =
\begin{pmatrix}
-\phi^* \\
\phi \\
-2\phi^* \\
2\Phi \\
0
\end{pmatrix} =
\begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix} .
\]

(14.2.12)

The above equation clearly shows that the gapless Goldstone excitation \( |G\rangle \) exists and its wave function is given by\(^{25}\) \((-\phi^*, \phi, -2\phi^*, 2\Phi, 0)\).

**Generalized Hugenholtz-Pines theorem**

Let us write (14.2.12) explicitly, by using the fact that \( \Gamma^{\alpha\beta}_0 \) is the inverse of the retarded Green’s function \( W^{\alpha\beta}_0 \), which can be written by using the self-energy function \( \Sigma \),

\[
\begin{pmatrix}
\mu - \hbar \Sigma_{\phi^*\phi}(k=0) & -\hbar \Sigma_{\phi^*\phi}(k=0) & \cdots & -\hbar \Sigma_{\phi\phi^*}(k=0) \\
-\hbar \Sigma_{\phi^*\phi}(k=0) & \mu - \hbar \Sigma_{\phi^*\phi}(k=0) & \cdots & -\hbar \Sigma_{\phi\phi^*}(k=0) \\
\cdots & \cdots & \cdots & \cdots \\
0 & 0 & \cdots & 0 \\
\end{pmatrix}
\times
\begin{pmatrix}
-\phi^* \\
\phi \\
-2\phi^* \\
2\Phi \\
0
\end{pmatrix} =
\begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix} .
\]

(14.2.13)

If the non-trivial solution \( \phi \) and \( \phi^* \) are assumed to be real, which is always possible
by a phase rotation, we get the following equation from (14.2.13), for example,
\begin{equation}
\mu = \hbar \Sigma_{\Phi}(k=0) - \hbar \Sigma_{\Phi}(k=0) + 2\sqrt{n_0} \hbar \Delta \{ \hbar \Sigma_{\Phi}(k=0) - \hbar \Sigma_{\Phi}(k=0) \},
\end{equation}
where $\phi = \phi^* = \sqrt{n_0}$ has been used. We have also defined $\Delta$ by $\hbar \Phi = - \phi \hbar \Delta$, $\hbar \Phi^* = - \phi^* \hbar \Delta$. Equation (14.2.14) is a generalization of the Hugenholtz-Pines theorem\(^{30}\) including the correction due to the pairing effect. Note the extra terms $\Sigma_{\Phi}$ and $\Sigma_{\Phi}$ on the right-hand side of (14.2.14), which assures the gapless character of phonon excitation. They come from the mixing of two order parameters $\langle \hat{\phi}^{(s)} \rangle$ and $\langle \hat{\phi}^{(s)} \hat{\phi}^{(s)} \rangle$. The last point is discussed in detail below.

**Gap and pairing effect**

Usually the pairing effect leads to the gap in single particle spectrum. For example in superconductor the pairing of two electrons results in the electron spectrum with finite gap.

The essential difference between the superconductor and our case above is the absence or the presence of non-vanishing $\langle \hat{\phi} \rangle$. Consider the superconductor where $\hat{\phi}$ represents electron field and $\phi = \langle \hat{\phi} \rangle$ is assumed to be zero. Therefore our mode determining equation is block diagonal and has the form,

\[
\begin{pmatrix}
2 \times 2 & 0 \\
0 & 3 \times 3
\end{pmatrix}
\begin{pmatrix}
-\phi^* = 0 \\
\phi = 0
\end{pmatrix} = 0.
\]

The vanishing of the off-diagonal part is easily seen by noting that $\Gamma$ is invariant under (14.2.6), (14.2.7) and hence $\Gamma$ is a function of $\phi \phi^*$ which vanishes after differentiating once by $\phi$ or $\phi^*$ and setting $\phi = \phi^* = 0$. Equation (14.2.15) says that $2 \times 2$ part has no Goldstone mode and a glance at Hartree-Fock expression of $\Gamma$ tells us that the gap exists for electron spectrum. In $3 \times 3$ part we of course have the Goldstone (phonon) mode which however decouples from single electron sector and, in the presence of electromagnetic field, is absorbed into the electromagnetic potential which is the cause of the Meissner effect.

The above situation is different from Helium case where non-zero character of $\phi$, $\phi^*$ assures a finite value of non-diagonal part of (14.2.15). This leads to the fact that the phonon mode couples to both single particle and pair channels as can be seen by the wave function of Goldstone mode. The excitation spectrum of all channels is the same and is gapless. (We have not studied the full on-shell equation (2.1.4a) so that it is not known whether this is the only excitation spectrum.) The reason why the gap appeared in the excitation mode in Refs. 17~22) is that only the lower $3 \times 3$ part is considered and off-diagonal $2 \times 3$ part and the upper $2 \times 2$ part are ignored in these references. It is easy to convince ourself that such a procedure violates the symmetry (14.2.6) and (14.2.7).

Although we know that the pairing indeed occurs, this effect is neglected below in deriving the phenomenological equations of the two fluid model. The inclusion of the pairing is left as a future study.
§ 14.3. Ward-Takahashi identities for mass flow

Now we take up the first step toward the derivation of the two fluid model. Below we present essential part of the derivation leaving the details to Ref. 27.

When the Hamiltonian of the system has the symmetry under some transformation group, there exist identities among Green’s functions which are called Ward-Takahashi (W-T) identities. Now we derive the various kinds of W-T identities involving the current corresponding to the mass flow. It is a consequence of the invariance of the action $I$ under the phase change $\tilde{\phi} \rightarrow e^{i\eta} \tilde{\phi}$, $\tilde{\phi}^* \rightarrow e^{-i\eta} \tilde{\phi}^*$. First the source terms are added to $\tilde{H}_I$ of (14.1.3) where the new external probes $K$ and $K^i$ $(i=1, 2, 3)$ couple to the number density $\bar{n}$ and current operator $\tilde{j}_i$, respectively:

$$\tilde{H}_{I,k^*}(t) = \tilde{H}_I - \int d^3x (K(x) \bar{n}(x) + K^i(x) \tilde{j}_i(x)),$$  \hspace{1cm} (14.3.1)

where $x = (t, \mathbf{x})$ and

$$\bar{n}(x) = \tilde{\phi}^*(x) \tilde{\phi}(x), \quad \tilde{j}_i(x) = -\frac{\hbar}{2m_i} \tilde{\phi}^*(x) \partial_i \tilde{\phi}(x).$$  \hspace{1cm} (14.3.2)

Here we have introduced the notation

$$\tilde{\phi}^*(x) \partial_i \tilde{\phi}(x) = \tilde{\phi}^*(x) (\partial_i - \partial_i) \tilde{\phi}(x) = \tilde{\phi}^*(x) \partial_i \tilde{\phi}(x) - (\partial_i \tilde{\phi}^*(x)) \tilde{\phi}(x).$$

When we discuss the conservation laws, it is convenient to adopt, besides $x = x^a = (x^0, x^1, x^2, x^3) = (t, \mathbf{x})$, the four dimensional notations as follows,

$$K^a(x) = (K(x), K^i(x), K^0(x), K^a(x)),$$

$$\tilde{j}_a(x) = (\bar{n}(x), \tilde{j}_i(x), \tilde{j}_2(x), \tilde{j}_3(x)).$$  \hspace{1cm} (14.3.3)

Two kinds of four vectors $A^a$ and $A_a$ are related as follows: let $A^a = (A^0, A^1, A^2, A^3)$ $\equiv (A^0, A^i)$, then $A_a = (A_0, A_i) = (A^0, -A^i)$. The inner product is defined to be $A^a B_a = A^a B^a + A^i B_i = A^0 B^0 - A^i B^i$. The space-time derivative is defined as $\partial^a = (\partial^0, \partial^i) = (\partial/\partial t, \mathbf{\nabla})$, $\partial_a = (\partial_0, \partial_i) = (\partial_0 - \partial^i) = (\partial/\partial t, \mathbf{\nabla})$. Remember however that we also use $\phi^i$ ($i=1, 2$) which means $(\phi, \phi)$.

14.3.1. Derivation of W-T identities

Let us start from the equation of motion in the presence of the source term and rewrite it by using the functional representation of the generating functional. The action functional $\tilde{I}_{J, k^*}$ corresponding to $\tilde{H}_{I, k^*}(t)$ is given in operator form by

$$\tilde{I}_{J, k^*} = \int d^4x \tilde{\phi}^*(x) \left( i\hbar \partial_t + \frac{\hbar}{2m} \mathbf{\nabla}^2 + \mu \right) \tilde{\phi}(x) - \frac{1}{2} \int d^4x \int d^4y \tilde{\phi}^*(x) \tilde{\phi}^*(y) U_0(x-y) \tilde{\phi}(y) \tilde{\phi}(x)$$

$$+ \int d^4x \left( J(x) \tilde{\phi}^*(x) + \mathcal{J}(x) \tilde{\phi}^*(x) + K(x) \tilde{\phi}^*(x) \tilde{\phi}(x) + K^i(x) \frac{\hbar}{2m_i} \tilde{\phi}^*(x) \partial_i \tilde{\phi}(x) \right),$$  \hspace{1cm} (14.3.4)
\[ I = \int d^4 x K^{\mu}(x) \tilde{J}^{\mu}(x). \] (14.3.5)

In (14.3.4) only one time integration is actually present because \( U_0(x-y) \) contains \( \delta(t_x - t_y) \). The Euler-Lagrange equation of motion in the operator formalism is obtained from the stationary condition of \( \tilde{I}_{\mu, \kappa^*} \),

\[
0 = \frac{\delta \tilde{I}_{\mu, \kappa^*}}{\delta \tilde{\phi}^\dagger(x)}
= \left( i\hbar \partial_t + \frac{\hbar}{2m} \partial^2 + \mu \right) \bar{\phi}(x) - \int d^4 y \bar{\phi}^\dagger(y) U_0(x-y) \bar{\phi}(y) \tilde{\phi}(x)
+ J(x) + K(x) \bar{\phi}(x) + \frac{\hbar}{2mi} \{ 2K'(x)(\partial_t \bar{\phi}(x)) + (\partial_t K'(x)) \bar{\phi}(x) \}, \quad (14.3.6)
\]

\[
0 = \frac{\delta \tilde{I}_{\mu, \kappa^*}}{\delta \tilde{\phi}(x)}
= \left( -i\hbar \partial_t + \frac{\hbar}{2m} \partial^2 + \mu \right) \tilde{\phi}^\dagger(x) - \int d^4 y \tilde{\phi}^\dagger(x) \tilde{\phi}^\dagger(y) U_0(x-y) \bar{\phi}(y)
+ \tilde{J}(x) + K(x) \tilde{\phi}^\dagger(x) + \frac{\hbar}{2mi} \{ -2K'(x)(\partial_t \tilde{\phi}^\dagger(x)) - (\partial_t K'(x)) \tilde{\phi}^\dagger(x) \}. \quad (14.3.7)
\]

In these equations any operator \( \tilde{O}(x) \) is in the Heisenberg representation which is related to the Schrödinger operator \( \tilde{O}(x) \) as follows,

\[
\tilde{O}(x) = U_{\mu, \kappa^*}(t, t_1) \tilde{O}(x) U_{\mu, \kappa^*}(t, t_1),
\]

\[
U_{\mu, \kappa^*}(t, t_1) = T \exp\left\{-\frac{i}{\hbar} \int_{t_1}^{t} dt' \tilde{H}_{\mu, \kappa^*}(t')\right\}. \quad (14.3.8)
\]

Here \( T \) stands for the time ordering operator. From (14.3.6) and (14.3.7), we are led to the following equation of motion:

\[
0 = \tilde{\phi}^\dagger(x) \frac{\delta \tilde{I}_{\mu, \kappa^*}}{\delta \tilde{\phi}^\dagger(x)} - \frac{\delta \tilde{I}_{\mu, \kappa^*}}{\delta \tilde{\phi}(x)} \tilde{\phi}(x)
= i\hbar \partial^\mu \tilde{J}_\mu(x) + J(x) \tilde{\phi}^\dagger(x) - \tilde{J}(x) \tilde{\phi}(x) + \frac{\hbar}{mi} \partial_t (K'(x) \tilde{\phi}^\dagger(x) \tilde{\phi}(x)). \quad (14.3.9)
\]

Now we take the expectation value by multiplying the initial density matrix \( \rho \) and by taking the trace. In order to write the desired expectation value by using the generating functional, we define \( W \) by introducing three kinds of sources \( J^\alpha(x) \) on three paths \( C_\alpha, \alpha = 1, 2, 3 \), see Fig. 14.1. (Similarly for \( K \).) We assume that the time variable of \( x \) or \( y \), etc., can be on one of three paths and define \( J'(x) \) in such a way that \( J'(x) = J^\alpha(x) \) if \( x \) is on \( C_\alpha \). \( W \) is then given by the contour (functional) path integral,
\[ \exp \frac{i}{\hbar} W[J_s^t, K_s^a] = \text{Tr} \{ \rho_{J_s^t, K_s^a} U_{J_s^t, K_s^a}(\infty, t_f) U_{J_s^t, K_s^a}(\infty, t_i) \} \]
\[ = \int \mathcal{D}[\phi^{\dagger}] \text{exp} \left( -\frac{i}{\hbar} I_c[\phi^{\dagger}, \phi, J^t, K^a] \right). \]  

(14.3.10)

In the above expressions \( \rho_{J_s^t, K_s^a} \) is defined, assuming the initial equilibrium with the temperature \((k_B\beta)^{-1}\), to be
\[ \rho_{J_s^t, K_s^a} = \text{Tr}_{\text{T}} \text{exp} \left\{ -\int_0^{\infty} d\tau H_{J_s^t, K_s^a}(\tau) \right\}, \]  

(14.3.11)

where \( \text{T} \) implies the time ordering with respect to the imaginary time \( \tau \). The functional path integral in (14.3.10) is performed along the contour \( C_a \) and \( I_c[\phi^{\dagger}, \phi, J^t, K^a] \) is the contour action which is given by (14.3.4) with the hat deleted and with the integration \( \int d^4 x \) or \( \int d^4 y \) replaced by the contour integral \( \int_c d^4 x \) or \( \int_c d^4 y \). The contour integration is defined as the time integration extending over the whole contour \( C_a \) made up of three paths \( C_1, C_2, C_3 \) of Fig. 14.1. The final time \( t_f \) in Fig. 14.1 is arbitrary as long as it is larger than the time we are interested in. The symbol B.C. implies the boundary conditions \( \phi(t_i, x) = \phi(t_i - i\hbar \beta, x) \), etc.

Now the expectation value of (14.3.9) is written in terms of the functional derivative of \( W \). For this purpose, we rewrite (14.3.10) using the variable
\[ \phi_s(x) = e^{i\theta(x)} \phi(x), \quad \phi_s^*(x) = e^{-i\theta(x)} \phi^*(x). \]

This method makes clear the relationship of the W-T identities and the phase transformation. The functional integration measure is invariant under this change, \( \int \mathcal{D}[\phi^{\dagger}] = \int \mathcal{D}[\phi^{\dagger}] \), therefore we get
\[ \int \mathcal{D}[\phi^{\dagger}] \text{exp} \left( -\frac{i}{\hbar} I_c[\phi^{\dagger}, \phi, J^t, K^a] \right) = \int \mathcal{D}[\phi] \text{exp} \left( -\frac{i}{\hbar} I_c[\phi, \phi, J^t, K^a] \right) \]
\[ = \int \mathcal{D}[\phi^{\dagger}] \text{exp} \left( -\frac{i}{\hbar} I_c[\phi^{\dagger}, \phi, J^t, K^a] \right). \]

For an infinitesimal \( \theta(x) \), we get the following identity:
\[ 0 = \frac{i}{\hbar} \int_c d^4 x \theta(x) \int \mathcal{D}[\phi^{\dagger}] \text{b.c.} \left\{ \phi(x) \frac{\delta I_c}{\delta \phi(x)} - \phi^*(x) \frac{\delta I_c}{\delta \phi^*(x)} \right\}. \]

Since \( \theta(x) \) is an arbitrary function of \( x \), we get
\[ 0 = \int \mathcal{D}[\phi^{\dagger}] \text{b.c.} \left\{ \phi(x) \frac{\delta I_c}{\delta \phi(x)} - \phi^*(x) \frac{\delta I_c}{\delta \phi^*(x)} \right\}, \]

which leads to the W-T relation we are looking for,
\[ 0 = i\hbar \partial_{\mu} \frac{\delta W}{\delta K_{a\mu}} - J_a(x) \frac{\delta W}{\delta J_a(x)} + J_a(x) \frac{\delta W}{\delta J_a(x)} + \frac{\hbar}{mi} \partial_{\mu} \left( K_{a\mu}(x) \frac{\delta W}{\delta K_{a\mu}(x)} \right). \]  

(14.3.12)

Here the notations \( J_a(x) \), etc., have been used and \( W \) is the functional of \( J_a^t \) and \( K_{a\mu}^i \),
i.e., $W = W[J^a_i, K^p_a]$. Equation (14.3.12) holds for $a = 1, 2, 3$. The physical expectation value is obtained if we set $J^a_i = K^p_a = 0$.

Now we perform the contour Legendre transformation from $W = W[J^a_i, K^p_a]$ to $\Gamma[\phi^a_s, K^p_a]$. It has to be remarked that $K^p_a$ is regarded as a spectator parameter in this case.

$$ \Gamma = W - \int_c d^4x \, J^a_i(x) \frac{\delta W}{\delta J^a_i(x)} \quad \phi^a_s(x) = (-1)^{a+1} \frac{\delta W}{\delta J^a_i(x)} . $$

Here we use the following identities of the Legendre transformation, see (A.5) and (A.11),

$$ \frac{\delta \Gamma}{\delta \phi^a_s(x)} = (-1)^a J^a_i(x) , \quad \frac{\delta \Gamma}{\delta K^p_a(x)} = (-1)^{a+1} \frac{\delta W}{\delta K^p_a(x)} . $$

For $a = 3$, we have to replace $(-1)^{a+1}$ by $\hbar/i$. Equation (14.3.13) is then rewritten as

$$ 0 = i\hbar \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} \right)_0 + \phi^a_s(x) \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} + \frac{\hbar}{mi} \partial^a \left( K^p_a(x) \frac{\delta W}{\delta K^p_a(x)} \right)_0 . $$

Taking the $n$-th ($n = 1, 2, 3, \cdots$) derivative of (14.3.12) by $J^a_i$, $K^p_a$ and evaluating the resulting expressions at $J^a_i = K^p_a = 0$, the following relations are obtained:

$n = 0$: $0 = \partial^a(n(x))_0 + \partial^a(j(x))_0 , \quad (14.3.15)$

$n = 1$: $0 = i\hbar \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} \right)_0 , \quad (14.3.16)$

$$ 0 = i\hbar \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} \right)_0 + \frac{\hbar}{mi} \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} \right)_0 , \quad (14.3.17) $$

$$ 0 = i\hbar \partial^a \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} \right)_0 + \frac{\hbar}{mi} \partial^a \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial K_s(y)} \right)_0 , \quad (14.3.18) $$

$$ 0 = i\hbar \partial^a \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial J^a_i(y)} \right)_0 + \delta_a \partial^a \left( \frac{\delta W}{\delta J^a_i(x)} \right)_0 , \quad (14.3.19) $$

$$ 0 = i\hbar \partial^a \partial^a \left( \frac{\delta W}{\delta K^p_a(x) \partial J^a_i(y)} \right)_0 - \delta_a \partial^a \left( \frac{\delta W}{\delta J^a_i(x)} \right)_0 , \quad (14.3.20) $$

etc.

We have introduced the notation that $(\cdots)_0$ is evaluated at $J^a_i = K^p_a = 0$. Equation (14.3.18) is derived by differentiating (14.3.16) with respect to $y^0$ and using the relation which is obtained by applying $\partial^a$ to (14.3.17). $(j(x))_0$ implies $(j(x))_0$ in (14.3.15) which is nothing but the continuity equation of the particle number. If we consider the uniform system, Eqs. (14.3.16)~(14.3.20) are expressed in Fourier representation as follows. Define
\[ W_{\kappa\kappa\alpha}^{(2)} = \left( \frac{\delta^2 W}{\delta K_{\alpha} \delta K_{\beta}} \right)_0, \]

then we get

\[ 0 = i\hbar \left( -ik_0 W_{\kappa\kappa\alpha}^{(2)}(k) - ik_1 W_{\kappa\kappa\alpha}^{(2)}(k) \right), \quad (14.3.21) \]

\[ 0 = i\hbar \left( -ik_0 W_{\kappa\kappa\alpha}^{(2)}(k) - ik_1 W_{\kappa\kappa\alpha}^{(2)}(k) \right) - \frac{\hbar}{mi} ik_1 \delta_{\alpha,\beta} (-1)^{\alpha+1} n, \quad (14.3.22) \]

\[ 0 = i\hbar k_0^2 W_{\kappa\kappa\alpha}^{(2)}(k) - i\hbar k_1 k_3 W_{\kappa\kappa\alpha}^{(2)}(k) - \frac{\hbar}{mi} k_1 k_3 \delta_{\alpha,\beta} (-1)^{\alpha+1} n, \quad (14.3.23) \]

\[ 0 = i\hbar \left( -ik_0 W_{\kappa\kappa\alpha}^{(2)}(k) - ik_1 W_{\kappa\kappa\alpha}^{(2)}(k) \right) + \delta_{\alpha,\beta} (-1)^{\alpha+1} \phi^{(0)}, \quad (14.3.24) \]

\[ 0 = i\hbar \left( -ik_0 W_{\kappa\kappa\alpha}^{(2)}(k) - ik_1 W_{\kappa\kappa\alpha}^{(2)}(k) \right) - \delta_{\alpha,\beta} (-1)^{\alpha+1} \phi^{(0)}. \quad (14.3.25) \]

Taking \( \alpha=1 \) and summing up over \( \beta=(1, 2) \), Eqs. (14.3.21) \(~14.3.25\) lead the well-known identities among the retarded Green's functions. Note here that writing only the indices in the \( \alpha \)-space, \( W_1 + W_2 \) is the retarded Green's function.

In the same way, we get the identities involving \( \Gamma \) by differentiating (14.3.14) with respect to \( \phi^{(i)} \), \( K_{\alpha}^{(i)} \) and evaluation at the stationary solution \( \phi^{(0)} \) (corresponding to \( J^{(i)} = 0 \)) and \( K_{\alpha}^{(0)} = 0 \). In doing so we use (14.3.13):

\[ n=0: \quad 0 = \partial_x F(n(x))_0 + \partial_x (n(x))_0, \quad (14.3.26) \]

\[ n=1: \]

\[ 0 = i\hbar \partial_x^2 \left( \frac{\delta^2 \Gamma}{\delta K_{\alpha}^{(i)}(x) \delta \phi(y)} \right)_0 + \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0 - \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0, \quad (14.3.27) \]

\[ 0 = i\hbar \partial_x^2 \left( \frac{\delta^2 \Gamma}{\delta K_{\alpha}^{(i)}(x) \delta \phi(y)} \right)_0 + \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0 - \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0, \quad (14.3.28) \]

\[ 0 = i\hbar \partial_x^2 \left( \frac{\delta^2 \Gamma}{\delta K_{\alpha}^{(i)}(x) \delta \phi(y)} \right)_0 + \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0 - \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0, \quad (14.3.29) \]

\[ 0 = i\hbar \partial_x^2 \left( \frac{\delta^2 \Gamma}{\delta K_{\alpha}^{(i)}(x) \delta \phi(y)} \right)_0 + \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0 - \phi^{(0)}(x) \left( \frac{\delta^2 \Gamma}{\delta \phi \delta \phi^{(i)}(y)} \right)_0, \quad (14.3.30) \]

etc. Actually, Eqs. (14.3.26) \(~14.3.30\) hold for \( K_{\alpha} = 0 \) without inserting the stationary value of \( \phi^{(i)} \) because only the condition \( K_{\alpha} = 0 \) has been used. However, since all the physically observable quantities correspond to the stationary solution, in the following we use the notation \( \cdots \) for the value at \( K_{\alpha}^{(i)} = J^{(i)} = 0 \).

In the uniform system, Fourier representation of (14.3.27) \(~14.3.30\) is given as
\[ 0 = i \hbar \left( -i k \Gamma^{(2)}_{\alpha \beta}(k) - ik \Gamma^{(2)}_{\alpha \beta}(k) \right) + \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k) - \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k), \quad (14.3.31) \]
\[ 0 = i \hbar \left( -i k \Gamma^{(2)}_{\alpha \beta}(k) - ik \Gamma^{(2)}_{\alpha \beta}(k) \right) + \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k) - \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k), \quad (14.3.32) \]
\[ 0 = i \hbar \left( -i k \Gamma^{(2)}_{\alpha \beta}(k) - ik \Gamma^{(2)}_{\alpha \beta}(k) \right) + \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k) - \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k), \quad (14.3.33) \]
\[ 0 = i \hbar \left( -i k \Gamma^{(2)}_{\alpha \beta}(k) - ik \Gamma^{(2)}_{\alpha \beta}(k) \right) + \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k) - \phi^{(0)} \Gamma^{(2)}_{\alpha \beta}(k) \]
\[ -\frac{\hbar}{m \alpha} - ik \delta_{\alpha \beta} (1)^{a+1} n. \quad (14.3.34) \]

Equations (14.3.31) ~ (14.3.34) are the W-T identities in the presence of the condensation. The advantage of making the Legendre transformation and using \( \Gamma \) instead of \( W \) is clear; since we take order parameter \( \phi \) itself as independent variables, separation of its contribution to any equation is automatic in the sense that the Green's functions appearing in the equations are irreducible ones with respect to \( \phi \)-field. This is expressed in the 1PI (one-particle irreducible) property of \( \Gamma \). The usual identities are expressed by the retarded Green's functions. They are obtained, as before, by setting \( \alpha = 1 \) and summing over \( \beta = 1, 2 \). Note that \( \Gamma_{11} + \Gamma_{12} \) is the (minus) inverse of \( W_{11} + W_{12} \). These identities are used to define the super (i.e., condensed) and normal part in the next subsection.

14.3.2. Condensation and correlation functions — definition of \( n_n \) and \( n_s \) —

When the correlation function derived from \( W[J_\alpha^i, K_\beta^a] \) is rewritten using that from \( \Gamma[\phi_\alpha^i, K_\beta^a] \), this function separates automatically into two terms without artificial technique. These terms just correspond to the usually adopted definition of the super part and normal part.

The expectation value of \( \bar{\mathcal{J}}_{\alpha \nu}(x) \) is given by the second expression of (14.3.13). Let us differentiate this equation with respect to \( K_\beta^a(y) \). Then we can obtain the current-current correlation function,

\[ \frac{i}{\hbar} (-1)^{a+s} \langle \bar{\mathcal{J}}_{\alpha \nu}(x) \bar{\mathcal{J}}_{\beta \mu}(y) \rangle_{\text{conn}} = \frac{\delta^2 W[J_\alpha^i, K_\beta^a]}{\delta K_\beta^a(x) \delta K_\beta^a(y)} \cdot \frac{\delta}{\delta \phi_\alpha^i(w)}. \quad (14.3.35) \]

The relation between the derivative by \( K_\beta^a \) with \( J_\alpha^i \) fixed and that with \( \phi_\alpha^i \) fixed is

\[ \left. \frac{\delta}{\delta K_\beta^a(x)} \right|_{\phi = \phi[J_\alpha^i, K_\beta^a]} = \left. \frac{\delta}{\delta K_\beta^a(x)} \right|_{\phi} + \left. \frac{\delta^2 \Gamma}{\delta K_\beta^a(x) \delta \phi_\alpha^i(z)} \right|_{\phi} \cdot \left. \frac{\delta^2 W}{\delta \phi_\alpha^i(w)} \right|_{\phi} \cdot \left. \frac{\delta}{\delta \phi_\alpha^i(w)} \right|_{\phi}. \quad (14.3.36) \]

The second term of (14.3.36) appears as a result of the \( K_\beta^a \)-dependence in \( \phi \), i.e., \( \phi = \phi[J_\alpha^i, K_\beta^a] \). After Eq. (14.3.36) is put into (14.3.35), the correlation function is given as

\[ \frac{i}{\hbar} (-1)^{a+s} \langle \bar{\mathcal{J}}_{\alpha \nu}(x) \bar{\mathcal{J}}_{\beta \mu}(y) \rangle_{\text{conn}} \]
\[ \frac{\delta^2 \Gamma}{\delta K_a'(x) \delta K_b'(y)} - \sum_{\nu} \int d^4 x' d^4 y' \frac{\delta^2 \Gamma}{\delta K_\nu''(x) \delta \phi'(z)} \left( \frac{\delta^2 \Gamma}{\delta \phi' \delta \phi} \right)_{ji}^{(1)B} (z, w) \frac{\delta^2 \Gamma}{\delta \phi'(w) \delta K_\nu''(y)} . \]

(14.3.37)

Here we have used the identity (A.7). Equation (14.3.38) below expresses (14.3.37) in a diagrammatical representation:

\[ \Gamma^{(2)}_{\kappa \kappa'} K_{\kappa} \Phi_{\kappa'} + \Gamma^{(2)}_{\Phi \Phi'} K_{\Phi} . \]

(14.3.38)

The first and second terms are the regular part and singular part respectively.

Let us consider the case \((\mu, \nu) = (i, j) \) \((i, j = 1, 2, 3)\). The retarded Green's function \((i/\hbar) \theta(t_x - t_y) [\bar{f}_\mu(x), \bar{f}_\nu(y)] \equiv W_{\kappa}^{(2)}(x, y)\) is obtained by setting \(a = 1\) and summing up over \(\beta = 1, 2\) in (14.3.37) and then setting \(K_\mu'' = K_\mu'' = K''\), \(j_i' = j_i'' = j_i\). For example, taking \(K'' = j_i' = 0\), Eq. (14.3.38) can be written by the retarded Green's functions as follows. In the equations below the integration is the ordinary one, not the contour integration;

\[ \frac{i}{\hbar} \theta(t_x - t_y) [\bar{f}_\mu(x), \bar{f}_\nu(y)] = \sum_{\nu = 1, 2} W_{\kappa}^{(2)\nu}(x, y) \]

\[ = \Gamma_{\kappa \kappa'}^{(2)\nu}(x, y) + \int d^4 z d^4 w \Gamma_{\kappa \Phi}^{(2)\nu}(x, z) W_{\kappa}^{(2)}(z, w) \Gamma_{\Phi \Phi'}^{(2)\nu}(w, y) \]

(14.3.39)

\[ = \Gamma_{\kappa \kappa'}^{(2)\nu}(x, y) - \int d^4 z d^4 w \Gamma_{\kappa \Phi}^{(2)\nu}(x, z) (\Gamma_{\Phi \Phi'}^{(2)\nu})^{-1}(z, w) \Gamma_{\Phi \Phi'}^{(2)\nu}(w, y) . \]

(14.3.40)

The derivation of (14.3.40) requires some algebra but it is straightforward to see the reason why only the retarded Green's functions appear. As is well known, the regular and singular parts of (14.3.40) correspond respectively to the super part and normal part in the limit \(k \to 0\). Let us discuss this fact in our terminology.

After taking \(k_0 \to 0\), Eq. (14.3.22) becomes in the low-momentum limit

\[ \lim_{k_0 \to 0} W_{\kappa}^{(2)\nu}(k^0 = 0, k) = \frac{n}{m} \frac{\rho}{m} = \frac{\rho}{m^2} , \]

(14.3.41)

where \(\rho\) is the density and the superscript (l) implies the longitudinal part. This is the well-known \(f\)-sum rule. We divide \(W_{\kappa}^{(2)\nu}(k)\) into the regular and singular part in a similar manner as (14.3.40). Here we note that the regular part of \(W_{\kappa}^{(2)\nu}(k)\) does not have singularity; therefore this part is proportional to \(g_{ij} = (\delta_{ij} - k_i k_j/k^2) k_i k_j/k^2\). Accordingly both longitudinal and transverse part are present in the regular part. On the other hand, \(\Gamma_{\kappa \Phi}^{(2)\nu}(k)\) or \(\Gamma_{\kappa \Phi'}^{(2)\nu}(k)\) becomes proportional to \(k_i\) or \(k_j\) coming from the current vertex and \((\Gamma_{\Phi \Phi'}^{(2)\nu})^{-1}(k)\) has the singularity \(1/k^2\). As a result, the singular part has the factor \(k_i k_j/k^2\). In this way the singular part includes only the longitudinal part.

Let us study the regular part of the longitudinal component. Consider the case \(T > T_c\). Then the stationary solution is a trivial one \((\phi_x(x) = 0)\) and in this case, the
singular part vanishes because $\Gamma_{\phi}^{(2)_{K} K'}(k)$ (or $\Gamma_{\phi}^{(2)_{K} \phi_{m_{K}}}(k)$) has the factor $\phi^{(x)(0)}$, which appears due to the differentiation $(\delta/\delta \phi_{x}^{(0)})$. Therefore only the regular part is present for $T > T_c$. Collecting these observations it is natural to conclude: the regular part gives the normal part and the singular part is regarded as the super one. Thus we define

$$\lim_{k \to 0} W_{\phi}^{(2)_{K} K'}(k^{0} = 0, k) = \lim_{k \to 0} \Gamma_{\phi}^{(2)_{K} K'}(k^{0} = 0, k) = \frac{n_{n}}{m} \equiv \frac{\rho_{n}}{m^{2}}$$, \hspace{1cm} (14.3.42)

$$\lim_{k \to 0} W_{\phi}^{(2)_{K} \phi_{m_{K}}}(k^{0} = 0, k)$$

$$= - \lim_{k \to 0} \frac{k_{i} k_{j}}{k^{2}} \Gamma_{\phi}^{(2)_{K} \phi_{m_{K}}}(k^{0} = 0, k) \left( \Gamma_{\phi}^{(2)_{K} \phi}(k^{0} = 0, k) \right)^{-1} \Omega_{\phi_{m_{K}}}(k^{0} = 0, k)$$

$$= \frac{n_{s}}{m} \equiv \frac{\rho_{s}}{m^{2}}$$, \hspace{1cm} (14.3.43)

where the superscript $(r)$ and $(s)$ signify the regular and singular part respectively and $n_{n}(\rho_{n})$ and $n_{s}(\rho_{s})$ are the normal and super number density (super density) respectively. Total number density $n$ has thus been divided into two parts,

$$n = n_{n} + n_{s}$$, \hspace{1cm} (14.3.44)

Furthermore the following relation holds through the above discussions:

$$\lim_{k \to 0} W_{\phi}^{(2)_{K} K'}(k^{0} = 0, k) = \delta_{i,j} \frac{n_{n}}{m} = \delta_{i,j} \frac{\rho_{n}}{m^{2}}$$, \hspace{1cm} (14.3.45)

§ 14.4. Superfluid flow

The superfluid flow can also be discussed as a stationary solution of $\Gamma[\phi_{x}^{(0)}]$. Thus, taking $J_{x} = K_{x} = 0$, we look for the solution $\phi^{(0)}(x)$ of the equation $\delta \Gamma[\phi_{x}^{(0)}]/\delta \phi_{x}^{(0)}(x) = 0$ where $\phi^{(0)}(x)$ has a necessary space-time dependence. The present section is the heart of the microscopic derivation of the superfluidity since the presence of the superfluid solution is the starting point of the whole story. However in the literature this has not been fully discussed.

14.4.1. Existence of solution of superflow

Let us discuss the problem in full order. Explicit calculation based on the one-loop approximation will be given later. The solution we are looking for is the one which corresponds to the homogeneous, i.e., space-time independent, velocity of the superflow. It is proved that the solution does exist which has the form,

$$\phi^{(0)}(x) = e^{-iqx} \bar{\phi}^{(0)} = \phi_{Q}^{(0)}(x), \hspace{0.5cm} \phi^{(t)(0)}(x) = e^{iQx} \bar{\phi}^{(t)(0)} = \phi_{Q}^{(t)(0)}(x)$$, \hspace{1cm} (14.4.1)

where $Qx = Qt - Q \cdot x$ and $\bar{\phi}^{(t)}$ is a constant which may depend on $Q$. As we shall see below this solution is not the Galilean transformation of the constant solution found in § 14.1.
We define the superfluid velocity as

$$v_s = \frac{\hbar Q}{m}. \quad (14.4.2)$$

In order to show that Eq. (14.4.1) is indeed the solution, we rely on the diagrammatic expansion of $\Gamma$. For this purpose it is convenient to introduce a new variable $\phi^*_s(x)$ defined as

$$\phi_s(x) = e^{-i\alpha x} \phi_s(x), \quad \phi^*_s(x) = e^{i\alpha x} \phi^*_s(x). \quad (14.4.3)$$

Looking at the expression (14.9), the inverse of the propagator $I^{(2)}(x,y)$ can be rewritten by using $\phi^*_s(x)$ as

$$I^{(2)}(x,y) \equiv \begin{pmatrix}
-i\hbar \partial_{tx} + \frac{\hbar^2}{2m} V^2_x + \mu - 2 \phi^*(x) \phi(x) U_0 & - \phi^*(x) \phi^*(x) U_0 e^{2i\alpha x} \\
- \phi(x) \phi(x) U_0 e^{-2i\alpha x} & i\hbar \partial_{tx} + \frac{\hbar^2}{2m} V^2_x + \mu - 2 \phi^*(x) \phi(x) U_0
\end{pmatrix} \times \delta^4(x-y)$$

$$= \begin{pmatrix}
-i\hbar \partial_{tx} + \frac{\hbar^2}{2m} V^2_x + \mu & 0 \\
0 & i\hbar \partial_{tx} + \frac{\hbar^2}{2m} V^2_x + \mu
\end{pmatrix} \delta^4(x-y) + V(x,y) \quad (14.4.4)$$

$$= \begin{pmatrix}
e^{i\alpha x} & 0 \\
e^{-i\alpha x} & 0
\end{pmatrix} \begin{pmatrix}
\tilde{I}^{(2)}(x,y) \\
0 & e^{i\alpha y}
\end{pmatrix} \begin{pmatrix}e^{-i\alpha y} & 0 \\
e^{i\alpha y} & 0
\end{pmatrix} \quad (14.4.5)$$

$$\tilde{I}^{(2)}(x,y) \equiv \begin{pmatrix}
-i\hbar \partial_{tx} + \frac{\hbar^2}{2m} V^2_x + \tilde{\mu} + \frac{\hbar Q}{m} \frac{\hbar}{i} \partial_x & 0 \\
0 & i\hbar \partial_{tx} + \frac{\hbar^2}{2m} V^2_x + \frac{\hbar Q}{m} \frac{\hbar}{i} \partial_x
\end{pmatrix} \times \delta^4(x-y) + \tilde{V}(x,y), \quad (14.4.6)$$

where $\tilde{\mu}$ is defined as

$$\tilde{\mu} = \mu + \hbar Q_0 - \epsilon a^0. \quad (14.4.7)$$

In the above expressions, $V(x,y)$ and $\tilde{V}(x,y)$ are given as follows,

$$V(x,y) = \begin{pmatrix}
-2 \phi^*(x) \phi(x) U_0 & - \phi^*(x) \phi^*(x) U_0 e^{2i\alpha x} \\
- \phi(x) \phi(x) U_0 e^{-2i\alpha x} & -2 \phi^*(x) \phi(x) U_0
\end{pmatrix} \delta^4(x-y)$$

$$= \begin{pmatrix}e^{i\alpha x} & 0 \\
e^{-i\alpha x}
\end{pmatrix} \begin{pmatrix}V(x,y) \\
0 & e^{i\alpha y}
\end{pmatrix} \begin{pmatrix}e^{-i\alpha y} & 0 \\
e^{i\alpha y} & 0
\end{pmatrix}, \quad (14.4.8)$$
\[ \tilde{V}(x, y) = \begin{pmatrix} -2 \tilde{\phi}^\dagger(x) \tilde{\phi}(x) U_0 & -\tilde{\phi}^\dagger(x) \tilde{\phi}^\dagger(x) U_0 \\ -\tilde{\phi}(x) \tilde{\phi}(x) U_0 & -2 \tilde{\phi}^\dagger(x) \tilde{\phi}(x) U_0 \end{pmatrix} \delta^4(x-y). \] (14.4.9)

For the fluctuation field which is integrated over in the path integral representation we introduce the new field \( \tilde{\varphi}_a \) similarly as
\[ \tilde{\varphi}_a(x) \equiv e^{i\alpha x} \varphi_a(x), \quad \tilde{\varphi}_a^\dagger(x) \equiv e^{-i\alpha x} \varphi_a^\dagger(x). \] (14.4.10)

In terms of \( \tilde{\varphi}_a(x) \) and \( \tilde{\varphi}_a(x) \), the phase factor \( e^{i\alpha x} \) disappears from all the expressions. Consider (J.1). The second order term of the action \( I[\phi^\dagger + \varphi^\dagger, \phi + \varphi] \) in \( \varphi_a^\dagger \), which is related to the propagator, can be written as
\[ (\varphi_a(x) \varphi_a^\dagger(y)) (I_{\varphi_a}^{(2)}(x, y)) (\varphi_a^\dagger(y) \varphi_a(y)) = (\tilde{\varphi}_a(x) \tilde{\varphi}_a^\dagger(x)) (\tilde{I}_{\varphi_a}^{(2)}(x, y)) (\tilde{\varphi}_a^\dagger(y) \tilde{\varphi}_a(y)), \] (14.4.11)

where \( I_{\varphi_a}^{(2)} = \delta_{a, a} I, \quad \tilde{I}_{\varphi_a}^{(2)} = \delta_{a, a} \tilde{I} \). From the diagrammatic rule of the Legendre transformation, the propagator of \( \tilde{\varphi}_a^\dagger \) field is given by \( \tilde{D}_{\varphi_a}^{(2)} \), which satisfies
\[ (\tilde{I}_{\varphi_a}^{(2)}(x, y)) \tilde{D}(y, z) = \delta_c(t_x - t_z) \delta^3(x - z) 1. \] (14.4.12)

Here \( \tilde{D} = \tilde{I}_{\varphi_a}^{(-1)} \) is written by \( D = I_{\varphi_a}^{(-1)} \) through the inverse relation of (14.4.5),
\[ \tilde{D}(x, y) = \begin{pmatrix} e^{-i\alpha x} & 0 \\ 0 & e^{i\alpha y} \end{pmatrix} \begin{pmatrix} D(x, y) & 0 \\ 0 & e^{-i\omega y} \end{pmatrix}. \] (14.4.13)

For later use we present here the expression of \( \tilde{D} \) in the case of constant \( \tilde{\varphi}_a^\dagger(x) \). We first write (14.4.12) in Fourier representation in this case,
\[ \begin{pmatrix} -i\hbar \partial_t - \epsilon_{0} - \tilde{\mu} - 2 \tilde{\phi}^\dagger \tilde{\phi} + \frac{\hbar Q}{m} \cdot \hbar \mathbf{k} & -U_0 \tilde{\phi}^\dagger \\
-\hbar \partial_t - \epsilon_{0} - \tilde{\mu} - 2 \tilde{\phi}^\dagger \tilde{\phi} - \frac{\hbar Q}{m} \cdot \hbar \mathbf{k} & i\hbar \partial_t - \epsilon_{0} - \tilde{\mu} - 2 \tilde{\phi}^\dagger \tilde{\phi} + \frac{\hbar Q}{m} \cdot \hbar \mathbf{k} \end{pmatrix} \times \begin{pmatrix} \tilde{D}_{11}(t, t', \mathbf{k}) & \tilde{D}_{12}(t, t', \mathbf{k}) \\
\tilde{D}_{21}(t, t', \mathbf{k}) & \tilde{D}_{22}(t, t', \mathbf{k}) \end{pmatrix} = \delta_c(t-t') \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \] (14.4.14)

After solving this differential equation, \( \tilde{D} \) is obtained as follows (see Appendix J and Ref. 28),
\[ \begin{pmatrix} \tilde{D}_{11}(t, t', \mathbf{k}) & \tilde{D}_{12}(t, t', \mathbf{k}) \\
\tilde{D}_{21}(t, t', \mathbf{k}) & \tilde{D}_{22}(t, t', \mathbf{k}) \end{pmatrix} = -\frac{i}{\hbar} \{ \theta_c(t-t') + f_\delta(\tilde{E}_0 + a_\delta) e^{-(i/\hbar)(\tilde{E}_0 + a_\delta)(t-t')} \tilde{R}_1(\mathbf{k}) \\
-\frac{i}{\hbar} \{ \theta_c(t'-t) + f_\delta(\tilde{E}_0 - a_\delta) e^{(i/\hbar)(\tilde{E}_0 - a_\delta)(t-t')} \tilde{R}_2(\mathbf{k}) \}, \] (14.4.15)

where
\[ E_k = \left( \epsilon_k^0 - \tilde \mu + 2 \tilde \phi \cdot U_0 \right)^2 - \left( \tilde \phi \cdot U_0 \right)^2 \right)^{1/2}, \quad \alpha_k = \frac{\hbar Q}{m} \cdot \hbar k, \]

\[ \tilde R_1(k) = \begin{pmatrix} \tilde v_k & \tilde C_k \\ \tilde \tilde C_k & \tilde \tilde u_k \end{pmatrix}, \quad \tilde R_2(k) = \begin{pmatrix} \tilde u_k & \tilde \tilde C_k \\ \tilde \tilde C_k & \tilde \tilde v_k \end{pmatrix}, \quad (14.4.16) \]

and \( \tilde \phi, \tilde \phi \tilde \phi \) and \( \tilde C \tilde C \) are defined by replacing \( E_k \) contained in \( u_k, v_k \) and \( C \) by \( \tilde E_k \), see Appendix J.

Let us come back to the general case where \( \tilde \phi(x) \) is not a constant. The third or higher order terms of \( \phi(x) \) in the expression \( I[F' + \phi', \phi + \phi] \) represent the interaction among the fluctuation field \( \phi(x) \). When the vertices of \( \phi_a \) field and those of \( \phi \) field are compared, we find the cancellation of the phase factor \( e^{i\alpha} \):

\[ O(\phi^3): \quad U_0 \phi^3(x) \phi^3(x) \phi \phi = U_0 \phi^3(x) \phi^3(x) \phi \phi, \quad (14.4.17) \]

\[ O(\phi^4): \quad U_0 \phi^4(x) \phi^4(x) \phi \phi = U_0 \phi^4(x) \phi^4(x) \phi \phi. \quad (14.4.18) \]

From the above discussion, \( \Gamma' = \Gamma[\phi^a] \) is expressed as the function of \( \phi_a \). We write this \( \Gamma' \) as \( \Gamma[\phi_a] \):

\[ \tilde \Gamma[\phi^a] = \Gamma[\phi^a], \quad (14.4.20) \]

where \( \phi_s^a(x) \) and \( \phi^a(x) \) are related by the relation (14.4.3). The tree term of \( \tilde \Gamma \), for example, becomes

\[ \tilde \Gamma_{\text{tree}}[\phi^a] = \int_c dt \int d^3 \phi^a(x) \left( i \hbar \partial_t - \frac{\hbar Q}{m} \cdot \vec \nabla + \frac{\hbar^2}{2m} \partial^2 + \tilde \mu \right) \phi(x) \]

\[ - \frac{1}{2} \int_c dt ds dt_y \int d^3 \phi^a(x) \phi^a(y) U_0(x-y) \phi(y) \phi(x). \quad (14.4.21) \]

The loop terms are given by the loop graphs whose propagator is \( \tilde D \) and interaction vertices are on the right-hand side of (14.4.17)~(14.4.19). The graphical rule is equivalent to that derived from the action

\[ \tilde \Gamma[\phi^a] = \int_c dt \int d^3 \phi^a(x) \left( i \hbar \partial_t + \frac{\hbar Q}{m} \cdot \vec \nabla + \frac{\hbar^2}{2m} \partial^2 + \tilde \mu \right) \phi(x) \]

\[ - \frac{1}{2} \int_c dt ds dt_y \int d^3 \phi^a(x) \phi^a(y) U_0(x-y) \phi(y) \phi(x). \quad (14.4.22) \]

The relation \( \tilde \Gamma[\phi^a] = \Gamma[\phi^a] \) holds of course if we substitute

\[ \phi^a(x) = e^{i\alpha} \phi^a(x), \quad \tilde \phi^a(x) = e^{-i\alpha} \tilde \phi^a(x). \quad (14.4.23) \]

Now we are in a position to prove that Eq. (14.4.1) is the solution. For this purpose let us evaluate the derivative of \( \Gamma' \) with respect to \( \phi^a(x) \) at the solution (14.4.1). For the tree term, we get

\[ \left( \frac{\delta \Gamma_{\text{tree}}}{\delta \phi^a(x)} \right)_{\phi^a(x)} = e^{-i\alpha} \left( \frac{\delta \tilde \Gamma_{\text{tree}}}{\delta \tilde \phi^a(x)} \right)_{\tilde \phi^a(x)}, \quad \left( \frac{\delta \Gamma_{\text{tree}}}{\delta \phi^a(x)} \right)_{\phi^a(x)} = e^{i\alpha} \left( \frac{\delta \tilde \Gamma_{\text{tree}}}{\delta \tilde \phi^a(x)} \right)_{\tilde \phi^a(x)}. \quad (14.4.24) \]
The loop term can be studied by using diagrams. In the diagrams of $\Gamma[\phi^i]$, $\phi^i(x)$ appears in the propagator and the vertices (14.4.17) and (14.4.18). The derivative of the propagator by $\phi^i(x)$ evaluated at $\phi^i(x) = \phi^i(0)(x)$ is (see (14.4.4))

\[
\frac{\delta}{\delta \phi^a(x)} D(y,z)\bigg|_{\phi^0(x)} = -(D(y_1, z_1) \left( \frac{\delta V(y_1, y_2)}{\delta \phi^a(x)} \right) (D(z_1, z))\bigg|_{\phi^0(x)}
\]

\[
= - e^{-iqa} U^{(-q)}(y_1) \left( \tilde{D}(y, y_1) \right) \phi^0(\tilde{D}(z_1, z)) \phi^0(U^{(q)}(z)),
\]

(14.4.25)

\[
\frac{\delta}{\delta \phi^a(x)} D(y,z)\bigg|_{\phi^0(x)} = -(D(y_1, z_1) \left( \frac{\delta V(y_1, y_2)}{\delta \phi^a(x)} \right) (D(z_1, z))\bigg|_{\phi^0(x)}
\]

\[
= - e^{iqa} U^{(-q)}(y_1) \left( \tilde{D}(y, y_1) \right) \phi^0(\tilde{D}(z_1, z)) \phi^0(U^{(q)}(z)),
\]

(14.4.26)

where we have defined $\tilde{V}(y_1, z_1) = [V(y_1, z_1)]_{\phi^0(x) = \phi^0(x)}$ and have used the following relation:

\[
D(x,y) = U^{(-q)}(x)\tilde{D}(x,y) U^{(q)}(y), \quad U_{ab}(x) = \delta_{ab} \begin{pmatrix} e^{-iqa} & 0 \\ 0 & e^{iqa} \end{pmatrix}.
\]

(14.4.27)

The factor $U^{(q)}$ is absorbed when we have changed the field $\phi^a$ into $\tilde{\phi}^a$. The differentiation of the three point vertex leads to the relation,

\[
\frac{\delta}{\delta \phi^a(x)} \left[ U_0 \phi^a(y) \phi^b(y) \phi^c(y) \right]_{\phi^0(x)} = e^{-iqa} \frac{\delta}{\delta \phi^a(x)} \left[ U_0 \tilde{\phi}^b(y) \tilde{\phi}^c(y) \tilde{\phi}^c(y) \right]_{\phi^0},
\]

(14.4.28)

\[
\frac{\delta}{\delta \phi^a(x)} \left[ U_0 \phi^a(y) \phi^b(y) \phi^b(y) \right]_{\phi^0(x)} = e^{iqa} \frac{\delta}{\delta \phi^a(x)} \left[ U_0 \tilde{\phi}^b(y) \tilde{\phi}^c(y) \tilde{\phi}^c(y) \right]_{\phi^0}.
\]

(14.4.29)

From (14.4.25)~(14.4.29), we see that

\[
\left( \frac{\delta \Gamma_{\text{loop}}}{\delta \phi^a(x)} \right)_{\phi^0(x)} = e^{-iqa} \left( \frac{\delta \tilde{\Gamma}_{\text{loop}}}{\delta \phi^a(x)} \right)_{\phi^0}, \quad \left( \frac{\delta \Gamma_{\text{loop}}}{\delta \phi^a(x)} \right)_{\phi^0(x)} = e^{iqa} \left( \frac{\delta \tilde{\Gamma}_{\text{loop}}}{\delta \phi^a(x)} \right)_{\phi^0}.
\]

(14.4.30)
Then we conclude that the solution of the stationary equation \( \phi^{(0)}(x) \) satisfies
\[
\left( \frac{\delta \Gamma}{\delta \tilde{\phi}_1^i(x)} \right)_{\tilde{\phi}_1(x) = \tilde{\phi}_2(x) = \phi^{(0)}(x)} = e^{-i\alpha} \left( \frac{\delta \tilde{\Gamma}}{\delta \tilde{\phi}_1^i(x)} \right)_{\tilde{\phi}_1 = \tilde{\phi}_2 = \tilde{\phi}^{(0)}} = 0, \tag{14.4.31}
\]
\[
\left( \frac{\delta \Gamma}{\delta \tilde{\phi}_1^i(x)} \right)_{\tilde{\phi}_1(x) = \tilde{\phi}_2(x) = \phi^{(0)}(x)} = e^{+i\alpha} \left( \frac{\delta \tilde{\Gamma}}{\delta \tilde{\phi}_2^i(x)} \right)_{\tilde{\phi}_1 = \tilde{\phi}_2 = \tilde{\phi}^{(0)}} = 0. \tag{14.4.32}
\]

This implies that one can get the solution describing the superfluid flow by solving \( \delta \tilde{\Gamma}[\tilde{\phi}^i] \delta \tilde{\phi}_1(x) = 0 \) with \( x \)-independent configurations; \( \tilde{\phi}_1 = \tilde{\phi}_2 = \tilde{\phi}^{(0)} \). It is shown below that the solution \( \tilde{\phi}^{(0)} \) does exist at least in the form of loop expansion and that it depends on \( Q^2 \) for non-zero temperature.

In order to look into these problems, the propagator \( \tilde{D} \) given by (14.4.15) is first Fourier transformed in time variable,
\[
\tilde{D}_{11}(k) = \left( \frac{f_s(\tilde{E}_h + a_h) + 1}{\hbar k_0 - a_h - \tilde{E}_h + i\eta} - \frac{f_s(\tilde{E}_h + a_h)}{\hbar k_0 - a_h - \tilde{E}_h - i\eta} \right) \tilde{R}_1(k)
+ \left( \frac{f_s(\tilde{E}_h - a_h)}{\hbar k_0 - a_h + \tilde{E}_h + i\eta} - \frac{f_s(\tilde{E}_h - a_h) + 1}{\hbar k_0 - a_h + \tilde{E}_h - i\eta} \right) \tilde{R}_2(k), \tag{14.4.33}
\]
\[
\tilde{D}_{22}(k) = \left( \frac{f_s(\tilde{E}_h + a_h)}{\hbar k_0 - a_h - \tilde{E}_h + i\eta} - \frac{f_s(\tilde{E}_h + a_h) + 1}{\hbar k_0 - a_h + \tilde{E}_h - i\eta} \right) \tilde{R}_1(k)
+ \left( \frac{f_s(\tilde{E}_h - a_h) + 1}{\hbar k_0 - a_h + \tilde{E}_h + i\eta} - \frac{f_s(\tilde{E}_h - a_h)}{\hbar k_0 - a_h + \tilde{E}_h - i\eta} \right) \tilde{R}_2(k), \tag{14.4.34}
\]
\[
\tilde{D}_{12}(k) = -\frac{i}{\hbar} (2\pi) \left( f_s(\tilde{E}_h + a_h) \delta \left( k_0 - \frac{a_h}{\hbar} - \frac{\tilde{E}_h}{\hbar} \right) \tilde{R}_1(k) \right.
+ \left. (f_s(\tilde{E}_h - a_h) + 1) \delta \left( k_0 - \frac{a_h}{\hbar} + \frac{\tilde{E}_h}{\hbar} \right) \tilde{R}_3(k) \right), \tag{14.4.35}
\]
\[
\tilde{D}_{21}(k) = -\frac{i}{\hbar} (2\pi) \left( (f_s(\tilde{E}_h + a_h) + 1) \delta \left( k_0 - \frac{a_h}{\hbar} - \frac{\tilde{E}_h}{\hbar} \right) \tilde{R}_1(k) \right.
+ \left. f_s(\tilde{E}_h - a_h) \delta \left( k_0 - \frac{a_h}{\hbar} + \frac{\tilde{E}_h}{\hbar} \right) \tilde{R}_3(k) \right), \tag{14.4.36}
\]
\[
\tilde{D}_{33}(\epsilon_n, \hbar) = \frac{i}{\hbar} \left( \frac{1}{\epsilon_n - a_h \hbar - \tilde{E}_h} \tilde{R}_1(k) - \frac{1}{\epsilon_n - a_h \hbar + \tilde{E}_h} \tilde{R}_2(k) \right). \tag{14.4.37}
\]

Here \( \eta \) is a positive infinitesimal quantity, \( f_s \) is given in (J.17) and the explicit forms of \( \tilde{R}_i(k) \), etc., are shown in (14.4.16). Recall here that we can ignore \( \tilde{D}_{13}, \tilde{D}_{25}, \tilde{D}_{31} \) and \( \tilde{D}_{32} \) because of the assumption \( t_1 \rightarrow -\infty \).

Looking at the action (14.4.22), it is clear that the graphs of \( \delta \tilde{\Gamma}[\tilde{\phi}^i(x)] \delta \tilde{\phi}_1^{(0)} \) are topologically equivalent to those of \( \delta \Gamma[\phi_1(x)] \phi_1^{(0)} \). Here \( \Gamma \) represents the case without superflow. The former is obtained from the latter by replacing the propagator \( D \) and \( \phi_1^i \) (\( \phi_1^i \) appears in the three point vertex of the latter) by \( \tilde{D} \) and \( \tilde{\phi}_1^i \) respectively. The change of integration variable of internal line as \( \hbar k_0 = \hbar k_0 - a_h \) leaves the \( Q \) dependence of \( \tilde{\Gamma}[\tilde{\phi}^i] \) only in \( f_s(\tilde{E}_h \pm a_h) \) and \( \tilde{E}_h \).

At this point we assume that \( Q \) is small and that \( \tilde{\mu} = \mu + \hbar Q \), as defined in
(14.4.7), is of the zero-th order of $Q$. Later these are confirmed by the loop expansion where we will see that $Q_0$ is of the order $Q^2$ and therefore $\bar{\mu} \rightarrow \mu$ as $Q \rightarrow 0$. This $\mu$ has been calculated in (14.1.14) within one-loop approximation.

Now we use the fact that the number (density) is independent of $Q$:

$$\beta \hbar V_n = \frac{\partial \bar{\Gamma}[\phi_a^i, \mu]}{\partial \mu} = \frac{\partial \bar{\Gamma}[\phi_a^i, \bar{\mu}, Q]}{\partial \mu} = \frac{\partial \bar{\Gamma}[\phi_a^i, \bar{\mu}, Q]}{\partial \bar{\mu}}.$$  \hspace{1cm} (14.4.38)

Here we have written explicitly that $\Gamma$ has $\mu$ and $Q$ as its arguments. The $Q$ dependence of $\bar{\Gamma}$, apart from the implicit one through $\bar{\mu}$, comes from $\alpha_0$ of (14.4.16). We have the relation

$$\lim_{Q \rightarrow 0} \bar{\Gamma}[\phi_a^i, \bar{\mu}, Q] = \Gamma[\phi_a^i, \mu].$$ \hspace{1cm} (14.3.39)

Besides (14.4.38), we have the stationary equation by (14.4.31) and (14.4.32),

$$0 = \left( \frac{\delta \bar{\Gamma}[\phi_a^i, \bar{\mu}, Q]}{\delta \phi_a^i(x)} \right)_{\phi_a^i = \phi^{i(0)}}.$$ \hspace{1cm} (14.4.40)

The set of Eqs. (14.4.38) and (14.4.40) determines $\bar{\mu}$ and $\phi^{i(0)}$, both of which depend on $Q^2$ satisfying

$$\lim_{Q \rightarrow 0} \bar{\mu} = \mu, \quad \lim_{Q \rightarrow 0} \phi^{i(0)} = \phi^{i(0)}.$$ \hspace{1cm} (14.4.41)

Here $\phi^{i(0)}$ is nothing but the static solution found in § 14.1. For small $|Q|$, because of the rotational symmetry,

$$\bar{\mu} = \mu + \mathcal{O}(Q^2), \quad \phi^{i(0)} = \phi^{i(0)} + \mathcal{O}(Q^2), \quad \hbar Q_0 = \mathcal{O}(Q^2).$$ \hspace{1cm} (14.4.42)

Indeed we can prove (14.4.42) as follows: because of the rotational symmetry, (14.4.40) takes the form, for small $Q$,

$$0 = \left( \frac{\delta \bar{\Gamma}[\phi_a^i, \bar{\mu}]}{\delta \phi_a^i(x)} \right)_{\phi^{i(0)}} + \mathcal{O}(Q^2).$$ \hspace{1cm} (14.4.43)

Equation (14.4.43) tells us that $\phi^{i(0)}$ is expanded as

$$\phi^{i(0)}(\bar{\mu}, Q) = \phi^{i(0)}(\mu = \bar{\mu}) + \mathcal{O}(Q^2).$$ \hspace{1cm} (14.4.44)

From (14.4.38) the number density is written as

$$n = n(\phi_a^i, \mu) = f(\phi_a^i, \mu)$$ \hspace{1cm} (14.4.45)

$$= n(\phi_a^i, \bar{\mu}, Q) = f(\phi_a^i, \bar{\mu}) + \mathcal{O}(Q^2).$$ \hspace{1cm} (14.4.46)

The rotational symmetry of the system has been used again. We take the inverse relation of (14.4.45) and (14.4.46) at the stationary solution $\phi^{i(0)}$ and $\phi^{i(0)}$ respectively. In this way it is obtained that

$$\mu = f^{-1}(\phi^{i(0)}, n), \quad \bar{\mu} = f^{-1}(\phi^{i(0)}(\mu = \bar{\mu}) + \mathcal{O}(Q^2), n - \mathcal{O}(Q^2)).$$ \hspace{1cm} (14.4.47)

From (14.4.47) we get
\[\hat{h}Q_0 - \varepsilon_\alpha = \mu = \mathcal{O}(Q^2), \quad (14.4.48)\]

\[\tilde{\phi}^{(0)}(\vec{\mu}, Q) = \phi^{(0)}(\mu) + \mathcal{O}(Q^2). \quad (14.4.49)\]

Thus Eq. (14.4.42) has been proved. Now we observe the following facts.

(i) For \(\beta = \infty\), the solution with the constant superfluid flow is simply given, by using the static solution \(\phi_q^{(0)}\) as

\[\phi_q^{(0)}(x) = e^{-i\alpha x}\phi_0^{(0)}, \quad \phi_q^{(0)}(x) = e^{i\alpha x}\phi_0^{(0)}.\]

This is the Galilean transformation of the static solution \(\phi^{(0)}\) but this situation is limited to the zero-temperature case.

(ii) For the case finite temperature, we have checked Eq. (14.4.42) up to one-loop level and found in fact that the condensation \(\bar{n}_0^{(0)}\) depends on \(Q^2\) and, compared with \(n_0^{(0)}\), which is \(\bar{n}_0^{(0)}\) evaluated at \(Q = 0\), is smaller for \(Q^2 \neq 0\).\(^{27}\) This is due to the fact that when the supercurrent flows through the environment which contains at finite temperature the thermally excited excitation modes (phonon modes), the flow is blocked and its magnitude is reduced. When this picture persists for large \(|Q|\), the superflow (i.e., the density of the condensed mode \(\bar{n}_0\)) ceases to exist at some finite value of \(|Q|\). This is another reason, besides the usual one, for the existence of the critical velocity.

144.2. W-T identities in presence of superflow

Let us study how the W-T identities derived in § 14.3.1 are modified in the presence of superflow. This is used in deriving the hydrodynamical equations in the next section. We assume that the background flow is of the form (14.4.1) where \(\tilde{\phi}^{(0)}\) is independent of \(x\).

The theory in the presence of superflow is summarized in the action (14.4.22) in the tilde variables (where the contour integral can be replaced by the integration over \(C_1\) and \(C_2\) if we take \(t_1 = -\infty\)). The phase factor \(e^{\pm i\alpha x}\) has disappeared and the \(Q^2\)-dependence is contained in the bilinear term of \(\tilde{\phi}(x)\). From this action we can construct \(\tilde{I}\) by the standard process; write \(\tilde{\phi}_a^{(1)}(x) = \tilde{\phi}^{(0)} + \tilde{\phi}_a^{(1)}(x)\), and discard from the action \(\tilde{I}\) of (14.4.22) the linear term in \(\tilde{\phi}_a^{(1)}\). Then we perform the integration over the fluctuating field \(\tilde{\phi}_a^{(1)}\) which can be done in the graphical expansion with constraint of 1PI. Apart from the term

\[\tilde{\phi}^{(1)}(x)\left( -\frac{\hbar}{m}\frac{\hbar}{i\nabla} \right)\tilde{\phi}(x), \quad (14.4.50)\]

the action in the presence of superflow is equivalent to the action in the absence of the superflow, i.e., \(Q = 0\), provided that we replace \(\phi_a^{(0)}\) by \(\tilde{\phi}_a^{(0)}\) and \(\mu\) by \(\tilde{\mu}\). Since we are considering constant \(\tilde{\phi}^{(0)}\) the above term does not contribute to the tree term \(\tilde{I}_{\text{tree}}\) and the only change is in the propagator of any loop diagram: \(\tilde{D}\) is replaced by \(\tilde{D}\) which contains, besides \(\tilde{\mu}\) and \(\tilde{\phi}^{(0)}\), the term \(a_k\) of (14.4.16) coming from (14.4.50).

We write the above situation as

\[\tilde{I}[\tilde{\phi}_a^{(1)}, \tilde{\mu}, 0] = \tilde{I}[\tilde{\phi}_a^{(1)}, \tilde{\mu}], \quad (14.4.51)\]

where \(0\) in the last argument of \(\tilde{I}\) implies that we have set \(Q = 0\) or \(a_k = 0\).
Now consider the expectation value of any operator in the background where the superflow is present and make the expansion in powers of $Q^2$ regarding $|Q|$ as a small quantity. In performing such an expansion, we first expand in $a_k$ keeping $\tilde{\mu}$ and $\phi^{(0)}$ fixed. However taking the derivative in terms of $a_k$ and setting $a_k=0$ is equal to the zero-momentum insertion of the current operator $\tilde{J}(x) = (\hbar/2mi) \tilde{\phi}^\dagger(x) \phi(x)$ in the theory $a_k=0$. Therefore the conclusion is that the coefficients in the Tailor expansion in terms of $a_k$ obey the W-T identities in the form (14.3.14) when we replace $\phi^{(0)}$ by $\phi^{(0)}$ and $\mu$ by $\tilde{\mu}$.

Summarizing, we have the following relations. Let us define $\Gamma[\phi_a^i, \mu, K']$ by writing the dependence on $\mu$ and $K'$ explicitly. Here $K'$ is the probe coupled to the zero-momentum part of the current operator $\tilde{J}(x)$, i.e., the term $-K' xd^3 x \tilde{J}(x)$. Then

$$
\Gamma[\phi_a^i, \tilde{\mu}, Q]
= \Gamma[\phi_a^i, \mu]
= \Gamma[\phi_a^i, \tilde{\mu}] + \hbar Q_i \frac{\delta \Gamma[\phi_a^i, \tilde{\mu}, K']}{\delta K^i} \bigg|_{K=0} + \frac{1}{2} \hbar^2 Q_i Q_j \frac{\delta^2 \Gamma[\phi_a^i, \tilde{\mu}, K']}{\delta K^i \delta K^j} \bigg|_{K=0} + \cdots .
$$

(14.4.52)

Each term of these expansion coefficients can be used in the W-T identities which have been derived from (14.3.14) through the differentiation by $K'$ and by setting $K'=0$. As is easily understood, W-T identities of the types (14.3.27)~(14.3.30) hold away from the stationary solution of $\phi$ (they are written at $J'=0$). Therefore,

**W-T identities are valid for the expansion coefficients of (14.4.52) in the form of (14.3.27)~(14.3.30) if we replace**: $\phi_a^{(0)} \rightarrow \phi_a^{(0)}, \mu \rightarrow \tilde{\mu}$.

This statement plays an important role when we derive the hydrodynamic equations. One important observation has to be given here. When we use the physical quantities as $n$, $n_n$ or $n_s$, etc., these have to be evaluated at the solution $\phi^{(0)}$ which satisfies the stationarity of $\Gamma$, otherwise a non-vanishing probe is present, i.e., $J' \neq 0$, and hence we are working with a theory different from the starting one. Therefore, if we use $n$, $n_n$ or $n_s$ in W-T identities for the expansion coefficients appearing in (14.4.52), then there arise the correction terms of the order $\mathcal{O}(Q^2)$ since the difference between $\phi^{(0)}$ and $\phi^{(0)}$ is $\mathcal{O}(Q^2)$, see (14.4.42).

In § 14.5, W-T identities involving energy-momentum tensor are considered and similar arguments as above can also be applied there.

**§ 14.5. Hydrodynamic equation of two fluid model**

In this section, we come to our final aim: the derivation Landau’s hydrodynamic equations from a microscopic point of view. We assume for the moment that the normal flow is absent and it is included in later stage.

It turns out that the basic hydrodynamic equations are obtained by the laws of number, momentum and energy conservation in the presence of the superflow. These relations lead to the W-T type identities in the situation where the background
superflow is described by \( \phi^{(0)}_q(x) \) given in (14.4.1) which is found as a solution of the stationary equation of \( \Gamma \). The number conservation law in such a case has already been discussed in § 14.3.1. In the following we shall first investigate the remaining conservation laws in the operator formalism and then derive the W-T type identities among Green’s functions. The energy-momentum tensor is introduced in this process and then this tensor and the corresponding flow will be evaluated under the existence of the superflow. Expanding in powers of \( Q \) and using the W-T relations, we are able to establish the well-known phenomenological set of equations in the absence of normal flow. Finally we study these results in the presence of normal flow by performing the Galilean transformation.

It is known that the definition and the conservation law of the energy and momentum tensor can be derived by the invariance of the theory under the space-time translation. This is most clearly done in the field theoretical Lagrangian formalism. Let us investigate the problem in the case of \(^4\text{He}\) using our Lagrangian explicitly.

14.5.1. Derivation of energy-momentum tensor through space-time translation invariance

Consider the action \( I \) and define its transformation property under the space-time translation, \( x'' \rightarrow x'' = x'' - \epsilon'' \), where \( \epsilon \) is an infinitesimal constant four vector. The field \( \tilde{\phi}''(x) \) is defined as follows,

\[
\tilde{\phi}''(x) = \tilde{\phi}''(x).
\]

Then the action is invariant in the following sense:

\[
0 = \delta I = \tilde{I} - \tilde{I}
\]

\[
= \int_\Omega d^4x \tilde{\mathcal{L}} \left( \tilde{\phi}''(x'), \partial_\nu \tilde{\phi}''(x'), \partial_\nu \partial_\nu \tilde{\phi}''(x') \right) - \int_\Omega d^4x \tilde{\mathcal{L}} \left( \tilde{\phi}''(x), \partial_\nu \tilde{\phi}''(x), \partial_\nu \partial_\nu \tilde{\phi}''(x) \right),
\]

where \( \tilde{\mathcal{L}} \) is our Lagrangian density

\[
\tilde{\mathcal{L}}(x) = \hat{\phi}^*(x) \left( i\hbar \partial_0 + \frac{\hbar^2}{2m} \nabla^2 + \mu \right) \hat{\phi}(x) - \frac{1}{2} U_0 \hat{\phi}^*(x) \hat{\phi}^*(x) \hat{\phi}(x) \hat{\phi}(x).
\]

The integration region \( \Omega \) of the first term in (14.5.2) is the same as that of the second term. For example, if \( \Omega \) is represented as \( a < x < b \) (in one dimensional case) in the second term, it becomes \( \Omega' \) defined by \( a - \epsilon < x < b - \epsilon \) in the first term. On the other hand, by rewriting the first integral by \( x \), \( \delta \tilde{I} \) is also written as

\[
\delta \tilde{I} = \int_\Omega \left\{ \delta \hat{\phi}^*(x) \frac{\partial \tilde{\mathcal{L}}}{\partial \tilde{\phi}^*(x)} + \frac{\partial \tilde{\mathcal{L}}}{\partial \tilde{\phi}(x)} \delta \hat{\phi}(x) + \frac{\partial \tilde{\mathcal{L}}}{\partial (\partial_0 \hat{\phi}(x))} \delta (\partial_0 \hat{\phi}(x)) \right\} + \sum \frac{\partial \tilde{\mathcal{L}}}{\partial (\partial_0 \partial_i \hat{\phi}(x))} \delta (\partial_0 \partial_i \hat{\phi}(x))
\]

where we have used the relation \( d^4x' = d^4x \) and the symbol \( \delta \) means
\[ \delta \bar{O}(x) \equiv \bar{O}'(x') - \bar{O}(x). \quad (14.5.5) \]

Now we define the local \( \delta L \)-operation as
\[ \delta_L \bar{O}(x) \equiv \bar{O}(x') - \bar{O}(x). \quad (14.5.6) \]

Then we have
\[ \delta \bar{O}(x) = (\bar{O}(x') - \bar{O}(x)) + (\bar{O}(x) - \bar{O}(x)). \quad (14.5.7) \]

The first term on the right-hand side of the above equation can be replaced by \( \bar{O}(x') - \bar{O}(x) \) for an infinitesimal \( \epsilon \). Since \( \delta L \) commutes with \( \partial_\mu, \delta_L \partial_\mu = \partial_\mu \delta_L \), the variation of the field \( \bar{\phi}_i(x) \) is expressed in terms of \( \delta L \) as follows,
\[ \delta \bar{\phi}_i(x) = \delta_L \bar{\phi}_i(x) = \epsilon^\alpha \partial_\alpha \bar{\phi}_i(x), \quad (14.5.8) \]
\[ \delta(\partial_\mu \bar{\phi}_i(x)) = \delta_L(\partial_\mu \bar{\phi}_i(x)) = \epsilon^\alpha \partial_\alpha \partial_\mu \bar{\phi}_i(x), \quad (14.5.9) \]
\[ \delta(\partial_\mu \partial_\nu \bar{\phi}_i(x)) = \delta_L(\partial_\mu \partial_\nu \bar{\phi}_i(x)) = \epsilon^\alpha \partial_\alpha \partial_\mu \partial_\nu \bar{\phi}_i(x). \quad (14.5.10) \]

Using (14.5.8)\textendash(14.5.10), Eq. (14.5.4) can be written as
\[ \delta \bar{I} = \int_B d^4x \left[ \delta L \bar{\phi}_i(x) \frac{\partial \bar{L}}{\partial \bar{\phi}_i(x)} \right. \]
\[ + \left( \frac{\partial \bar{L}}{\partial \bar{\phi}(x)} - \partial_\phi \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))} + \sum_i \partial_\phi \frac{\partial \bar{L}}{\partial (\partial_\mu \bar{\phi}(x))} \right) \partial_L \bar{\phi}(x) + \partial_\phi \left( \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))} \delta_L \bar{\phi}(x) \right) \]
\[ + \sum_i \partial_\phi \left( \frac{\partial \bar{L}}{\partial (\partial_\mu \bar{\phi}(x))} \partial_L \bar{\phi}(x) - \left( \frac{\partial L}{\partial (\partial_\mu \bar{\phi}(x))} \right) \delta_L \bar{\phi}(x) \right) - \epsilon^\alpha \partial_\alpha \bar{L}(x) \left( \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))} \right). \quad (14.5.11) \]

Equation (14.5.2) is valid for any space-time region \( \Omega \) so that we have form (14.5.11)
\[ \delta_L \bar{\phi}_i(x) \frac{\partial \bar{L}}{\partial \bar{\phi}_i(x)} + \left( \frac{\partial \bar{L}}{\partial \bar{\phi}(x)} - \partial_\phi \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))} + \sum_i \partial_\phi \frac{\partial \bar{L}}{\partial (\partial_\mu \bar{\phi}(x))} \right) \partial_L \bar{\phi}(x) \]
\[ + \partial_\phi \left( \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))} \delta_L \bar{\phi}(x) \right) \]
\[ + \sum_i \partial_\phi \left( \frac{\partial \bar{L}}{\partial (\partial_\mu \bar{\phi}(x))} \partial_L \bar{\phi}(x) - \left( \frac{\partial L}{\partial (\partial_\mu \bar{\phi}(x))} \right) \delta_L \bar{\phi}(x) \right) \]
\[ - \epsilon^\alpha \partial_\alpha \bar{L}(x) = 0. \quad (14.5.12) \]

Substituting the Euler-Lagrange equation
\[ 0 = \frac{\delta \bar{I}}{\delta \bar{\phi}_i(x)} = \frac{\partial \bar{L}}{\partial \bar{\phi}_i(x)}, \quad (14.5.13) \]
\[ 0 = \frac{\delta \bar{I}}{\delta \bar{\phi}(x)} = \frac{\partial \bar{L}}{\partial \bar{\phi}(x)} - \partial_\phi \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))} + \sum_i \partial_\phi \frac{\partial \bar{L}}{\partial (\partial_\mu \bar{\phi}(x))} \frac{\partial \bar{L}}{\partial (\partial_\phi \bar{\phi}(x))}, \quad (14.5.14) \]

and the relation
\begin{align}
\delta L \phi^t(x) &= \delta L \phi^t(x) - \phi^t(x) = \hat{\phi}^t(x) + \epsilon \partial_\epsilon \phi^t(x), \\
\delta L \partial_\nu \phi^t(x) &= \epsilon \partial_\nu \phi^t(x), \\
\delta L \partial_\mu \partial_\nu \phi^t(x) &= \epsilon \partial_\mu \partial_\nu \phi^t(x)
\end{align}

into (14.5.12), the latter can be cast into the form

\begin{align}
0 &= \partial_\epsilon \left\{ \frac{\partial L}{\partial \partial_\epsilon \phi} \right\} \\
&\quad + \sum_i \partial_i \left\{ \frac{\partial L}{\partial (\partial_\epsilon \partial_i \phi)} \partial_i (\epsilon \partial_\epsilon \phi) \right\} - \left( \partial_i \frac{\partial L}{\partial (\partial_\epsilon \partial_i \phi)} \right) \epsilon \partial_\epsilon \phi(x) - \epsilon \partial_\epsilon L(x) \\
&= \epsilon \partial_\epsilon T^\epsilon_{\nu}(x). \tag{14.5.18}
\end{align}

Here the energy momentum tensor \( T^\epsilon_{\nu}(x) \) has been introduced. Equation (14.5.18) is valid for arbitrary small \( \epsilon \), so that \( T^\epsilon_{\nu} \) satisfies the conservation law. This tensor is explicitly written as

\begin{align}
T^0_\nu(x) &= \hat{\phi}^t(x) \left( -\frac{\hbar^2}{2m} \nabla^2 - \mu \right) \phi(x) + \frac{1}{2} U_\nu \hat{\phi}^t(x) \hat{\phi}^t(x) \phi(x) \phi(x) = \mathcal{H}(x), \\
T^i_\nu(x) &= \left( \partial^i \hat{\phi}^t(x) \right) \frac{\hbar^2}{2m} \partial_\nu \hat{\phi}(x), \\
\hat{T}_\nu(x) &= i \hbar \hat{\phi}^t(x) \partial_\nu \phi(x), \\
\hat{L}_\nu(x) &= \left( \partial^i \hat{\phi}^t(x) \right) \frac{\hbar^2}{2m} \partial_\nu \phi(x) - \delta^i \nabla \phi(x). \tag{14.5.22}
\end{align}

Here \( \mathcal{H}(x) \) is the Hamiltonian density.

One comment is in order here. The expressions (14.5.19)~(14.5.22) are not Hermitian since we started from the non-Hermitian Lagrangian (14.5.3). It is known, however, that (14.5.3) can be made Hermitian by adding the term which is written as a total derivative of something. But it is also known that the addition of the total derivative term does not affect the physical content of the whole theory. Therefore we can use the above non-Hermitian form without any trouble so we work with the above expressions since the calculation is easier than the Hermitian form. See Ref. 27 for details.

### 14.5.2 W-T identities involving energy-momentum tensor

The problem of deriving the W-T identities involving energy-momentum tensor operator is now discussed. In this subsection W-T identities in the absence of superflow are derived and the superflow will be included later in § 14.5.4.

In the operator action \( \hat{I}_{\mu,\nu} \) of (14.3.4), let us introduce the source term for the energy-momentum tensor \( \hat{T}_\mu^\nu \),

\begin{align}
\int d^4 x \ \eta_\mu^\nu(x) \hat{T}_\mu^\nu(x) + \int d^4 x \ \eta_\nu(x) \hat{\eta}(x). \tag{14.5.23}
\end{align}
Here the second term is added for convenience of the later discussions where we encounter the operator $\tilde{h}(x)$ defined as

$$\tilde{h}(x) = \frac{i\hbar}{2} \tilde{\phi}^*(x) \tilde{\phi}'(x). \quad (14\cdot5\cdot24)$$

Thus we start with the action,

$$\tilde{I}_{\mu\nu}(x) = \tilde{I}_{\mu\nu} + \int d^4x \, \eta_{\mu\nu}(x) \tilde{T}_{\mu\nu}(x) + \int d^4x \, \eta_\h(x) \tilde{h}(x). \quad (14\cdot5\cdot25)$$

The Euler-Lagrange equation of motion in this case is obtained in a similar way as in §14.3.1,

$$0 = -\frac{\delta \tilde{I}_{\mu\nu}(x)}{\delta \tilde{\phi}^*(x)}$$

$$= \left( i\hbar \frac{\partial}{\partial x} + \frac{\hbar^2}{2m} \vec{p}^2 + \mu \right) \tilde{\phi}(x) - U_0 \tilde{\phi}^*(x) \tilde{\phi}(x) + J(x) + K(x) \tilde{\phi}(x)$$

$$+ \frac{\hbar}{2m} \left[ 2K'(x)(\partial_i \tilde{\phi}(x)) + (\partial_i K'(x)) \tilde{\phi}(x) \right]$$

$$+ \eta_\h(x) \left( \left( i\hbar \frac{\partial}{\partial x} + \frac{\hbar^2}{2m} \vec{p}^2 + \mu \right) \tilde{\phi}(x) - U_0 \tilde{\phi}^*(x) \tilde{\phi}(x) \right) - \left( \partial_i \tilde{\eta}_\h(x) \right) \frac{\hbar^2}{2m} \left( \partial_i \tilde{\phi}(x) \right)$$

$$+ \eta_i(x) \left( \frac{\hbar^2}{m} \partial_i \tilde{\phi}(x) \right) + \eta_i(x) i\hbar \frac{\partial}{\partial x} \tilde{\phi}(x) - \left( \partial_i \eta_\nu(x) \right) \frac{\hbar^2}{2m} \partial_i \tilde{\phi}(x)$$

$$+ \eta_i(x) \left[ - \frac{\hbar^2}{m} \partial_i \tilde{\phi}(x) - \delta_i \left( \left( i\hbar \frac{\partial}{\partial x} + \frac{\hbar^2}{2m} \vec{p}^2 + \mu \right) \tilde{\phi}(x) - U_0 \tilde{\phi}^*(x) \tilde{\phi}(x) \right) \right]$$

$$+ \frac{i\hbar}{2} \left( \eta_\h(x) \partial_0 \tilde{\phi}(x) + (\partial_0 \eta_\h(x)) \tilde{\phi}(x) \right). \quad (14\cdot5\cdot26)$$

We deduce the following relation by using (14\cdot5\cdot26) (and its Hermite conjugate) and by looking at the expression of $\tilde{T}_{\mu\nu}$ given in (14\cdot5\cdot19)\sim(14\cdot5\cdot22),

$$0 = \left( \partial_0 \tilde{\phi}^*(x) \right) \frac{\delta \tilde{I}_{\mu\nu}(x)}{\delta \tilde{\phi}^*(x)} + \frac{\delta \tilde{I}_{\mu\nu}(x)}{\delta \tilde{\phi}^*(x)} \left( \partial_0 \tilde{\phi}(x) \right)$$

$$= - \partial_0 \tilde{T}_0(x) + \left( \partial_0 \tilde{\phi}^*(x) \right) J(x) + \tilde{J}(x) \partial_0 \tilde{\phi}(x) + K_0(x) \partial_0 \tilde{\phi}(x) + K_0(x) \partial_0 \tilde{\phi}(x)$$

$$+ K'(x) \partial_0 \tilde{J}_i(x) - \partial_i \tilde{K}(x) \left( \frac{\hbar}{2m} \tilde{\phi}^*(x) \tilde{\phi}(x) \right) \tilde{\phi}(x) \right) + \partial_i \tilde{\phi}(x), \quad (14\cdot5\cdot27)$$

$$0 = \left( \partial_i \tilde{\phi}^*(x) \right) \frac{\delta \tilde{I}_{\mu\nu}(x)}{\delta \tilde{\phi}^*(x)} + \frac{\delta \tilde{I}_{\mu\nu}(x)}{\delta \tilde{\phi}^*(x)} \left( \partial_i \tilde{\phi}(x) \right)$$

$$= - \partial_i \tilde{T}_i(x) + \left( \partial_i \tilde{\phi}^*(x) \right) J(x) + \tilde{J}(x) \partial_i \tilde{\phi}(x) + K_0(x) \partial_i \tilde{\phi}(x)$$

$$+ K'(x) \partial_i \tilde{J}_i(x) - \partial_i \tilde{K}(x) \left( \frac{\hbar}{2m} \tilde{\phi}^*(x) \tilde{\phi}(x) \right) \tilde{\phi}(x) \right) + \partial_i \tilde{\phi}(x), \quad (14\cdot5\cdot28)$$

where $\partial_0$ and $\partial_i$ are the linear terms of $\eta_\nu$, $\partial \eta_\nu$, $\partial \eta_\mu$, $\eta_\nu$, $\partial \eta_\nu$. The expectation
values of \(14\cdot5\cdot27\) and \(14\cdot5\cdot28\) are written by introducing the contour generating functional \(W=W[J_\alpha', K_\alpha'', \eta_{\alpha}(a), \eta_{h}(a)]\), as defined in \(14\cdot3\cdot10\). The suffix \(\alpha\) \((\alpha=1, 2, 3)\) discriminates the three paths on the contour \(C_\alpha\). Just like \(14\cdot3\cdot12\), the following identities are easily derived

\[
0 = -\partial_\alpha \frac{\delta W}{\delta \eta_{\alpha}(a)}(x) + J_\alpha(x) \partial_\alpha \frac{\delta W}{\delta J_\alpha(x)} + \bar{J}_\alpha(x) \partial_\alpha \frac{\delta W}{\delta \bar{J}_\alpha(x)} + K_\alpha''(x) \partial_\alpha \frac{\delta W}{\delta K_\alpha''(x)} \\
+ \frac{1}{m} \partial_\alpha \left( K_\alpha'(x) \frac{\delta W}{\delta \eta_{h}(a)}(x) \right) + \langle \tilde{O}_{\alpha}(x) \rangle, \tag{14\cdot5\cdot29}
\]

\[
0 = -\partial_\alpha \frac{\delta W}{\delta \eta_{\alpha}(a)}(x) + J_\alpha(x) \partial_\alpha \frac{\delta W}{\delta J_\alpha(x)} + \bar{J}_\alpha(x) \partial_\alpha \frac{\delta W}{\delta \bar{J}_\alpha(x)} + K_\alpha''(x) \partial_\alpha \frac{\delta W}{\delta K_\alpha''(x)} \\
- \partial_\alpha \left( K_\alpha'(x) \frac{\delta W}{\delta K_\alpha'(x)} \right) + \langle \tilde{O}_{h}(x) \rangle. \tag{14\cdot5\cdot30}
\]

When one makes the Legendre transformation from \(W[J_\alpha', K_\alpha'', \eta_{\alpha}(a), \eta_{h}(a)]\) to \(I[\phi_{\alpha}', K_\alpha'', \eta_{\alpha}(a), \eta_{h}(a)]\), the parameters \(K_\alpha'', \eta_{\alpha}(a), \eta_{h}(a)\) are regarded as spectators. In terms of \(I\), \(14\cdot5\cdot29\) and \(14\cdot5\cdot30\) are written as

\[
0 = -\partial_\alpha \frac{\partial I}{\partial \eta_{\alpha}(a)} - (\partial_\alpha \phi_\alpha')(x) \frac{\partial I}{\partial \phi_\alpha'}(x) - \frac{\delta I}{\delta \phi_\alpha''}(x) \partial_\alpha \frac{\delta I}{\delta K_\alpha''(x)} \\
+ \frac{1}{m} \partial_\alpha \left( K_\alpha'(x) \frac{\delta I}{\delta \eta_{h}(a)}(x) \right) + \langle \tilde{O}_{\alpha}(x) \rangle, \tag{14\cdot5\cdot31}
\]

\[
0 = -\partial_\alpha \frac{\partial I}{\partial \eta_{\alpha}(a)} - (\partial_\alpha \phi_\alpha')(x) \frac{\partial I}{\partial \phi_\alpha'}(x) - \frac{\delta I}{\delta \phi_\alpha''}(x) \partial_\alpha \frac{\delta I}{\delta K_\alpha''(x)} \\
- \partial_\alpha \left( K_\alpha'(x) \frac{\delta I}{\delta K_\alpha'(x)} \right) + \langle \tilde{O}_{h}(x) \rangle. \tag{14\cdot5\cdot32}
\]

Here we have made use of the identities of the Legendre transformation \(14\cdot3\cdot13\) and

\[
\frac{\delta I}{\delta \eta_{\alpha}(a)(x)} = \frac{\delta W}{\delta \eta_{\alpha}(a)(x)} = (-1)^{\alpha+1} \langle \tilde{T}_{\alpha}(x) \rangle. \tag{14\cdot5\cdot33}
\]

Now we take the \(n\)-derivative \((n=0, 1, 2, \ldots)\) of \(14\cdot5\cdot29\sim14\cdot5\cdot32\) by \(J_\alpha'\) (or \(\phi_\alpha'\) in the case of \(14\cdot5\cdot31\), \(14\cdot5\cdot32\)), \(K_\alpha''\), \(\eta_{\alpha}(a)\) or \(\eta_{h}(a)\) and evaluate them at \(J_\alpha''=K_\alpha''=\eta_{\alpha}(a)=\eta_{h}(a)=0\) (or at \(\phi^{(0)}\) satisfying \(\delta I/\delta \phi^{(0)}(x)=0\) in the case of \(14\cdot5\cdot31\), \(14\cdot5\cdot32\)). In this way we are led to various kinds of W-T identities involving \(T_{\alpha''}\). Below several examples of these identities are shown which are written in terms of \(I\) and obtained through the differentiation by \(K_\alpha''\). Some of them will be used later.

\[
n=0: \quad 0 = \partial_\alpha \langle \tilde{T}_{\alpha''}(x) \rangle_0. \tag{14\cdot5\cdot34}
\]

This is just the laws of momentum \((\mu=i)\) and energy \((\mu=0)\) conservation.

\[
n=1: \quad 0 = -\partial_\alpha \left( \frac{\delta^2 I}{\delta \eta_{\alpha}(a)(x) \delta K_\alpha''(y)} \right)_0 - (\partial_\alpha \phi^{(0)}_\alpha(x)) \left( \frac{\delta^2 I}{\delta \phi^{(0)}_\alpha(x) \delta K_\alpha''(y)} \right)_0
\]
\[-\left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a'(y)}\right)_0 \left(\phi_b^{(0)}(x)\right) + \delta_{a, e} \delta^2(x - y) \partial_y^2 \left(\frac{\delta \Gamma}{\delta K_a'(x)}\right)_0 \]
\[+ \frac{1}{m} \partial^2 \left\{ \delta_{a, e} \delta^2(x - y) \left(\frac{\delta \Gamma}{\delta \eta_{h(a)}(x)}\right)_0 \right\}, \quad (14.5.35)\]

\[0 = -\partial^2 \left(\frac{\delta^2 \Gamma}{\delta \eta_{h(a)}(x) \delta K_a'(y)}\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a'(y)}\right)_0 \]
\[+ \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a'(y)}\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) + \delta_{a, e} \delta^2(x - y) \partial_y^2 \left(\frac{\delta^2 \Gamma}{\delta K_a^m(x) \delta K_a'(y)}\right)_0 \]
\[-\partial^2 \left\{ \delta_{a, e} \delta^2(x - y) \left(\frac{\delta \Gamma}{\delta \eta_{h(a)}(x) \delta K_a'(y)}\right)_0 \right\}, \quad (14.5.36)\]

\(n = 2:\)

\[0 = -\partial^2 \left(\frac{\delta^2 \Gamma}{\delta \eta_{h(a)}(x) \delta K_a^m(z)}\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a^m(z)}\right)_0 \]
\[+ \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a^m(z)}\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) + \delta_{a, e} \delta^2(x - z) \partial_y^2 \left(\frac{\delta^2 \Gamma}{\delta K_a^m(x) \delta K_a'(y)}\right)_0 \]
\[+ \frac{1}{m} \partial^2 \left\{ \delta_{a, e} \delta^2(x - y) \left(\frac{\delta \Gamma}{\delta \eta_{h(a)}(x) \delta K_a'(y)}\right)_0 \right\}, \quad (14.5.37)\]

\[0 = -\partial^2 \left(\frac{\delta^2 \Gamma}{\delta \eta_{h(a)}(x) \delta K_a^m(z)}\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a^m(z)}\right)_0 \]
\[+ \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a^m(z)}\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) + \delta_{a, e} \delta^2(x - z) \partial_y^2 \left(\frac{\delta^2 \Gamma}{\delta K_a^m(x) \delta K_a'(y)}\right)_0 \]
\[+ \delta_{a, e} \delta^2(x - y) \partial_y^2 \left(\frac{\delta^2 \Gamma}{\delta K_a^m(x) \delta K_a'(z)}\right)_0 \]
\[-\partial^2 \left\{ \delta_{a, e} \delta^2(x - y) \left(\frac{\delta \Gamma}{\delta \eta_{h(a)}(x) \delta K_a'(z)}\right)_0 \right\}, \quad (14.5.38)\]

\(n = 3:\)

\[0 = -\partial^2 \left(\frac{\delta^2 \Gamma}{\delta \eta_{h(a)}(x) \delta K_a^m(z)} \delta K_a^m(w)\right)_0 \]
\[+ \left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a^m(z)} \delta K_a^m(w)\right)_0 \]
\[-\left(\frac{\delta^2 \Gamma}{\delta \phi_a(x) \delta K_a^m(z)} \delta K_a^m(w)\right)_0 \left(\partial_y \phi_a^{(0)}(x)\right) \]
\[+ \delta_{a, e} \delta^2(x - w) \partial_y^2 \left(\frac{\delta^2 \Gamma}{\delta K_a^m(x) \delta K_a^m(z)} \delta K_a^m(w)\right)_0 \]
\[+ \delta_{a, e} \delta^2(x - z) \partial_y^2 \left(\frac{\delta^2 \Gamma}{\delta K_a^m(x) \delta K_a^m(z)} \delta K_a^m(w)\right)_0 \]
\[
+ \delta_{a,b} \delta^4(x-y) \partial_x^2 \left( \frac{\partial^3 \Gamma}{\partial K_\alpha(x) \partial K_\beta(y) \partial K_\gamma(w)} \right)_0 \\
+ \frac{1}{m} \partial_x \left( \delta_{a,b} \delta^4(x-w) \left( \frac{\partial^3 \Gamma}{\partial \eta_{h(a)}(x) \partial K_\beta(y) \partial K_\gamma(w)} \right)_0 \right) \\
+ \frac{1}{m} \partial_y \left( \delta_{a,b} \delta^4(x-z) \left( \frac{\partial^3 \Gamma}{\partial \eta_{h(a)}(x) \partial K_\beta(y) \partial K_\gamma(w)} \right)_0 \right) \\
+ \frac{1}{m} \partial_z \left( \delta_{a,b} \delta^4(x-w) \left( \frac{\partial^3 \Gamma}{\partial \eta_{h(a)}(x) \partial K_\beta(y) \partial K_\gamma(w)} \right)_0 \right),
\] (14.5.39)

e tc.

In the absence of superflow, where \( \phi^{(0)}(x) \) is independent of \( x \), one finds Eqs. (14.5.35) \sim (14.5.39) to be expressed in Fourier representation as follows,

\[
0 = ik_0 \Gamma_{\delta h(a),K_\alpha,K_\beta}(k) + ik_1 \Gamma_{\delta h(a),K_\alpha,K_\beta}(k) + \delta_{a,b} \frac{1}{m} (-ik_1)(k)_0,
\] (14.5.40)

\[
0 = ik_0 \Gamma_{\delta h(a),K_\alpha,K_\beta}(k) + ik_1 \Gamma_{\delta h(a),K_\alpha,K_\beta}(k) + \delta_{a,b} i k_1(n)_0,
\] (14.5.41)

\[
0 = i(p_0 + q_0) \Gamma_{\delta h(a),K_\alpha,K_\beta}(p,q) + i(p_1 + q_1) \Gamma_{\delta h(a),K_\alpha,K_\beta}(p,q) - \delta_{a,b} i p_0 \Gamma_{\delta h(a),K_\alpha,K_\beta}(p)
\]

\[
- \delta_{a,b} i q_0 \Gamma_{\delta h(a),K_\alpha,K_\beta}(q) + \frac{1}{m} (-i p_m - i q_m) \delta_{a,b} \Gamma_{\delta h(a),K_\alpha,K_\beta}(p)
\]

\[
+ \frac{1}{m} (-i p_1 + i q_1) \delta_{a,b} \Gamma_{\delta h(a),K_\alpha,K_\beta}(q),
\] (14.5.42)

\[
0 = i(p_0 + q_0) \Gamma_{\delta h(a),K_\alpha,K_\beta}(p,q) + i(p_1 + q_1) \Gamma_{\delta h(a),K_\alpha,K_\beta}(p,q) - \delta_{a,b} i p_1 \Gamma_{\delta h(a),K_\alpha,K_\beta}(p)
\]

\[
- \delta_{a,b} i q_1 \Gamma_{\delta h(a),K_\alpha,K_\beta}(q) + (i p_m + i q_m) \delta_{a,b} \Gamma_{\delta h(a),K_\alpha,K_\beta}(p) + (i p_1 + i q_1) \delta_{a,b} \Gamma_{\delta h(a),K_\alpha,K_\beta}(q),
\] (14.5.43)

\[
0 = i(k_{20} + k_{30} + k_{40}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_2, k_3, k_4) + i(k_{21} + k_{31} + k_{41}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_2, k_3, k_4)
\]

\[
- \delta_{a,e} i(k_{20} + k_{30}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_2, k_3) - \delta_{a,e} i(k_{20} + k_{40}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_2, k_4)
\]

\[
- \delta_{a,e} i(k_{30} + k_{40}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_3, k_4) - \frac{1}{m} \delta_{a,e} i(k_{2n} + k_{3n} + k_{4n}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_2, k_3)
\]

\[
- \frac{1}{m} \delta_{a,e} i(k_{2m} + k_{3m} + k_{4m}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_2, k_4)
\]

\[
- \frac{1}{m} \delta_{a,e} i(k_{21} + k_{31} + k_{41}) \Gamma_{\delta h(a),K_\alpha,K_\beta,K_\gamma}(k_3, k_4).
\] (14.5.44)

In these equations the superscript 0 in \( \Gamma^{(0)} \) for example and suffix 0 in \((\cdots)_0\) imply that they are evaluated at the constant solution \( \phi^{(0)} \). We have used the notations,

\[h = \langle \hat{h}(x) \rangle,
\]

\[
\Gamma_{\delta h(x),y}^{(20)}(x,y) \xrightarrow{F.T.} \Gamma_{\delta h}(x,-q) = \Gamma_{\delta h}^{(20)}(k) \delta^4(k-q),
\]

\[
\begin{array}{c}
\text{Diagram} \\
\end{array}
\]

\[
\begin{array}{c}
\xrightarrow{\Gamma_{\delta h(x),y}^{(20)}(x,y)} \\
\end{array}
\]
The graphical representations for $\Gamma^{(3)}$, $\Gamma^{(4)}$ and $\Gamma^{(4)}$ have also been given at the right end. Now we list some of the identities derived from (14.5.40)~(14.5.44). They are obtained by taking the limit of zero energy and zero momentum and will be used in the discussion of next subsection. The essential point in deriving these identities is, as stated repeatedly, the fact that $\Gamma$ is regular in the limit $k \to 0$. They are given in the form of the multiple retarded Green's functions by setting $\alpha=1$ and summing over 1 and 2 over $\beta$, $\gamma$ and $\epsilon$,

$$\lim_{k \to 0} \sum_{\beta, \gamma, \epsilon} \Gamma^{(3)}_{\beta \gamma \epsilon}(k^0=0, \mathbf{p}, \mathbf{q}) = \frac{n}{m} \left( \delta^{\beta \gamma} \delta_{\beta \gamma} - \delta_{\beta \gamma} \delta^{\beta \gamma} - \delta_{\beta \gamma} \delta_{\beta \gamma} \right), \quad (14.5.45)$$

$$\lim_{k \to 0} \sum_{\beta, \gamma, \epsilon} \Gamma^{(4)}_{\beta \gamma \epsilon K_{\beta \gamma \epsilon}}(k^0=0, \mathbf{h}) = \frac{1}{m} \delta_{\beta \gamma}'(h)_0, \quad (14.5.46)$$

$$\lim_{k \to 0} \sum_{\beta, \gamma, \epsilon} \Gamma^{(4)}_{\beta \gamma \epsilon K_{\beta \gamma \epsilon}}(k^0=0, \mathbf{h}) = \frac{1}{m} \delta_{\beta \gamma}'(h)_0, \quad (14.5.47)$$

$$\lim_{k \to 0} \Gamma^{(4)}_{\beta \gamma \epsilon K_{\beta \gamma \epsilon}}(k^0=0, \mathbf{h}) = 0, \quad (14.5.48)$$

etc.

Indeed the identities (14.5.45) and (14.5.47) can be derived from (14.5.43) and (14.5.44) respectively. The essential point in this process is that $\Gamma$ is regular when any of its arguments go to zero if we assume the "fictitious gap" (to regularize the logarithmic divergences) of Ref. 1) as explained in the beginning of this chapter. As has been stated repeatedly, this is due to the property of $\Gamma$, which is 1PI because it is the Legendre transformed function. In the following we use the word "regular" or
"not singular" in the above sense.
First we consider (14.5.45). Setting \( \rho^0 = q^0 = 0 \) in (14.5.43),
\[
0 = i(p_i + q_i) \Gamma^{(3)0}_{\eta_{il},K_{\alpha}K_{\beta}K_{\rho}}(\rho^0 = q^0 = 0; \ p, q)
- \delta_{\alpha,\gamma}ip_\gamma \Gamma^{(2)0}_{K_{\alpha}'K_{\beta}K_{\rho}}(\rho^0 = 0, p) - \delta_{\alpha,\eta}iq_\eta \Gamma^{(2)0}_{K_{\alpha}'K_{\beta}K_{\rho}}(q^0 = 0, q)
+ i/(p_m + q_m) \delta_{\alpha,\gamma}p_\gamma \Gamma^{(2)0}_{K_{\alpha}'K_{\beta}K_{\rho}}(\rho^0 = 0, p) + i/(p_i + q_i) \delta_{\alpha,\eta}q_\eta \Gamma^{(2)0}_{K_{\alpha}'K_{\beta}K_{\rho}}(q^0 = 0, q). \tag{14.5.49}
\]
After setting \( a = 1 \) and summing up over \( \beta, \gamma = 1, 2 \), we differentiate (14.5.49) by \( p^\prime \) and then set \( p = q = 0 \). In the resulting expression, Eq. (14.3.42) is used which leads to (14.5.45).

Equation (14.5.47) is derived as follows. Setting \( k_2^0 = k_3^0 = k_4^0 = 0 \) in (14.5.44), we get
\[
0 = i(k_{2i} + k_{3i} + k_{4i}) \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_2^0 = k_3^0 = k_4^0 = 0; \ k_2, k_3, k_4)
+ \frac{1}{m} \delta_{\alpha,e}(-i)(k_{2m} + k_{3n} + k_{4n}) \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_2^0 = k_3^0 = 0; \ k_3, k_2)
+ \frac{1}{m} \delta_{\alpha,f}(-i)(k_{2m} + k_{3m} + k_{4m}) \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_2^0 = k_4^0 = 0; \ k_2, k_4)
+ \frac{i}{m} \delta_{\alpha,\rho}(-i)(k_{2i} + k_{3i} + k_{4i}) \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_3^0 = k_4^0 = 0; \ k_3, k_4)
= i(k_{2i} + k_{3i} + k_{4i}) \left[ \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_2^0 = k_3^0 = k_4^0 = 0; \ k_2, k_3, k_4)
- \frac{1}{m} \delta_{\alpha,e} \delta_{\rho} \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_2^0 = k_3^0 = 0; \ k_2, k_3)
- \frac{1}{m} \delta_{\alpha,f} \delta_m \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_2^0 = k_4^0 = 0; \ k_2, k_4)
- \frac{1}{m} \delta_{\alpha,\rho} \delta_m \Gamma^{(3)0}_{\eta_{il},K_{\alpha}'K_{\beta}K_{\rho}}(k_3^0 = k_4^0 = 0; \ k_3, k_4) \right]. \tag{14.5.50}
\]
Differentiate (14.5.50) by \( k_{\alpha}' \) and take the limit \( k_2, k_3, k_4 \to 0 \). Then after summing up over \( \beta, \gamma, e = 1, 2 \), we arrive at the identity (14.5.47).

By using the above derived W-T identities, we shall evaluate the expectation value of the current density in the presence of the superfluid flow. The well-known basic phenomenological equation of the two fluid model is thus derived. It is the exact equation obtained by starting from the microscopic Hamiltonian. (Lowest order derivation by the Bogoliubov transformation has been done in Ref. 6.)

For this purpose it is crucial to use \( \Gamma \). We first introduce the \( c \)-number probe \( J'(x) \) which is coupled to \( \hat{O}_I \) in the form \( -i \int d^3 x J'(x) \hat{O}_I(x) \). Then the expectation value \( \langle \hat{O}_I \rangle \) with the background superflow is given by
\[
O_I(x; \nu_\alpha) = \langle \hat{O}_I \rangle \nu_\alpha = \langle \hat{O}_I \rangle \phi_{0\omega}(x) = \left( \frac{\delta \Gamma}{\delta \hat{J}_I'(x)} \right)_{\phi_0^{\omega}(x)}. \tag{14.5.51}
\]
The notation \( (\cdots)_{\phi_0^{\omega}(x)} \) implies that the order parameter \( \phi_0'(x) \) is replaced by the
solution $\phi^{(0)}(x)$ which has been obtained in § 14.4, therefore the artificially introduced probe $J_{\alpha}^{\prime}(x)$ is made to vanish.

14.5.3. Mass flux

The current density is obtained from (14·5·51),

$$j_{\alpha}(x, v_{s}) = (\frac{\partial \Gamma}{\partial K_{1}(x)})_{\phi^{(0)}(x)} = \left(\frac{\delta I}{\delta K_{1}(x)}\right)_{\phi^{(0)}(x)}.$$  \hspace{1cm} (14·5·52)

Assuming $v_{s}$ is small, we expand the current in powers of $v_{s}$ and use the W·T identities. There are two ways, (a) and (b), to accomplish the purpose and we present both of them below.

(a) Let us expand $j_{\alpha}(x, v_{s})$ around $v_{s} = 0$:

$$j_{\alpha}(x, v_{s}) = \left(\frac{\delta I}{\delta K_{1}(x)}\right)_{\phi^{(0)}(x)}$$

$$= \left(\frac{\delta I}{\delta K_{1}(x)}\right)_{\phi^{(0)}} + v_{s}^{2} \left\{ \frac{\partial}{\partial v_{s}} \left(\frac{\delta I}{\delta K_{1}(x)}\right)_{\phi^{(0)}} \right\}_{q=0} + O\left(v_{s}^{2}\right)$$

$$= v_{s}^{2} \sum_{a} d^{4}y \left\{ -i \frac{m}{\hbar} \gamma_{a} \left[ \phi^{(0)} \left(\frac{\delta^{2} I}{\delta \phi_{a}^{(0)}(y) \delta K_{1}(x)}\right)_{0} - \phi^{(0)} \left(\frac{\delta^{2} I}{\delta \phi_{a}^{(0)}(y) \delta K_{1}(x)}\right)_{0} \right] \right\} + O\left(v_{s}^{2}\right)$$

$$= v_{s}^{2} \sum_{a} d^{4}y \left\{ -i \frac{m}{\hbar} \gamma_{a} \left[ -i \hbar \partial_{\gamma} \left(\frac{\delta^{2} I}{\delta K_{a}(y) \delta K_{1}(x)}\right)_{0} - \frac{\hbar}{mi} \delta_{\gamma,0} \delta^{4}(y - x) \left(\frac{\delta I}{\delta K_{a}(x)}\right)_{0} \right] \right\} + O\left(v_{s}^{2}\right).$$

Here the identity (14·3·30) has been used. Integration-by-parts leads to

$$j_{\alpha}(x, v_{s})$$

$$= v_{s}^{2} \int d^{4}y \left\{ -i \frac{m}{\hbar} \gamma_{a} \left[ -i \hbar \sum_{a} \left(\frac{\delta^{2} I}{\delta K_{a}(y) \delta K_{1}(x)}\right)_{0} - \frac{\hbar}{mi} \delta_{\gamma,0} \delta^{4}(y - x) n_{a} \right] \right\} + O\left(v_{s}^{2}\right).$$

Substituting (14·3·42) into the above equation, it is found that

$$j_{\alpha}(x, v_{s}) = (n - n_{\alpha}) v_{s}^{2} + O\left(v_{s}^{2}\right) = n_{\alpha} v_{s}^{2} + O\left(v_{s}^{2}\right),$$  \hspace{1cm} (14·5·53)

which is the relation we are looking for.

(b) Another method consists in adopting the new variable $\tilde{\phi}_{a}(x)$ introduced in § 14.4. This method relies on the diagrammatical rule and will be used for subsequent studies. See Appendix J. Consider the action $I_{\omega, K_{\alpha}^{\omega}, n_{\alpha}, n_{\alpha}}$ of (14·5·25) and its Legendre transform (by $f$) $I_{\omega, K_{\alpha}^{\omega}, n_{\alpha}, n_{\alpha}}$. The inverse of the propagator $D^{-1}(x, y)$ is divided into two parts:

$$D^{-1}(x, y) = \left(\frac{\delta^{2} I_{\omega, K_{\alpha}^{\omega}, n_{\alpha}, n_{\alpha}}}{\delta \phi_{a}(x) \delta \phi_{a}(y)}\right)_{\phi = \phi^{(0)}(x)} = D_{0}^{-1}(x, y) + V_{\omega, K_{\alpha}^{\omega}, n_{\alpha}, n_{\alpha}}(x, y).$$  \hspace{1cm} (14·5·54)
We proceed by taking the loop expansion scheme. For the tree term, one finds

\[
(j_i(x, v_s))_{\text{tree}} = -\frac{\hbar Q_i}{m} \tilde{n}_0(0) = - v_{at} \tilde{n}_0(0).
\] (14.5.55)

As for the loop term, we notice that the propagator has the dependence on \(K^\mu, \eta^\nu, \eta_h\) and both the three and four point vertices also depend on \(\eta^\mu(\mu = \nu)\). When the propagator is differentiated by \(K_a'(x)\), it is easy to see that

\[
\frac{\delta}{\delta K_a'(x)} D_{\sigma\tau}(y, z) = (-1)^{\sigma+1} \left(D_{\sigma\tau}(y, x) \begin{pmatrix} \frac{\hbar}{2mi \partial_t^2} & 0 \\ 0 & \frac{\hbar}{2mi \partial_t^2} \end{pmatrix} \delta^4(x - z) \right)
\times \left(D_{\sigma\tau}(z_1, z) \right).
\] (14.5.56)

Note that, if \(\sigma = 3\), the factor \((-1)^{\sigma+1}\) is replaced by \(\hbar / i\). Using \(\tilde{D}\) of (14.4.27), Eq. (14.5.56) is expressed as

\[
\frac{\delta}{\delta K_a'(x)} D_{\sigma\tau}(y, z)
\]

\[
= (-1)^{\sigma+1} \left(U^{(\sigma)}(y) \tilde{D}_{\sigma\tau}(y, x) \begin{pmatrix} \frac{\hbar}{2mi \partial_t^2} - \frac{\hbar Q_i}{m} & 0 \\ 0 & \frac{\hbar}{2mi \partial_t^2} - \frac{\hbar Q_i}{m} \end{pmatrix} \delta^4(x - z) \tilde{D}_{\sigma\tau}(z_1, z) \right) (U^{(\sigma)}(z)).
\] (14.5.57)

Equation (14.5.56) tells us that the current vertex is shifted by \((-\hbar Q_i/m)\) 1 in the \(\tilde{\phi}\)-formalism. Then \(j_i(x, v_s)\) is graphically represented as

\[
\left[ \begin{array}{c}
\text{\ldots} \quad \Gamma \\
\vdots
\end{array} \right]_{\text{v}_s}
= \left[ \begin{array}{c}
\text{\ldots} \quad \tilde{\Gamma} \\
\vdots
\end{array} \right] - \frac{\hbar Q_i}{m} 1 \quad \left[ \begin{array}{c}
\text{\ldots} \quad \Gamma \\
\vdots
\end{array} \right]_{\tilde{\phi}^{(0)}}.
\] (14.5.58)

Several comments will be necessary concerning the graphs presented above:

(1) \(\tilde{\Gamma}\) in the figures implies that the propagator in the graph is \(\tilde{D}^{(0)} = \tilde{D}(\tilde{\phi}_a^{(i)} = \tilde{\phi}^{(i)(0)}, \ K^\mu = \eta^\mu = \eta_h = 0)\). Explicitly \(\tilde{D}\) has been given in (14.4.15).

(2) The graphical relation such as (14.5.58) holds not only for the total sum of the graphs but also for the subset. The subset consists of the fixed number of the propagators (\(N_P\)), vertices (\(N_V\)) and loops (\(N_L\)). It is convenient to define \(N_V\) as the number of the interaction part of the Hamiltonian (it contains \(\phi^3\) and \(\phi^4\) type with a definite weight, see (14.4.17) ~ (14.4.19)) which is used in the graphs we are considering. Thus Eq. (14.5.58) is valid if we replace \(\Gamma\) and \(\tilde{\Gamma}\) by \(\Gamma_{N_P, N_V, N_L}\) and \(\tilde{\Gamma}_{N_P, N_V, N_L}\) respectively. The reason for this is that we can count \(N_V\), for example, by multiplying the vertex part in the Hamiltonian by the parameter \(\kappa\), say, and identify the power of \(\kappa\) on both sides of (14.5.58). Inclusion of \(\kappa\) does not invalidate the derivation of
(14.5.58) itself. In order to count $N_L$, it is known that the power of $\hbar$ essentially does this job. For $N_F$ we can rely on the topological relation $N_L + N_V - N_F = 1$ which is easily established.

In the following $\Gamma$ and $\bar{\Gamma}$ in the figure which is inside the circle represent those with fixed number of $N_L$, $N_V$ and $N_F$ while those without the circle are the total sum over $N_L$, $N_V$ and $N_F$.

(3) The vertex

\[ \begin{array}{c}
\Gamma \\
1 \quad \alpha
\end{array} \]  \hspace{1cm} (14.5.59)

is obtained by differentiating the propagator with respect to $K_\alpha(x)$.

Let us expand $j_i(x, v_s)$ in powers of $v_s$, taking notice of the fact that $v_s$ dependence comes from the propagator $\bar{D}^{(0)}$. Here we take into account of the $Q$-dependence except for the one coming from $\bar{\mu}$ and $\bar{\phi}^{(0)}$ and thus expand by $a_\alpha$ contained in $\bar{D}^{(0)}$. The $v_s$ expansion, i.e., $a_\alpha$ expansion, of $\bar{D}^{(0)}$ is thus written as

\begin{align}
\frac{\partial}{\partial v_s} \bar{D}^{(0)}(x, y) & = \bar{D}^{(0)}_{v_s=0} + v_s \left( \frac{\partial \bar{D}^{(0)}}{\partial v_s} \right)_{v_s=0} + \frac{1}{2!} v_s^2 \left( \frac{\partial^2 \bar{D}^{(0)}}{\partial v_s \partial v_s} \right)_{v_s=0} + \cdots, \\
& = -(-1)^{\sigma+1} \sum_\mathcal{I} \int d^4 z d^4 w \left( \bar{D}^{(0)}_{\mathcal{I}}(x, z) \right) \begin{pmatrix}
\frac{\hbar}{i} \partial^\tau \\
0
\end{pmatrix} \delta^4(z-w) \left( \bar{D}^{(0)}_{\mathcal{I}}(w, y) \right)
\end{align}

\begin{align}
& = -(-1)^{\sigma+1} \sum_\mathcal{I} \int d^4 z d^4 w \left( \bar{D}^{(0)}_{\mathcal{I}}(x, z) \right) \begin{pmatrix}
\frac{\hbar}{i} \partial^\tau \\
0
\end{pmatrix} \delta^4(z-w) \left( \bar{D}^{(0)}_{\mathcal{I}}(w, z) \right). \\
& = -(-1)^{\sigma+1} \sum_\mathcal{I} \int d^4 z d^4 w \left( \bar{D}^{(0)}_{\mathcal{I}}(x, z) \right) \begin{pmatrix}
\frac{\hbar}{i} \partial^\tau \\
0
\end{pmatrix} \delta^4(z-w) \left( \bar{D}^{(0)}_{\mathcal{I}}(w, z) \right). \\
& \begin{array}{c}
\begin{pmatrix}
\Gamma \\
\Gamma
\end{pmatrix}
\end{array}
\end{align}

We find

\[ \begin{pmatrix}
\partial_i(x) \\
\partial_i(x)
\end{pmatrix} = \begin{pmatrix}
\Gamma & - v_{si} \frac{1}{x} \Gamma \\
\partial_i(x) & \partial_i(x)
\end{pmatrix} \\
+ \begin{pmatrix}
\frac{d}{d \gamma} \\
\frac{d}{d \gamma}
\end{pmatrix} \begin{pmatrix}
\Gamma & - mv_{ji} \frac{1}{x} \\
\partial_i(x) & \partial_i(x)
\end{pmatrix} \begin{pmatrix}
\begin{pmatrix}
\Gamma, q_1 \\
\Gamma, q_1
\end{pmatrix} \\
\begin{pmatrix}
\Gamma, q_1 \\
\Gamma, q_1
\end{pmatrix}
\end{pmatrix} \begin{pmatrix}
\phi^{(0)} \\
\phi^{(0)}
\end{pmatrix}. \hspace{1cm} (14.5.62)
\]

In the figures, $\Gamma$ is evaluated at $\phi^i = \bar{\phi}^{(0)}$ and $\mu = \bar{\mu}$ so that the propagator is $D_{\phi^i = \bar{\phi}^{(0)}, \mu = \bar{\mu}}$. One rewrites (14.5.62) in the form,
\((j_i(x; v_s))_{\text{loop}}\)

\[ = (j_i(x; v_s=0))_{\text{loop}} - v_s n_{\text{loop}} + (-m)v_s^i \int d^4 y \Gamma_{\text{loop}}^i(k)_{K} \xi_1(x-y) + O(v_s^2) \]

\[ = (j_i(x; v_s=0))_{\text{loop}} - v_s n_{\text{loop}} - mv_s^i \Gamma_{\text{loop}}^i(k)_{K} \xi_1(k=0) + O(v_s^2). \quad (14.5.63) \]

The superscript \(\tilde{0}\) implies the estimation at \(\phi^i = \tilde{\phi}^{(0)}\) and \(\mu = \tilde{\mu}\). Recall here that, since we have used the number density \(n_{\text{loop}}\), it causes the correction of \(O(v_s^2)\) besides the expansion \((14.5.60)\) in terms of \(a_k\), see the discussion in §14.4.2. Now the first term of \((14.5.63)\) vanishes because of the rotational symmetry. As for the third term, we get by \((14.3.42)\), which is the relation at \(Q=0\),

\[ \lim_{k \to 0} \Gamma_{K}^{\tilde{0}}(k=0, k) = \delta_0 \left( \frac{n_n}{m} + O(v_s^2) \right). \quad (14.5.64) \]

Collecting \((14.5.55)\) and \((14.5.63)\), and using

\[ n = \tilde{n}^{(0)}_n + n_{\text{loop}}, \quad \tilde{n}^{(0)}_n = n^{(0)}_n, \quad (14.5.65) \]

we are led to \((14.5.53)\) again,

\[ j_i(x; v_s) = (n^{(0)}_n + n_{\text{loop}})v_s^i - n_nv_s^i + O(v_s^2) = (n_n - n_n)v_s^i + O(v_s^2) \]

\[ = n_s v_s^i + O(v_s^2). \]

In zero temperature case, the first term on the right-hand side of \((14.5.58)\) vanishes, because \(f_\beta(E_\pm a_k) = 0\) in this case and the change of integration variable \(\hbar q_0^i = \hbar q_0 - a_q\) leads to the fact that the internal line is even in \(q\). Then one finds easily

\[ j_i(x; v_s) = v_s^i n. \quad (14.5.66) \]

Equation \((14.5.66)\) tells that \(n_s = n\) at zero temperature.

In passing we note that

\[ (n_s)_{\text{tree}} = \tilde{n}_0^{(0)} = n_{\text{tree}}, \quad (n_n)_{\text{tree}} = 0. \quad (14.5.67) \]

This will often be used in later calculation.

14.5.4. *Energy-momentum tensor with superflow*

Now we come to the problem of the small-\(v_s\) expansion for the energy-momentum tensor. A diagrammatic analysis in terms of loop expansion is adopted and the W-T equations obtained in §14.5.2 play an essential role in this analysis.

(i) **Momentum density**

Using \((14.5.21)\), the momentum density is defined by

\[ T_i^0(x; v_s) = \langle \hat{T}_i^0(x) \rangle_{\phi^{(0)}(x)} = \left( \frac{\delta \Gamma}{\delta \hat{\eta}^{(1)}(x)} \right)_{\phi^{(0)}(x)}. \quad (14.5.68) \]

The expression \((14.5.21)\) for \(\hat{T}_i^0(x)\) is not Hermitian but, as shown in §14.5.9 below, if we had started with the Hermitian form of the Lagrangian, the operator \(\hat{T}_i^0(x)\) is equal to \(-m \hat{f}_i(x)\). From the discussion at the end of §14.5.1, this suggests that the physical results are the same if we replace our \(\hat{T}_i^0(x)\) by the Hermitian form.
Therefore we expect
\[ T_i^0(x; \nu_x) = -m \nu_x \nu_y. \]  \hspace{1cm} (14.5.69)

Indeed one can check (14.5.69) explicitly.

(ii) **Momentum flux**

Let us study the momentum flux defined in (14.5.22),
\[ T_i'(x; \nu_x) = \langle \tilde{T}_i'(x) \rangle_{\phi_{\nu_x}(x)} = \left( \frac{\delta \Gamma'}{\delta \eta_{ij}(x)} \right)_{\phi_{\nu_x}(x)}. \]  \hspace{1cm} (14.5.70)

The tree term contributes to this quantity as
\[ (T_i'(x; \nu_x))_{\text{tree}} = -\frac{h^2}{m} \tilde{\eta}_0^{(0)} Q_i Q_j - \delta_i^j \left( \tilde{\eta}_0^{(0)} - \frac{1}{2} U_0 \tilde{\eta}_0^{(0)2} \right). \]  \hspace{1cm} (14.5.71)

We shall study the loop contribution as follows. Since the operator \( \tilde{T}_i'(x) \) contains the term higher than bilinear in the field through the term \(-\delta_i^j \tilde{L}_0 \) of (14.5.22), \( \eta_i' \) appears in the propagator and also in the three and four vertices. Our interests are the derivative of those quantities. Taking the differentiation of the propagator, one obtains
\[
\frac{\delta}{\delta \eta_{j}(x)} D_{\nu}(y, z) = -(-1)^{\sigma + 1} (D_{\nu}(y, x))
\]
\[
\times \begin{pmatrix}
\frac{h^2}{2m} \left( \overline{\partial} \tilde{\zeta}' \overline{\partial} \zeta' - \overline{\partial} \zeta' \overline{\partial} \tilde{\zeta}' \right), & 0 \\
0, & \frac{h^2}{2m} \left( \overline{\partial} \zeta' \overline{\partial} \tilde{\zeta}' - \overline{\partial} \tilde{\zeta}' \overline{\partial} \zeta' \right)
\end{pmatrix}
\]
\[
- \delta_i^j \begin{pmatrix}
i \overline{\partial} \tilde{\zeta}' + \frac{h^2}{2m} \overline{\partial} \overline{\partial} \tilde{\zeta}' + \mu - 2U_0 \phi(x) \phi(x), & -U_0 \phi(x) \phi(x) \\
- U_0 \phi(x) \phi(x), & i \overline{\partial} \tilde{\zeta}' + \frac{h^2}{2m} \overline{\partial} \overline{\partial} \tilde{\zeta}' + \mu - 2U_0 \phi(x) \phi(x)
\end{pmatrix}
\]
\[
\times \delta^d(x - z_i) (D_{\nu}(z_i, x))
\]
\[
= -(-1)^{\sigma + 1} (U^{(-\nu)}(y))(D_{\nu}(y, x))
\]
\[
\times \begin{pmatrix}
\frac{h^2}{2m} \left( \overline{\partial} \tilde{\zeta}' - iQ_i \right) \left( \overline{\partial} \zeta' + iQ_i \right) - \left( \overline{\partial} \zeta' - iQ_i \right) \left( \overline{\partial} \tilde{\zeta}' - iQ_i \right), & 0 \\
0, & \frac{h^2}{2m} \left( \overline{\partial} \zeta' + iQ_i \right) \left( \overline{\partial} \tilde{\zeta}' - iQ_i \right) - \left( \overline{\partial} \tilde{\zeta}' - iQ_i \right) \left( \overline{\partial} \zeta' - iQ_i \right)
\end{pmatrix}
\]
\[ -\delta i \left( i\hbar (\vec{\partial} \delta - iQ_0) - \frac{\hbar^2}{2m} (\vec{\partial} \cdot \vec{r} - iQ) (\vec{\partial} \cdot \vec{r} - iQ) + \mu - 2U_0 \bar{\phi}^*(x) \bar{\phi}(x), \\
- U_0 \bar{\phi}(x) \bar{\phi}(x), \\
- U_0 \bar{\phi}^*(x) \bar{\phi}(x) \right) \]
\[ \times \delta^4(x - z_i)(\bar{D}_{\sigma}(z_i, z_i))(U^{(q)}(z_i)). \]  

The derivative of the three or four point vertex leads to
\[ \frac{\partial}{\partial \eta^{(a)}(x)} \left[ (-1)^{t+1} \delta_i \eta^{(a)}(y) U_0 \phi^a(y) \phi^a(y) \varphi(y) \varphi(y) \right] 
\[ = (-1)^{t+1} \delta \iota \delta^4(y - x) \delta_{a,a} U_0 \phi^a(x) \phi^a(x) \varphi_a(x) \varphi_a(x), \]  

(14.5.73)

\[ \frac{\partial}{\partial \eta^{(a)}(x)} \left[ (-1)^{t+1} \delta_i \eta^{(a)}(y) U_0 \phi^a(y) \phi^a(y) \varphi_a(y) \varphi_a(y) \right] 
\[ = (-1)^{t+1} \delta \iota \delta^4(y - x) \delta_{a,a} U_0 \phi^a(x) \phi^a(x) \varphi_a(x) \varphi_a(x), \]  

(14.5.74)

\[ \frac{\partial}{\partial \eta^{(a)}(x)} \left[ (-1)^{t+1+1/2} \delta_i \eta^{(a)}(y) U_0 \phi^a(y) \phi^a(y) \varphi_a(y) \varphi_a(y) \right] 
\[ = (-1)^{t+1+1/2} \delta \iota \delta^4(y - x) \delta_{a,a} U_0 \phi^a(x) \phi^a(x) \varphi_a(x) \varphi_a(x), \]  

(14.5.75)

These relations imply that, if a three or four point vertex is differentiated, one gets the same three or four point vertex as the original action. This is expected since \( \eta^{(i)} \) couples to \(- \delta \iota \bar{L} \). When \( a = 3 \) in (14.5.73) \sim (14.5.75), the weight \(-1^{t+1}\) is replaced by \( \hbar/i \).

Now the small \( v_s \) expansion (i.e., expansion in \( a_s \)) is performed. Although the process is similar to the case of mass flux, the actual calculation is rather involved so that we present only the results together with important relations to be used in the derivation. See Ref. 27 for details.

The zero-order of \( v_s \) is given as
\[ \left( \langle \bar{T}_i(x) \rangle_{v_s=0} \right)_{\text{loop}} = -\delta \iota \frac{i}{\beta \hbar V} \Gamma_{\text{loop}}[\bar{\phi}^{(0)}; \mu = \bar{\mu}]. \]  

(14.5.76)

Here we have used the topological relation \( N_p - N_r - N_t = -1 \). The first order is zero because of the rotational symmetry and the symmetry under the space reflection.

The second order contribution can be summed up into a rather simple form:
\[ hQ_i \frac{Q^j}{m} \left( \frac{n_s}{2m} \right) \left( \frac{1}{\hbar} \right) \left( \frac{1}{2} \right) = \frac{1}{2} \frac{n_n}{m} \left( \frac{\hbar Q^2}{2m} \right). \] (14.5.77)

Here (14.5.45), (14.5.64) and (14.5.67) have been used. From (14.5.71), (14.5.76) and (14.5.77), one finally finds

\[ T_i(x; v_s) = m v_n v_s n_s - \delta^j_i \left( \frac{i}{\beta \hbar V} \Gamma[\tilde{v}^{(0)}; \mu = \tilde{\mu}] + \frac{n_n}{2m} (\hbar Q^2) \right). \] (14.5.78)

This is the expectation value of the momentum flux up to \( \mathcal{O}(v_s^2) \).

Let us write (14.5.78) in terms of the pressure. The pressure \( P \) of the uniform system without superflow is given by using the thermodynamic potential \( \Omega \) as

\[ P = -\frac{\partial \Omega}{\partial V} = \frac{i \Gamma[\phi]}{\beta \hbar V}. \quad (\phi: \text{const}) \] (14.5.79)

Extending this argument, the pressure in the presence of the superfluid flow is defined as

\[ P = \frac{i \Gamma[\tilde{\phi}^{(0)}(x)]}{\beta \hbar V} = \frac{i \tilde{\Gamma}[\tilde{\phi}^{(0)}]}{\beta \hbar V}. \] (14.5.80)

We expand \( P \) in powers of \( v_s \) (\( a_s \)-expansion). The contribution of the tree diagram is

\[ P = \tilde{\mu} \tilde{n}_0 - \frac{1}{2} U_0 \tilde{n}_0 \tilde{n}_0. \] (14.5.81)

The total sum of the loop contribution is

zero-th order: \( P^{(0)} = \frac{i \Gamma[\phi^{(0)}; \mu = \tilde{\mu}]}{\beta \hbar V} \),

first order: zero because of rotational symmetry,

second order: \( P^{(2)} = \frac{1}{2} \left( \frac{\partial^2 \tilde{\Gamma}_{\text{loop}}[\tilde{\phi}^{(0)}]}{\beta \hbar V} \right)_{\phi = 0, \mu = \tilde{\mu}} Q_i Q^i \)

\[ = \frac{1}{2} \sum_a \int d^4 y \left( \frac{\delta^2 \tilde{\Gamma}_{\text{loop}}}{\delta K_{a}^i(x) \delta K_{a}^j(y)} \right) \tilde{v}^{a, \tilde{\mu}} \left( -\hbar Q^i \right) \left( -\hbar Q^j \right) \]

\[ = \frac{n_n}{2m} \left( \frac{\hbar Q^2}{2m} \right). \] (14.5.84)

In (14.5.84), we have used (14.5.64) and (14.5.67) again. In this way Eqs. (14.5.81) ~ (14.5.84) lead to

\[ P = \frac{i \Gamma[\tilde{\phi}^{(0)}; \mu = \tilde{\mu}]}{\beta \hbar V} + \frac{1}{2} mn_s v_s^2 + \mathcal{O}(v_s^4). \] (14.5.85)

We conclude from (14.5.78) and (14.5.85) that

\[ \langle \hat{T}_i(x) \rangle_{v_s} = mn_s v_s v_s' - \delta^j_i P, \] (14.5.86)

which coincides with the expression commonly adopted in the phenomenological
approach.

(iii) Energy flux
The energy flux is studied in a similar way which is defined by

$$T_0^i(x; \nu_s) \equiv \langle \bar{T}_0^i(x) \rangle_{\nu_s^\omega(x)} = \left( \frac{\delta \Gamma}{\delta \eta_{11}(x)} \right)_{\nu_s^\omega(x)} \cdot \tag{14.5.87}$$

Here the operator $\bar{T}_0^i(x)$ is defined in (14.5.20). First, we get easily within tree approximation as

$$\langle T_0^i(x; \nu_s) \rangle_{\text{tree}} = \hbar Q_0 \frac{\hbar Q^i}{m} \bar{\eta}_0^{(0)} = \hbar Q_0 v_s^i \langle n_s \rangle_{\text{tree}}. \tag{14.5.88}$$

The loop term is obtained as follows. Since (14.5.20) is bilinear in the field, $\eta_i^\alpha$ dependence appears only in the propagator. As the propagator depends on $\eta_i^\alpha$, we differentiate the propagator with respect to $\eta_i^\alpha$,

$$\frac{\delta}{\delta \eta_{i0}(x)} D_{sa}(y, z) = -(-1)^{a+1}(D_{sa}(y, x))$$

$$\times \left( \begin{array}{cc}
\frac{\hbar^2}{2m} (\bar{\partial}_i^x \bar{\partial}_j^x - \bar{\partial}_j^x \bar{\partial}_i^x) & 0 \\
0 & \frac{\hbar^2}{2m} (\bar{\partial}_i^x \bar{\partial}_0^x - \bar{\partial}_0^x \bar{\partial}_i^x)
\end{array} \right) \delta^4(x-z_1)(D_{sa}(z_1, z))$$

$$= -(-1)^{a+1}(U^{(-)(y)})(\bar{D}_{sa}(y, x))$$

$$\times \left( \begin{array}{cc}
\frac{\hbar^2}{2m} \{(\bar{\partial}_0^x - iQ_0)(\bar{\partial}_i^x + iQ^i) - (\bar{\partial}_i^x - iQ^i)(\bar{\partial}_0^x - iQ_0)\} \\
0 \\
0 \\
\frac{\hbar^2}{2m} \{(\bar{\partial}_i^x + iQ^i)(\bar{\partial}_0^x - iQ_0) - (\bar{\partial}_0^x - iQ^i)(\bar{\partial}_i^x - iQ_0)\}
\end{array} \right)$$

$$\times \delta^4(x-z_1)(D_{sa}(z_1, z))(U^{(0)}(z)). \tag{14.5.89}$$

Since we know that $Q_0 \sim \mathcal{O}(Q^2)$, see (14.4.42), the small-$v_s$ expansion ($\alpha_k$-expansion) leads to the following result. First of all the zero-th order is zero due to the rotational symmetry. It is remarkable that the first order vanishes due to the identity (14.5.46),

$$(\text{first order}) = \sum_a \int d^4 y \left( \frac{\delta^2 \Gamma_{\text{loop}}}{\delta \eta_{11}(x) \delta \Omega^a_{\eta}(y)} \right) \rho_{m, \beta} \left( -\hbar Q^i \right) + \frac{\hbar}{m} Q^i \left( \frac{\delta}{\delta \eta_{0}(x)} \right)_{\text{loop}}$$

$$= \Gamma_{\text{loop}}^{(2)\delta} \eta_{\alpha \beta} (k=0) (-\hbar Q^i) + \frac{\hbar Q^i}{m} \rho_{0}^{(0) \delta}$$
\[ \frac{1}{m} \delta_i \left( -\hbar \mathcal{Q}^i \right) h_{\text{loop}}^{(0)} + \frac{\hbar \mathcal{Q}^i}{m} h_{\text{loop}}^{(0)} = 0, \quad (14.5.90) \]

where the identity \((14.5.46)\) has been put into the fourth equation. Actually we need the formula \((14.5.46)\) where \(\phi^{(0)}\) and \(\mu\) are replaced by \(\overline{\phi}^{(0)}\) and \(\overline{\mu}\). But this replacement is allowed since the only requirement to get \((14.5.46)\) from \((14.5.35)\) is that \(\phi^{(0)}(x)\) or \(\overline{\phi}^{(0)}(x)\) is independent of \(x\). The important remark here is that the first order is zero without expanding \(\overline{\phi}^{(0)}\) or \(\overline{\mu}\) in \(v_s^2\) so that \((14.5.90)\) has no influence on the third order term discussed below.

The second order vanishes due to the rotational symmetry and the third order term is rather involved but it turns out to be written in a compact form,

\[ (\text{third order}) = v_s^i \hbar \mathcal{Q}_0 (n_{\text{loop}} - n_s) = v_s^i \hbar \mathcal{Q}_0 (n_s)_{\text{loop}}. \quad (14.5.91) \]

Here \((14.5.47)\) has been used. Equations \((14.5.90)\) and \((14.5.91)\) lead to

\[ T_0^i(x; v_s)_{\text{loop}} = \hbar \mathcal{Q}_0 v_s^i (n_s)_{\text{loop}}. \quad (14.5.92) \]

Thus, from \((14.5.88)\) and \((14.5.92)\), the energy flux is finally given by\(^{28}\)

\[ T_0^i(x; v_s) = \hbar \mathcal{Q}_0 v_s^i n_s. \quad (14.5.93) \]

This result is not familiar in that \(T_0^i(x; v_s)\) has the dependence on \(\mathcal{Q}_0\) explicitly. However one will get the well-known form by introducing the “reduced” energy flux in § 14.5.5.

(iv) Hamiltonian density

Let us calculate the density of Hamiltonian given in \((14.5.19)\) in the presence of superflow,

\[ \mathcal{H}(x; v_s) = T_0^0(x; v_s) = \left( \frac{\delta \Gamma}{\delta \eta_0(x)} \right)_{\eta_0(x)} \quad (14.5.94) \]

in the same manner as the previous argument. We show the outline of derivation and result.\(^{27}\)

First, the tree term contribution is

\[ (T_0^0(x; v_s))_{\text{tree}} = \left( \frac{1}{2} m v_s^2 - \mu \right) \bar{n}_0^{(0)} + \frac{1}{2} U_0 \bar{n}_0^{(0)2} = \hbar \mathcal{Q}_0 - \hbar \bar{n}_0^{(0)} + \frac{1}{2} U_0 \bar{n}_0^{(0)2}. \quad (14.5.95) \]

As for the loop terms, the \(\eta_0^{(0)}\)-dependence is found in the propagator and also in the three and four point vertices. Taking the derivative of the propagator, we get

\[ \frac{\delta}{\delta \eta_0(x)} D_{\alpha}(y, z) \]

\[ = -(-1)^{a+1} (D_{\nu\alpha}(y, z)) \]
\begin{align*}
&\times \left( \frac{\hbar^2}{2m} \bar{r} \frac{\partial}{\partial r} - \mu + 2U_0 \phi(x) \phi(x) \quad U_0 \phi(x) \phi(x) \right) \\
&\times \left( \frac{\hbar^2}{2m} \bar{r} \frac{\partial}{\partial r} - \mu + 2U_0 \phi^*(x) \phi^*(x) \right) \\
&\times \delta^4(x - z_i)(D_{\alpha\beta}(z_i, z)) \\
&= -(-1)^{a+1}(U^{(\phi)}(y))(D_{\alpha\beta}(y, z)) \\
&\times \left( \frac{\hbar^2}{2m} \left( \bar{r} - iQ_i \right) \left( \bar{r}^\dagger - iQ_i^\dagger \right) - \mu + 2U_0 \phi^*(x) \phi(x), \\
&\quad U_0 \phi(x) \phi(x), \\
&\quad \frac{\hbar^2}{2m} \left( \bar{r} - iQ_i \right) \left( \bar{r}^\dagger - iQ_i^\dagger \right) - \mu + 2U_0 \phi^*(x) \phi(x) \\
&\times \delta^4(x - z_i)(D_{\alpha\beta}(z_i, z))(U^{(\phi)}(z)). \tag{14\cdot5\cdot96}
\end{align*}

Differentiation of the three and four point vertex gives us

\begin{align*}
\frac{\delta}{\delta \eta_{\alpha\beta}(x)} \left[ (-1)^{a+1} \eta_{\alpha\beta}(y) U_0 \phi^*(y) \phi^*(y) \phi^*(y) \phi^*(y) \right] \\
&= (-1)^{a+1} \delta^4(y - x) \delta_{\alpha\beta} U_0 \phi^*(x) \phi^*(x) \phi^*(x) \phi^*(x) \\
&= (-1)^{a+1} \delta^4(y - x) \delta_{\alpha\beta} U_0 \phi^*(x) \phi^*(x) \phi^*(x) \phi^*(x), \\
\frac{\delta}{\delta \eta_{\alpha\beta}(x)} \left[ (-1)^{a+1} \eta_{\alpha\beta}(y) U_0 \phi^*(y) \phi^*(y) \phi^*(y) \phi^*(y) \right] \\
&= (-1)^{a+1} \delta^4(y - x) \delta_{\alpha\beta} U_0 \phi^*(x) \phi^*(x) \phi^*(x) \phi^*(x) \\
&= (-1)^{a+1} \delta^4(y - x) \delta_{\alpha\beta} U_0 \phi^*(x) \phi^*(x) \phi^*(x) \phi^*(x), \\
\frac{\delta}{\delta \phi_{\alpha}(x)} \left[ (-1)^{a+1} \frac{1}{2} \eta_{\alpha\beta}(y) U_0 \phi^*(y) \phi^*(y) \phi^*(y) \phi^*(y) \right] \\
&= (-1)^{a+1} \frac{1}{2} \delta^4(y - x) \delta_{\alpha\beta} U_0 \phi^*(x) \phi^*(x) \phi^*(x) \phi^*(x) \\
&= (-1)^{a+1} \frac{1}{2} \delta^4(y - x) \delta_{\alpha\beta} U_0 \phi^*(x) \phi^*(x) \phi^*(x) \phi^*(x).
\end{align*}

Let us expand in \( v_s \),

\begin{align*}
(T_0^\phi(x, v_s))_{\text{loop}} &= \left(T_0^\phi(x; \mu = \bar{\mu})\right)_{\text{loop}} \\
&\quad + \frac{1}{2!} \sum_{\alpha\beta, \alpha', \beta'} \left( T_{\text{loop}}^{(2)} \delta_{\alpha\beta} \delta_{\alpha'\beta'} \delta_{k_1} \delta_{k_2} \delta_{k_1} \delta_{k_2} = 0 \right)(-\hbar Q^{(4)})(-\hbar Q^{(4)}) \\
&\quad + \hbar Q^{(4)} T_{\text{loop}}^{(2)} \delta_{\alpha\beta} \delta_{k_1} \delta_{k_2} \delta_{k_3} \delta_{k_4} = 0 \right)(-\hbar Q^{(4)}) + \hbar Q^{(4)} n_{\text{loop}}. \tag{14\cdot5\cdot97}
\end{align*}

Equations (14\cdot5\cdot95) and (14\cdot5\cdot97) sum up into
\[ T_0^0(x; \mathbf{v}_e) = (T_0^0(x; \mu = \bar{\mu})) \tilde{\phi}^{(0)} + \hbar Q^0 n - m \mathbf{v}_e \cdot \mathbf{n} \]
\[ + \frac{1}{2} m^2 \mathbf{v}_e \cdot \mathbf{v}_e \sum_{\sigma_1, \sigma_2} \left( \Gamma^{(2)}_{\sigma_1, \sigma_2} \right) \phi^{(0)}(k_1 = k_2 = 0) \].

The last term cannot be rewritten in another form by using W-T identities of § 14.5.2. In § 14.5.6, \( T_0^0(x; \mathbf{v}_e) \) will be calculated by another approach.

14.5.5. Energy and energy flux

Let us introduce the "reduced" energy and its flux as is announced in the previous subsection. It is used by many authors and is written as \( \tilde{E} \) and \( \tilde{j}_e(x) \),
\[ \tilde{E}(x) = \tilde{T}_0^0(x) + \mu \tilde{n}(x), \quad \tilde{j}_e(x) = \tilde{T}_0^i(x) + \mu \tilde{j}_e(x). \]

The extra term \( \mu \tilde{n}(x) \) or \( \mu \tilde{j}_e(x) \) cancels the corresponding term in \( \tilde{T}_0^0 \) or \( \tilde{T}_0^i \). From (14·3·14) and (14·5·27), the following conservation law holds in the case where any probe term is absent
\[ \partial_0 \tilde{E}(x) + \partial_i \tilde{j}_e(x) = 0, \]

Eqs. (14·5·53) and (14·5·93) lead to the expectation value of \( \tilde{j}_e(x) \) in the presence of superfluid flow
\[ j_e(x; \mathbf{v}_e) = (\hbar Q^0 + \mu) \mathbf{v}_e \cdot \mathbf{n} \]
\[ = (\tilde{\mu} + \frac{1}{2} m \mathbf{v}_e \cdot \mathbf{v}_e) \mathbf{n} \cdot \mathbf{v}_e. \]

The energy density is given by
\[ E(x; \mathbf{v}_e) = (T_0^0(x; \mu = \bar{\mu})) \tilde{\phi}^{(0)} + (\tilde{\mu} + \frac{1}{2} m \mathbf{v}_e \cdot \mathbf{v}_e) n - m \mathbf{v}_e \cdot \mathbf{n} \]
\[ + \frac{1}{2} m^2 \mathbf{v}_e \cdot \mathbf{v}_e \sum_{\sigma_1, \sigma_2} \left( \Gamma^{(2)}_{\sigma_1, \sigma_2} \right) \phi^{(0)}(k_1 = k_2 = 0) \].

14.5.6. Entropy conservation

When the normal flow is absent, the entropy conservation is represented as
\[ \frac{\partial s}{\partial t} = 0. \]

Here \( s \) is the entropy density. In this section, we derive Eq. (14·5·104) in our formalism. For this purpose we need the local expansion of \( \tilde{\Gamma} \) assuming the space-time dependent order parameters in the beginning. This problem is discussed in Ref. 27) and we assume here that all the quantities below are the ones at the space-time point \( x \) we are looking at.

First, we note that the differential of \( \Gamma[\phi] = \tilde{\Gamma}[\tilde{\phi}] \), which is a function of \( T, V, \mu, Q^0, Q = m \mathbf{v}_e \) and \( \tilde{\phi} \), can be written as
\[ d(i \tilde{\Gamma}) = \frac{\partial i \tilde{\Gamma}}{\partial T} dT + \frac{\partial i \tilde{\Gamma}}{\partial V} dV + \frac{\partial i \tilde{\Gamma}}{\partial \mu} d\mu + \frac{\partial i \tilde{\Gamma}}{\partial (\hbar Q^0)} d(\hbar Q^0) + \frac{\partial i \tilde{\Gamma}}{\partial \mathbf{v}_e} d\mathbf{v}_e + \frac{\partial i \tilde{\Gamma}}{\partial \tilde{\phi}} d\tilde{\phi}, \]

(14·5·105)
where we have assumed that $\tilde{\phi}_i = \tilde{\phi}_i = \text{const}$. Then all the $x$-dependence goes away and the problem becomes the equilibrium one, see §12.2.2 and Ref. 27). The entropy density is defined by

$$ s = \frac{1}{V} \frac{\partial (\text{Tr} (\tilde{\phi}_i / \beta \hbar))}{\partial T} = \frac{1}{V} \frac{\partial (\text{Tr} (\tilde{\phi}_i / \beta \hbar))}{\partial T} . \quad (14\cdot5\cdot106) $$

Note that $\tilde{\Gamma}$ is related to the pressure $P$ by (14\cdot5\cdot80). Using (14\cdot5\cdot105), $P$ is expressed as

$$ dP = s dT + n d\mu + \frac{1}{\beta \hbar V} \left\{ \left( \frac{\partial i \tilde{\Gamma}}{\partial (h Q^0)} \right)_{\tilde{\phi}^{(0)}} d(h Q^0) + \left( \frac{\partial i \tilde{\Gamma}}{\partial v_s^i} \right)_{\tilde{\phi}^{(0)}} d v_s^i + \left( \frac{\partial i \tilde{\Gamma}}{\partial \tilde{\phi}_i} \right)_{\tilde{\phi}^{(0)}} d \tilde{\phi}_i \right\} . \quad (14\cdot5\cdot107) $$

The last term in the curly bracket vanishes by the stationary condition. Within the lowest order of $v_s$, (14\cdot5\cdot107) reduces to

$$ dP = s dT + n d\mu + n d(h Q^0) - m n_s v_s^i d v_s^i . \quad (14\cdot5\cdot108) $$

Here we have used the expression (14\cdot4\cdot14) which tells us that $Q^0$ appears in the combination $\mu + h Q^0$ and

$$ \frac{1}{\beta \hbar V} \left( \frac{\partial i \tilde{\Gamma}}{\partial v_s^i} \right)_{\tilde{\phi}^{(0)}} = - m j_s^i $$

in the lowest order of $v_s$, since the situation is the same as we expand in $a_h$ defined in (14\cdot4\cdot16). In the absence of superflow, the energy density is given by the familiar relation,

$$ - \mathcal{E} = P - \mu n - T_s . \quad (14\cdot5\cdot109) $$

We find this is consistent with (14\cdot5\cdot99). Extending this definition to the system with superfluid flow, the energy density is given by

$$ - \mathcal{E} = P - \mu n - T_s - h Q^0 n . \quad (14\cdot5\cdot110) $$

The relation (14\cdot5\cdot110) can be established by deriving the relation,

$$ P - T_s = - T_s^0 (x; v_s, \mu = \tilde{\mu}) + h Q^0 n (x; v_s) . \quad (14\cdot5\cdot111) $$

The proof is performed diagrammatically using the topological identity $N_L - N_F + N_T = 1$, see Ref. 27) for details.

The energy density is now written by using (14\cdot5\cdot110) as

$$ d \mathcal{E} = \left( T d s + (h Q^0 + \mu) d n + m n_s v_s^i d v_s^i \right) $$

$$ = T d s + \left( \frac{1}{2} m v_s^2 + \tilde{\mu} \right) d n + m j_s^i d v_s^i . \quad (14\cdot5\cdot112) $$

Here we have put (14\cdot4\cdot7) and (14\cdot5\cdot53) into the second equation. By the local equilibrium assumption, the conservation law (14\cdot5\cdot100) leads to
\[ 0 = \partial \mathcal{E} + \partial \mathcal{J} \]
\[ = T \frac{\partial \mathcal{S}}{\partial t} + \left( \frac{1}{2} m v_s^2 + \bar{\mu} \right) \frac{\partial n}{\partial t} + m \bar{v}_s \frac{\partial \phi_s}{\partial t} + \partial_i \left( \bar{\mu} + \frac{1}{2} m v_s^2 \right) j_i \]
\[ = T \frac{\partial \mathcal{S}}{\partial t}, \quad (14.5 \cdot 113) \]

where we have used the relation \((14.5 \cdot 121)\) derived below. Thus we have proved the entropy conservation in the case where the superfluid flow is present.

14.5.7. Inhomogeneous superflow

If the velocity of superflow depends on space-time coordinates, we write the condensation \(\phi_s(x)\) as
\[ \phi_\pm(x) = e^{i\tau(x)} \tilde{\phi}_s(x), \quad \phi_s(x) = e^{-i\tau(x)} \tilde{\phi}_s(x), \quad (14.5 \cdot 114) \]
instead of \((14.4 \cdot 3)\). In this case the inverse of the propagator is represented as
\[ I^{(0)}(x, y) = \begin{pmatrix} e^{i\tau(x)} & 0 \\ 0 & e^{-i\tau(y)} \end{pmatrix}, \quad \tilde{I}^{(0)}(x, y) = \begin{pmatrix} e^{-i\tau(y)} & 0 \\ 0 & e^{i\tau(y)} \end{pmatrix}, \quad (14.5 \cdot 115) \]
\[ \tilde{I}^{(2)}(x, y) = \begin{pmatrix} -i\hbar \partial_x - \frac{\hbar^2}{m_i} (\partial_x f(x))\partial_x + \frac{\hbar^2}{2m} iV_x^2 f(x) + \bar{\mu}(x) - 2\bar{\phi}^*(x)\bar{\phi}(x) U_0, \\ -\bar{\phi}(x)\bar{\phi}(x) U_0, \\ - \frac{\hbar^2}{2m} iV_x^2 f(x) + \bar{\mu}(x) - 2\bar{\phi}^*(x)\bar{\phi}(x) U_0 \end{pmatrix} \times \delta^4(x - y). \quad (14.5 \cdot 116) \]

Here \(x\)-dependent \(\bar{\mu}(x)\) has been defined by
\[ \bar{\mu}(x) = \mu + \hbar \partial_x f(x) - \frac{\hbar^2}{2m} (\nabla f(x))^2. \quad (14.5 \cdot 117) \]

The fluctuating part of the field \(\tilde{\phi}_s\) is introduced in an analogous way as \((14.5 \cdot 114)\). The propagator of \(\tilde{\phi}_s\)-field is given by \(\tilde{I}^{(2)-1}\). The three and four vertices satisfy the relations similar to those of \(\phi_s\)-field; \((14.4 \cdot 17)\)~\((14.4 \cdot 19)\). If one wants to get physical quantity at \(x\), both propagators and vertices are expanded around the point \(x\). After this process, the propagators and the vertices are expressed in terms of the derivative of \(f(x)\) or \(\sqrt{\hbar_0^{(0)}(x)}\).

Note that the phase \(e^{\pm i\tau(x)}\) disappears from the theory and \(f(x)\) is contained only in the propagator in the form of derivative. Thus, using the diagrammatical rule, we find
\[ \Gamma = \Gamma^{(0)}[\tilde{\phi}_s^i, \mu, \hbar \partial f, -\frac{\hbar^2}{2m} (\nabla f)^2, \nabla f, \nabla^2 f, \ldots] \]
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\[
= \Gamma \left[ \delta \phi^i, \mu + \hbar \delta f - \frac{\hbar^2}{2m} (\nabla f)^2, \nabla f, \nabla^2 f, \ldots \right]
\]

(14.5.118)

and

\[
\frac{\delta \Gamma}{\delta \mu(x)} = n(x).
\]

(14.5.119)

We call $\mu$ the "reduced chemical potential". The velocity of superfluid flow is defined by

\[
v_s(x) = -\frac{\hbar}{m} \nabla f(x).
\]

(14.5.120)

If we put $f(x) = Qx$ into (14.5.114), the argument presented above is identified with that of § 14.4. From (14.5.117) and (14.5.120), one is led to

\[
m \frac{\partial v_s(x)}{\partial t} + \nabla \left( \frac{1}{2} m v_s(x)^2 + \mu(x) \right) = 0.
\]

(14.5.121)

14.5.8. Galilean transformation

We have discussed the system where the superfluid flow is present but without the normal flow. In this section, we introduce the normal flow by using the Galilean transformation. Then one will find the complete set of phenomenological equations. This part of study is well-known but for completeness the derivation is shown below within our formalism.

Now the argument we have presented up to now is regarded as that in a frame $F_0$ where the normal fluid is at rest, i.e., the normal fluid velocity $v_n^{(0)}$ is zero in this frame. The velocity of superfluid flow in this frame is written as $v_s^{(0)}$. The Galilean transformation from $F_0$ to the laboratory frame $F$, where the normal fluid flows with the velocity $v_n$, is generated by the unitary operator $U_{v_n}$,

\[
U_{v_n} = \exp \left( \frac{Q_{v_n}}{\hbar} \right),
\]

(14.5.122)

\[
Q_{v_n} = i \int d^3x \left[ -v_n^t \cdot m \tilde{f}_s + v_n^t \cdot m \tilde{n} \right].
\]

(14.5.123)

It can be shown after some algebra that $U_{v_n}$ is independent of the time; $\partial_0 Q_{v_n} = 0$. Any quantities as seen in $F_0$ are expressed in terms of the corresponding quantities in the system $F$,

\[
\langle \tilde{O}_i(x) \rangle_{v_s^{(0)}} = \text{Tr} \{ \rho \tilde{O}_i(x) \} = \text{Tr} \{ U_{v_n} \rho U_{v_n}^{-1} \cdot U_{v_n} \tilde{O}_i(x) U_{v_n}^{-1} \}
\]

\[
= \text{Tr} \{ \rho_{v_n} \tilde{O}_i(t, x + v_n t) \} = \langle \tilde{O}_i(t, X) \rangle_{v_{s, v_n}} = \langle f(\tilde{O}(t, X)) \rangle_{v_{s, v_n}},
\]

(14.5.124)

\[
v_s = v_s^{(0)} + v_n, \quad X = x + v_n t, \quad \rho_{v_n} = U_{v_n} \rho U_{v_n}^{-1},
\]

\[
\tilde{O}_i(t, X) = U_{v_n} \tilde{O}_i(x) U_{v_n}^{-1} = f_i(\tilde{O}(t, X)).
\]

(14.5.125)

The function $f_i$ introduced in (14.5.125) is some function depending on the operator $\tilde{O}_i$. The inversion of (14.5.124) leads to $\langle \tilde{O}(t, X) \rangle_{v_{s, v_n}}$ written in terms of the
quantities in the system $F_{0}$,

$$
\langle \tilde{\tilde{O}}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle f^{-1}(\tilde{\tilde{O}}(t, x)) \rangle_{\nu^{(0)}}.
$$

(14·5·126)

The transformation of the field operator $\tilde{\theta}_{a}^{i}(x)$ is the well-known one,

$$
U_{\nu_{n}} \tilde{\theta}_{a}^{i}(x) U_{\nu_{n}}^{\dagger} = \exp \left\{ \pm \frac{i}{\hbar} \left( \frac{1}{2} m v_{n}^{i} v_{n} m + m v_{n}^{i} x_{i} \right) \right\} \tilde{\theta}_{a}^{i}(t, X).
$$

(14·5·127)

Using (14·5·127) and by explicit calculations, it is straightforward to get the transformation rules for the number density and its current and the energy-momentum tensor,

$$
\langle \tilde{n}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{n}(t, x) \rangle_{\nu^{(0)}},
$$

(14·5·128)

$$
\langle \tilde{j}^{i}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{j}^{i}(t, x) \rangle_{\nu^{(0)}},
$$

(14·5·129)

$$
\langle \tilde{T}_{a}^{i}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}},
$$

(14·5·130)

$$
\langle \tilde{T}_{a}^{i}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} - v_{n} m \langle \tilde{j}^{i}(t, x) \rangle_{\nu^{(0)}} + \nu_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}}
$$

$$
+ v_{n}^{i} v_{n} m \langle \tilde{n}(t, x) \rangle_{\nu^{(0)}},
$$

(14·5·131)

$$
\langle \tilde{T}_{a}^{0}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{T}_{a}^{0}(t, x) \rangle_{\nu^{(0)}} - v_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} - \frac{1}{2} v_{n}^{i} v_{n} m \langle \tilde{n}(t, x) \rangle_{\nu^{(0)}},
$$

(14·5·132)

$$
\langle \tilde{T}_{a}^{0}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{T}_{a}^{0}(t, x) \rangle_{\nu^{(0)}} - v_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} + \frac{1}{2} v_{n}^{i} v_{n} m \langle \tilde{j}^{i}(t, x) \rangle_{\nu^{(0)}}
$$

$$
- v_{n}^{i} v_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} + v_{n} \langle \tilde{T}_{a}^{0}(t, x) \rangle_{\nu^{(0)}}
$$

$$
- \frac{1}{2} v_{n}^{i} v_{n}^{i} v_{n} m \langle \tilde{n}(t, x) \rangle_{\nu^{(0)}}.
$$

(14·5·133)

The Lagrangian density does not change

$$
\langle \tilde{L}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{L}(t, x) \rangle_{\nu^{(0)}}.
$$

(14·5·134)

The density of energy and its flux is transformed into

$$
\langle \tilde{E}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{E}(t, x) \rangle_{\nu^{(0)}} - v_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} - \frac{1}{2} v_{n}^{i} v_{n} m \langle \tilde{n}(t, x) \rangle_{\nu^{(0)}},
$$

(14·5·135)

$$
\langle \tilde{j}^{i}(t, X) \rangle_{\nu_{n}, \nu_{n}} = \langle \tilde{j}^{i}(t, x) \rangle_{\nu^{(0)}} - v_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} + \frac{1}{2} v_{n}^{i} v_{n} m \langle \tilde{j}^{i}(t, x) \rangle_{\nu^{(0)}}
$$

$$
- v_{n}^{i} v_{n}^{i} \langle \tilde{T}_{a}^{i}(t, x) \rangle_{\nu^{(0)}} + v_{n} \langle \tilde{E}(t, x) \rangle_{\nu^{(0)}}
$$

$$
- \frac{1}{2} v_{n}^{i} v_{n}^{i} v_{n} m \langle \tilde{n}(t, x) \rangle_{\nu^{(0)}}.
$$

(14·5·136)

Putting (14·5·53), (14·5·69), (14·5·86), (14·5·93) and (14·5·102) into (14·5·129) \(\sim\) (14·5·131), (14·5·135) and (14·5·136), we arrive at the set of fundamental equations of the two fluid model,
\[ \langle \hat{\mathcal{J}}_i(t, X) \rangle_{v_n v_n} = n_n v_n^i + n_n^i v_n, \tag{14.5.137} \]
\[ \langle \hat{T}_i(t, X) \rangle_{v_n v_n} = -m(n_s v_s^i + n_n^i v_n), \tag{14.5.138} \]
\[ \langle \hat{T}_i(t, X) \rangle_{v_n v_n} = mn_v n_v n_v^i + mn_v n_v v_n^i - \delta^i P, \tag{14.5.139} \]
\[ \langle \hat{\mathcal{E}}(t, X) \rangle_{v_n v_n} = \mathcal{E}_s^{(0)}(v_s - v_n) + v_n^i mn_v (v_s^i - v_n^i) + \frac{1}{2} m v_n^2 n, \tag{14.5.140} \]
\[ \langle \hat{j}_e^i(t, X) \rangle_{v_n v_n} = \left( \hat{\mu} + \frac{1}{2} mv_s^2 \right)(n_s v_s^i + n_n v_n^i) \]
\[ + \left\{ \mathcal{E}_s^{(0)}(v_s - v_n) - \hat{\mu} n + P - mn_v (v_s - v_n) \cdot v_s \right. \]
\[ - \frac{1}{2} mn_v (v_s - v_n)^2 + \frac{1}{2} mn_v (v_s - v_n) \cdot v_s \left. \right\} v_n^i, \tag{14.5.141} \]

where
\[ \mathcal{E}_s^{(0)}(v_s - v_n) \equiv \langle \mathcal{E}(t, X) \rangle_{v_n}. \]

From (14.5.140), the energy \( \mathcal{E}_s^{(0)}(v_n - v_s) \) in the system where the velocity of superfluid flow is zero but the velocity of the normal flow is \( v_n - v_s \) can be seen to be related to \( \mathcal{E}_s^{(0)}(v_s - v_n) \) as
\[ \mathcal{E}_s^{(0)}(v_n - v_s) = \mathcal{E}_s^{(0)}(v_s - v_n) - \frac{1}{2} mn_v (v_s - v_n)^2 + mn_v (v_s - v_n) \cdot v_s^2. \tag{14.5.142} \]

Here we have used the fact that
\[ \mathcal{E}_s^{(0)}(v_s - v_n) = \mathcal{E}_s^{(0)}(v_n - v_s) \]

because of the rotational symmetry. By using (14.5.113), \( \mathcal{E}_s^{(0)}(v_n - v_s) \) satisfies the relation
\[ d \mathcal{E}_s^{(0)}(v_n - v_s) = Ts + \hat{\mu} d n + m(v_n - v_s) \cdot d[n_n(v_n - v_s)]. \tag{14.5.143} \]

Here we have identified \( \mathcal{E}_s^{(0)}(v_s - v_n) \) with \( \mathcal{E} \) of (14.5.103) and \( v_n - v_s \) with \( v_s \). The stationary condition \( \partial \mathcal{G} / \partial \hat{\phi} \equiv 0 \) has also been used.

By using \( \mathcal{E}_n^{(0)}(v_n - v_s) \) and (14.5.110) and also by noting that the definition (14.4.7) reads in the present case as
\[ \hat{\mu} = \mu + \hbar Q_n - \frac{1}{2} m(v_s - v_n)^2, \]
the pressure can be written as follows,
\[ P = -\mathcal{E}_s^{(0)} + Ts + \hat{\mu} n + mn_v (v_n - v_s)^2. \tag{14.5.144} \]

Inserting the above relation into (14.5.141), the energy flow has another expression,
\[ \langle \hat{j}_e^i(t, X) \rangle_{v_n v_n} = \left( \hat{\mu} + \frac{1}{2} mv_s^2 \right)(n_s v_s^i + n_n v_n^i) + Ts v_n^i + mn_v n_v^i \{ v_n^i(v_n - v_s) \}. \tag{14.5.145} \]
It is possible\textsuperscript{27} to generalize the entropy conservation (14·5·104) to the case where $v_n \neq 0$. We get
\[
\frac{\partial s}{\partial t} + \mathbf{P} \cdot (s \mathbf{v}_n) = 0.
\]
Together with this equation, Eqs. (14·5·137)\textendash(14·5·141), (14·5·143), (14·5·144) and (14·5·145) are the fundamental equations in the two fluid model. Thus we have completed the microscopic derivation of the whole set of phenomenological equations in the absence of the dissipation.

Although we have considered the case of small $v_s$ in this article, the investigation on the arbitrary $v_s$ has been done in Ref. 27).

References

1) J. Gavoret and P. Nosieres, Ann. of Phys. 28 (1964), 349.
Appendix A

—— Formulas of Legendre Transformation ——

Here several formulas of the Legendre transformation are collected which are sufficient for the discussions in this article. The formulas below are written for the Bosonic (commuting) variables and in order to simplify the notation, conjugate variables of the Legendre transformation are denoted by $J_i$ and $\phi_i$. The index $i$ represents all the attributes characterizing the variable including space-time coordinate $x$: $\phi_i = \phi_a(x)$ where index $a$ represents discrete degrees of freedom other than $x$. Therefore $\Sigma_i$ implies actually $\int d^4x \Sigma_a$. Kronecker $\delta_{ij}$ signifies $\delta_{ab}\delta'(x-y)$ where $\delta'(x-y)$ is the four-dimensional Dirac $\delta$-function. For example $\partial \phi_i / \partial \phi_j = \delta_{ij}$ implies the functional derivative $\delta \phi_a(x)/\delta \phi_b(y) = \delta_{ab}\delta'(x-y)$. The following formulas are applicable also to composite field case like $\phi_i = \phi_a(x)\phi_b(y)$. In this case the subscript $i$ represents collectively $(a, x, b, y)$ and $\phi_i$ is regarded as if it is an elementary field.

The Legendre transformation between $W[J]$ and $\Gamma[\phi]$ is defined as follows,

$$\Gamma[\phi] = W[J] - J_i \frac{\partial W[J]}{\partial J_i}, \quad (A\cdot1)$$

where $\phi$ and $J$ are related by

$$\phi_i = \frac{\partial W[J]}{\partial J_i} \quad \rightarrow \quad J_i = J_i[\phi]. \quad (A\cdot2a, b)$$

Repeated index $i$ in (A·1) is summed or integrated over and the relation (A·2a) is inverted solving for $J_i$ to get (A·2b) which is inserted into (A·1). In this sense, Eq. (A·1) is written more explicitly as

$$\Gamma[\phi] = W[J[\phi]] - J_i[\phi] \phi_i. \quad (A\cdot3)$$

(1) Conjugate relation Differentiating (A·3) by $\phi_i$,

$$\frac{\partial \Gamma[\phi]}{\partial \phi_j} = \frac{\partial W[J]}{\partial J_i} \frac{\partial J_i}{\partial \phi_j} - \frac{\partial J_i}{\partial \phi_j} \phi_i - J_j. \quad (A\cdot4)$$

By (A·2a), we get

$$\frac{\partial J_i[\phi]}{\partial \phi_i} = -J_i \quad \text{or} \quad \Gamma_i^{(n)}[\phi] = -J_i. \quad (A\cdot5)$$

Here and in the following, the following notation is introduced

$$\Gamma_{i_1 i_2 \cdots i_n}[\phi] = \frac{\partial^n \Gamma[\phi]}{\partial \phi_{i_1} \partial \phi_{i_2} \cdots \partial \phi_{i_n}}, \quad (A\cdot6a)$$

$$W_{i_1 i_2 \cdots i_n}[J] = \frac{\partial^n W[J]}{\partial J_{i_1} \partial J_{i_2} \cdots \partial J_{i_n}}. \quad (A\cdot6b)$$

Note that $\Gamma^{(n)}$ and $W^{(n)}$ are symmetric with respect to the interchange of suffixes.
(2) **Inverse matrix relation**  Differentiate (A·2a) with respect to $\phi_j$, then we have, using (A·5),

$$\delta_i = \frac{\partial \phi_i}{\partial \phi_j} = \frac{\partial^2 W[J]}{\partial J_i \partial J_k} \frac{\partial J_k}{\partial \phi_j} = - \frac{\partial^2 W[J]}{\partial J_i \partial J_k} \frac{\partial^2 \Gamma[\phi]}{\partial \phi_k \partial \phi_j}.$$  

(A·7)

Therefore,

$$W^{(2)}_{ik} \Gamma^{(2)}_{kj} = W^{(2)}_{kij} \Gamma^{(2)}_{kij} = - \delta_{ij}. \quad \text{(A·8)}$$

The first equality is obtained by either noting that $\Gamma^{(2)}$ and $W^{(2)}$ are symmetric matrix or by differentiating (A·5) by $J_i$.

(3) **Differentiation by spectator parameter**  Let $a_a$ be some parameter which is regarded as a constant when we make the Legendre transformation. Then the inversion process (A·2a, b) is written more explicitly as

$$\phi_i = \frac{\partial W[J, a]}{\partial J_i} = \phi_i[J, a], \quad \text{(A·9a)}$$

$$\rightarrow J_i = J_i[\phi, a]. \quad \text{(A·9b)}$$

Now we take the derivative of $\Gamma[\phi, a]$ by $a_a$ with $\phi$ fixed. This is easily done as follows,

$$\Gamma[\phi, a] = W[J[\phi, a], a] - J_i[\phi, a] \phi_i, \quad \text{(A·10a)}$$

$$\frac{\partial \Gamma[\phi, a]}{\partial a_a} = \frac{\partial W[J, a]}{\partial a_a} + \frac{\partial W[J, a]}{\partial J_i} \frac{\partial J_i[\phi, a]}{\partial a_a} - \frac{\partial J_i[\phi, a]}{\partial a_a} \phi_i. \quad \text{(A·10b)}$$

Thus we get

$$\frac{\partial \Gamma[\phi, a]}{\partial a_a} = \frac{\partial W[J, a]}{\partial a_a}. \quad \text{(A·11)}$$

Higher derivatives are obtained straightforwardly by (A·11).

(4) **Successive Legendre transformation**  Take $W[J_1, J_2]$ and make the Legendre transformation in two steps,

$$\Gamma_1[\phi_1, J_2] = W[J_1, J_2] - J_1 \frac{\partial W[J_1, J_2]}{\partial J_1}, \quad \text{(A·12)}$$

$$\phi_1 = \frac{\partial W[J_1, J_2]}{\partial J_1} = \phi_1[J_1, J_2], \quad \text{(A·13)}$$

$$\Gamma_2[\phi_1, J_2] = \Gamma_1[\phi_1, J_2] - J_2 \frac{\partial \Gamma_1[\phi_1, J_2]}{\partial J_2}, \quad \text{(A·14)}$$

$$\phi_2 = \frac{\partial \Gamma_1[\phi_1, J_2]}{\partial J_2}. \quad \text{(A·15)}$$

We can show that $\Gamma_2[\phi_1, \phi_2]$ is equivalent to $\Gamma[\phi_1, \phi_2]$ defined by the double Legendre transformation,
\[ \Gamma[\phi_1, \phi_2] = W[J_1, J_2] - J_1 \frac{\partial W[J_1, J_2]}{\partial J_1} - J_2 \frac{\partial W[J_1, J_2]}{\partial J_2}, \quad (A\cdot16) \]

\[
\phi_1 = \frac{\partial W[J_1, J_2]}{\partial J_1}, \quad \phi_2 = \frac{\partial W[J_1, J_2]}{\partial J_2}. \quad (A\cdot17a, b)
\]

Note that Eqs. (A\cdot13) and (A\cdot17a) are the same. The key formula to prove the statement is (A\cdot11) which implies that \( \phi_2 \) defined by (A\cdot15) is given by

\[
\phi_2 = \frac{\partial}{\partial J_2} \left( W[J_1, J_2] - J_1(\phi_1, J_2) \phi_1 \right)_{J_1} = \frac{\partial W[J_1, J_2]}{\partial J_2} \Bigg|_{J_1} \phi_1 + \frac{\partial W[J_1, J_2]}{\partial J_1} \Bigg|_{J_2} - \frac{\partial J_1[J_1, J_2]}{\partial J_1} \Bigg|_{\phi_1} \phi_1
\]

\[
= \frac{\partial W[J_1, J_2]}{\partial J_2} \Bigg|_{J_1=J_2[J_1, J_2]} \quad (A\cdot18)
\]

where \( J_1[J_1, J_2] \) is the function obtained by solving (A\cdot13) in terms of \( J_1 \). Therefore the two functions \( \phi_2[J_1, J_2] \) and \( \phi_2[J_1, J_2] \) defined by (A\cdot13) and (A\cdot15) are the same with (A\cdot17a, b). The equivalence \( \Gamma[\phi_1, \phi_2] = \Gamma[\phi_1, \phi_2] \) is easily seen by inserting (A\cdot12) into (A\cdot14) and using (A\cdot15) and (A\cdot18). The statement is thus proved.

The generalization to \( N \)-variables is straightforward. We see that \( N \)-step successive Legendre transformation from \( W[J_1, J_2, \cdots, J_N] \) to \( \Gamma_N[\phi_1, \phi_2, \cdots, \phi_N] \) gives the same result as that from \( W[J_1, J_2, \cdots, J_N] \) to \( \Gamma[\phi_1, \phi_2, \cdots, \phi_N] \) in one step.

(5) **Higher derivatives and one particle irreducibility** The derivative of the relation (A\cdot8) is the starting process to get higher derivatives in terms of \( \phi_i \). We follow the procedure of Jona-Lasinio\(^1\) and for a historical review, see the Appendix of the review article by Haymaker.\(^2\) The chain rules obtained by (A\cdot2a), (A\cdot5) and (A\cdot8),

\[
\frac{\partial}{\partial J_i} = \frac{\partial \phi_j}{\partial J_i} \frac{\partial}{\partial \phi_j} = W_{j'i}^{(2)} \frac{\partial}{\partial \phi_j} = -(\Gamma^{(2)-1})_{j'i} \frac{\partial}{\partial \phi_j}, \quad (A\cdot19)
\]

\[
\frac{\partial}{\partial \phi_i} = \frac{\partial J_j}{\partial \phi_i} \frac{\partial}{\partial J_j} = -(\Gamma^{(2)-1})_{j'i} \frac{\partial}{\partial J_j}, \quad (A\cdot20)
\]

are frequently used when applied to appropriate functions. Let us proceed step by step.

(i) \( \Gamma^{(3)} \) and \( W^{(3)} \) Differentiating (A\cdot8) by \( \phi_i \) we get by using (A\cdot20),

\[
\Gamma^{(3)}_{m'k} W^{(3)}_{m'k} + \Gamma^{(3)}_{n'k} W^{(3)}_{k'n} (W^{(2)-1})_{m'i} = 0. \quad (A\cdot21)
\]

Thus the following relation is obtained, with the notation \((W^{(3)-1})_{m'} = W^{(3)}_{m'i}\)

\[
\Gamma^{(3)}_{n'k} = W^{(3)}_{n'k} W^{(2)-1} W^{(2)-1} W^{(2)-1}, \quad (A\cdot22)
\]

where Eq. (A\cdot8) has been used. In the case of quantum field theory, \( W^{(2)} \) is the propagator and, in this case, Eq. (A\cdot22) states that \( \Gamma^{(3)} \) is equal to \( W^{(3)} \) with three external legs amputated by \( W^{(2)} \).

(ii) \( \Gamma^{(4)} \) and \( W^{(4)} \) Here one of the most important properties of the Legendre transformation, one particle irreducibility, comes in. Let us take the derivative of (A\cdot22)
by $\phi_m$ and use (A·20),
\[
\Gamma^{(4)}_{ijkl} = W^{(4)}_{ij} W^{(2)-1}_{kl} W^{(2)-1}_{ij} W^{(2)-1}_{kl} - (W^{(2)-1}_{ij} W^{(2)-1}_{kl} W^{(2)-1}_{ij} W^{(2)-1}_{kl} W^{(2)-1}_{ij} W^{(2)-1}_{kl} + \text{two other terms}),
\]
(A·23)
where we have used
\[
\frac{\partial W^{(2)-1}_{ij}}{\partial J_{ij}} = - W^{(2)-1}_{ij} W^{(2)-1}_{ij} W^{(2)-1}_{ij}.
\] (A·24)
In (A·23) “two other terms” include the same terms as the preceding one with the suffixes properly interchanged. By using (A·22), subtracted terms on the right-hand side of (A·23) are written as
\[
\Gamma^{(3)}_{jkm} W^{(2)}_{mn} \Gamma^{(3)}_{nli} + \text{two other terms}.
\] (A·25)
We rewrite (A·23) symbolically as
\[
W^{(4)} = (W^{(2)})^3 \{ \Gamma^{(4)} + \Gamma^{(3)} W^{(2)} \Gamma^{(3)} + \text{two other terms} \}.
\] (A·26)
Equation (A·26) is represented graphically in Fig. A.1, where a line implies the propagator $W^{(2)}$. In Fig. A.1, by following the suffixes properly, two other terms in (A·26) are shown explicitly. We see that $W^{(4)}$ is written by the sum of tree diagrams constructed out of vertices $\Gamma^{(4)}$, $\Gamma^{(3)}$ and propagator $W^{(2)}$. Thus $\Gamma^{(4)}$ is called amputated one-particle irreducible (1PI) part of $W^{(4)}$ in the sense that it cannot be separated into two parts if one of the lines, i.e., propagator, contained in $\Gamma^{(4)}$ is cut. Such a graph is distinguished and added on the right-hand side of (A·26) as independent terms.

(iii) $\Gamma^{(N)}$ In order to show that $\Gamma^{(N)}$ is 1PI for general $N$, we rely on the mathematical induction. Let us assume that for $1 \leq i \leq N$, $\Gamma^{(i)}$ is the amputated 1PI part of $W^{(i)}$ and that $W^{(N)}$ has the tree graph expansion of the form,
\[
W^{(N)} = (W^{(2)})^N \{ \Gamma^{(N)} + \Gamma^{(N-k+1)} W^{(2)} \Gamma^{(k+1)} + \ldots \}, \quad (1 \leq k \leq N-2)
\] (A·27)
which is a function of $\Gamma^{(i)}$ with $3 \leq i \leq N$ and $W^{(2)}$. Now it is clear that $W^{(N+1)}$ is obtained from $W^{(N)}$ by adding one extra external leg in all possible ways. There are

\[
\begin{align*}
W^{(6)} &= \Gamma^{(6)} \\
&+ \Gamma^{(3)} \Gamma^{(3)} + \Gamma^{(3)} \Gamma^{(3)} + \Gamma^{(3)} \Gamma^{(3)}
\end{align*}
\]

Fig. A.1. The relation (A·26) between $W^{(4)}$ and $\Gamma^{(4)}$. Straight line represents $W^{(2)}$. 
two possibilities; one is to change $\Gamma^{(i)} \rightarrow \Gamma^{(i+1)} W^{(2)}$ and the others are $W^{(2)} \rightarrow W^{(3)}$. A new leg emerges from the vertex $\Gamma^{(i)}$ in the former case and from the line $W^{(2)}$ in the latter.

However, this is just realized by differentiating $W^{(N)}$ of (A·27) by $J$, as is seen from the chain rule (A·19). Therefore $W^{(N+1)}$ is again written as (A·27) where the right-hand side is the sum of tree graphs with $(N+1)$ external legs. Since the $N=4$ has been proven, we have shown that $\Gamma^{(N)}$ is the amputated 1PI for general $N$.

For the case of composite field $\phi_i = \phi_a(x) \phi_b(y)$, for example, the terminology 1PI has to be understood as if the index $i$ specifies collectively single line in the graph.

Since 1PI property is essential for the Legendre transformation, apart from the above inductive method, two different proofs are given; in Appendix C on the basis of the combinatorial properties of the vacuum graphs and in Chapter VI by establishing the summing up rule which holds for any diagrams having external legs. Therefore, for composite field, we see that 2PI (3PI and so forth) is more conventional and transparent terminology than 1PI.

(6) **Existence of physical source** Suppose the Hamiltonian has the term $-\nu_i \hat{O}_i$ with $\hat{O}_i$ some operator and $\nu_i$ represents a real external parameter which is a $c$-number field exerted on the system from outside. Then effective action $\langle \hat{O}_i \rangle$ is obtained by applying further the term $J_i \hat{O}_i$ to the Lagrangian. Thus in the presence of $\nu$, $W[J]$ becomes $W[J, \nu] = W[J + \nu]$. Therefore by inverting the relation

$$\phi_i = \frac{\partial W[J + \nu]}{\partial J_i},$$

$J + \nu$ becomes a function(al) of $\phi_i$. Effective action $\Gamma[\phi, \nu]$ in the presence of $\nu$ is therefore given by

$$\Gamma[\phi, \nu] = W[J + \nu] - \nu_i \frac{\partial W[J + \nu]}{\partial J_i}$$

$$= W[J + \nu] - (J_i + \nu) \frac{\partial W[J + \nu]}{\partial J_i} + \nu_i \frac{\partial W[J + \nu]}{\partial J_i}$$

$$= \Gamma[\phi] + \nu_i \phi_i,$$

(A·28)

where $\Gamma[\phi]$ is independent of $\nu$ and is equal to $\Gamma$ in the absence of $\nu$. All the $\nu$-dependence comes from the term $\nu_i \phi_i$. The stationary equation that has to be solved is

$$0 = \frac{\delta \Gamma[\phi, \nu]}{\delta \phi_i} = \frac{\delta \Gamma[\phi]}{\delta \phi_i} + \nu_i.$$

(A·29)

(7) **Legendre transformation in terms of Grassmann variables** All the above formulas hold with particular care about the sign factor for the case where $J_i$ and hence $\phi_i$ are Grassmann numbers. Instead of collecting their formulas here, § 2.5 contains necessary manipulations.
Appendix B

References


Appendix B

—— Feynman Prescription and Large Time Limit of Kernel ——

We discuss here how the formula \((1\cdot2\cdot4)\) or \((1\cdot2\cdot7)\) selects the vacuum state as a boundary states at \(t=\pm\infty\).

It is obvious that for any Hamiltonian \(H\),
\[
\exp(-\beta H) = \exp(-\beta H) \sum |n><n| \longrightarrow \exp(-\beta E_0)|0><0|, \quad (\beta \to +\infty) \quad (B\cdot1)
\]
where the summation is done over the complete set of eigenstates of the Hamiltonian and \(E_0\) is the energy of the ground state \(|0\rangle\). The problem is to find a proper analytic regularization which ensures
\[
\exp(-iT H) \longrightarrow \exp(-iT E_0)|0><0|, \quad (T \to +\infty) \quad (B\cdot2)
\]
Without regularization, Eq. \((B\cdot2)\) does not hold of course. The observation in this appendix is that the usual Feynman prescription,
\[
m^2 \longrightarrow m^2 - i\epsilon \equiv m^0, \quad (B\cdot3)
\]
giving infinitesimally small negative imaginary part to mass squared is sufficient for this purpose.\(^1\),\(^2\) This is equivalent to the statement that Eq. \((B\cdot3)\) assures the analytic continuation \(\beta \to iT \quad (\beta > 0, \quad T > 0)\) thus we have both \((B\cdot1)\) and \((B\cdot2)\).

To see whether Eq. \((B\cdot3)\) really satisfies \((B\cdot2)\) is an interesting subject and the fact that the answer is in fact yes is an important result since Eq. \((B\cdot3)\) naturally arises in any Feynman rule of the T-product of the operators and hence in any path integral formula: we do not have to introduce extra regularization scheme to assure \((B\cdot2)\).

In order to make the arguments transparent, let us take harmonic free Hamiltonian,
\[
H = \frac{1}{2m} p^2 + \frac{m\omega^2}{2} q^2, \quad (B\cdot4)
\]
where we assume \(\omega > 0\). In this form the Feynman replacement \((B\cdot3)\) is equivalent to
\[
\omega^2 \to \omega^2 - i\epsilon \equiv \omega^0. \quad (B\cdot5)
\]
Let us consider \(\langle q'|\exp(-iT H)|q\rangle\) with the Feynman replacement \((B\cdot5)\). By the well-known formula,\(^3\) it has the expression,
\[
\langle q'|e^{-i\tau n}|q\rangle = \sqrt{\frac{m\omega'}{2\pi i\sin \omega'T}} \exp \left( i\frac{m\omega'}{2} \frac{\cos \omega'T}{\sin \omega'T} (q^2 + q'^2) - i\frac{m\omega'}{\sin \omega'T} qq' \right). \quad (B\cdot6)
\]
It is easy to see that with \((B\cdot5)\) in mind the limit \(T \to \infty\) gives the following result,
\[ \langle q' | \exp(-iTH) | q \rangle \longrightarrow \sqrt{m\omega/\pi} \exp\left\{ -i\frac{1}{2} \omega' T - \frac{1}{2} m\omega'(q^2 + q'^2) \right\}. \] (B·7)

This is just \( q, q' \) representation of (B·2).

The above proof of free case is found in Ref. 1). Inclusion of unharmonic interaction \( V_i(q) \) has been discussed in Ref. 2) where the formula (B·2) is proved for all order of perturbation in the interaction. But we have to be careful:

Caution!! The proof of Ref. 2) relies on the perturbation theory. Although (B·2) holds for any order of perturbative expansion, it is not applicable when the interaction \( V' \) becomes strong: the case may occur where the limit \( T \to \infty \) and Taylor expansion in terms of \( V' \) do not commute. If this happens, our formula (B·2) will fail.

We have indeed constructed\(^2\) a model Hamiltonian in which \( \exp(-iTH) \) approaches an excited state when the coupling strength \( g \) multiplying \( V' \) exceeds some critical value. The model Hamiltonian is given by, taking \( m^2 = 0 \) in (B·4) and \( g > 0 \),

\[ H = \frac{p^2}{2m} + \begin{cases} \infty & \text{for } |q| \geq 2L, \\ -g(\delta(q + L) + \delta(q - L)) & \text{for } |q| < 2L. \end{cases} \]

In any realistic field theoretical system, the interaction is polynomial in the field so that the above potential looks artificial. However the fact that we can construct a model that invalidates (B·2) has to be kept in mind.

References


Appendix C

— Diagrammatic Rule of Legendre Transformation —

Here we present a review of De Dominicis-Martin’s rule of the Legendre transformation\(^1\) up to three-body channels. Originally this rule was derived in the framework of non-relativistic quantum statistical mechanics, but it can also be applied to any case with a small notational modifications.\(^3\) We shall explain in the following this (slightly modified) rule, by which we can directly derive an explicit form of the effective action in field theory. The proof of the rule especially clarifies the graphical meaning of the Legendre transformation. The relation to the rules given by Jackiw\(^2\) and Cornwall-Jackiw-Tomboulis\(^3\) is also discussed. For another way of performing inversion process between the source and the expectation value of operator, which is an essential part of the Legendre transformation, is given in Chapters VI, VII and XI, see also Ref. 5).

Let us examine the bose field case following De Dominicis-Martin and start from
the generating functional $W[v_\nu]$ defined in (3·1·1). Incidentally this starting point is different from the original one in Ref. 1, where $W$ is defined through the partition function $e^W = \text{Tr} e^{-H}$. The notations employed by De Dominicis-Martin are recapitulated as follows (see also Chapter III). By using the generating functional $W[v_\nu]$, $G_\nu$ is first introduced for $\nu=1, 2, 3$,

$$G_\nu(j, k, \cdots) = \nu! \frac{\delta W[v_\nu]}{\delta v_\nu(j, k, \cdots)} . \tag{C·1}$$

The connected part of (C·1) is denoted by $\bar{G}_\nu$ as shown in (3·1·3) and, for convenience of diagrammatical representation, $C_3$-vertex is further introduced as in (3·1·4) which is the amputated part of $\bar{G}_3$. With these notations, the Legendre transformation is carried out step by step. De Dominicis and Martin introduced the following functional $F_\nu$, which is the Legendre transform of $W$ from the variable $v_\nu$ to $G_\nu$:

$$F_1[G_1, v_2, v_3] = W[v_\nu] - v_1(j)G_1(j) , \tag{C·2a}$$

$$F_2[G_1, \bar{G}_2, v_3] = F_1[G_1, v_2, v_3] - \frac{1}{2!} v_2(j, k)G_2(j, k) , \tag{C·2b}$$

$$F_3[G_1, \bar{G}_2, C_3] = F_2[G_1, \bar{G}_2, v_3] - \frac{1}{3!} v_3(j, k, l)G_3(j, k, l) . \tag{C·2c}$$

Recall that each $v_\nu$ has the form $v_\nu = v_\nu^0 + J_\nu$ ($\nu=1, 2, 3$), where $J_\nu$ is the external source used as a probe and $v_\nu^0$ denotes the original bare vertex. On the other hand, the effective action $\Gamma$ in field theory is defined by the Legendre transformation for $J$ instead of $v$. So they are related by, using the formula (A·28)

$$\Gamma_1[G_1, J_2, J_3] = F_1[G_1, v_2, v_3] + v_1^0(j)G_1(j) , \tag{C·3a}$$

$$\Gamma_2[G_1, \bar{G}_2, J_3] = F_2[G_1, \bar{G}_2, v_3] + v_2^0(j)G_2(j) + \frac{1}{2!} v_2^0(j, k)G_2(j, k) , \tag{C·3b}$$

$$\Gamma_3[G_1, \bar{G}_2, C_3] = F_3[G_1, \bar{G}_2, C_3] + v_3^0(j)G_3(j) + \frac{1}{2!} v_3^0(j, k)G_3(j, k) + \frac{1}{3!} v_3^0(j, k, l)G_3(j, k, l) . \tag{C·3c}$$

Namely, once the functional $F_\nu$ is obtained by De Dominicis-Martin's approach, we can derive effective action $\Gamma_\nu$ straightforwardly.

C.1. Legendre transformation for one-body channel

In order to calculate $F_1[G_1, v_2, v_3]$ defined in (C·2a), the following definitions are first introduced.

A diagram with $\nu$ external lines is called $\nu$-diagram. Vacuum graph is a 0-diagram. If there exists at least one continuous path joining any two internal vertices or external points, the $\nu$-diagram is called connected. The generating functional $iW$ is constructed upon all distinct connected 0-diagrams. Here and hereafter, we concentrate on such a class of diagrams. In the same way, the graphical meaning of $\bar{G}_\nu$ is given as the sum of all distinct connected $\nu$-diagrams. The $\nu$ external points
are generated of course through the derivative by \( v_1 \) as in (C.1). Let us consider a line in a connected 0-diagram. It is named an articulation line if the diagram is separated into two parts when it is cut. If one and only one of those parts is a single \( v_1 \)-vertex, the articulation line is said to be trivial. With these preliminaries, a 1-particle irreducible (1PI) 0-diagram is defined as the connected vacuum diagram containing only trivial articulation lines. The class of all 1PI 0-diagrams is written as \( \kappa^{(1)}(iG_2^0(j, k)v_1(k)) \), where \( G_2^0(j, k) \) is the bare propagator defined by \( v_2(j, k) \equiv i[G_2^0]^{-1}(j, k) \). The general connected 1-diagram, or \( G_1 = G_i \), is then generated as follows by a simple iteration of diagrams,

\[
G_i(j) = G_2^0(j, k)(iv_1(k) + K_i(k; G_i)) \tag{C.4}
\]

\[
K_i(k; G_i) = \frac{\delta \kappa^{(1)}(iG_2^0v_1)}{\delta (iG_2^0(k, l)v_1(l))} \bigg|_{iG_2^0v_1 = G_i}. \tag{C.5}
\]

Therefore all possible one particle reducible 1-diagrams (written in terms of \( iv_1 \)) can be summed up into the new variable \( G_i \) itself. Here the direct resummation procedure is possible for 1-diagrams because “these diagrams have some element distinguished (in this case, one external point”). However, such resummation is no longer possible for the vacuum diagram, we cannot write \( W[v_1, v_2, v_3] \) as \( W[G_1, v_2, v_3] \) for example. To sum up the subdiagrams of \( W \) unambiguously, let us use the following topological relation for a 0-diagram,

\[-N(\text{art } l) + N(\kappa^{(1)}) + N(v_1) = 1, \tag{C.6}\]

where \( N(\text{art } l) \) is the number of articulation lines, and \( N(v_1) \) the number of \( v_1 \)-vertices. \( N(\kappa^{(1)}) \) is the number of 1-irreducible skeletons, or the number of ways in which one can generate the 0-diagram out of the diagrams of \( \kappa^{(1)}(G_i) \) by using the relation (C.4). (Note that, since \( G_i \) includes all possible one particle reducible diagrams, \( \kappa^{(1)}(G_i) \) covers all connected 0-diagrams.) An example of (C.6) is given now.

**Example of (C.6):** Consider the diagram of Fig. C.1, where the cross represents \( v_1 \)

![Fig. C.1. An example of (C.6).](image-url)
Appendix C

and the line is \( G_2^0 \). Here \( N(\text{art } l)=8 \), \( N(v_i)=6 \), \( N(\kappa^{(l)})=3 \) (A, B and C parts). Recall here that there are three ways to generate the diagram starting from each skeleton A or B or C: one starts from A part replacing the part which extends to the right originating from the \( l_i \) line by the full \( G_1 \). Alternatively one starts from B and replace A, C part by \( G_1 \). The similar process applies when one starts from C. Thus \( N(\kappa^{(l)})=3 \) and the relation \( (C\cdot6) \) holds.

The general proof of (C\cdot6) is very simple. Since the number of trivial articulation lines is equal to \( N(v_i) \), \( N(\text{art } l)−N(v_i) \) is the number of non-trivial articulation lines, \( l_1, l_2 \) in Fig. C.1. This is easily seen to be equal to \( N(\kappa^{(l)})−1 \).

Now, if we distinguish one articulation line, any diagram of \( iW[v_1, v_2, v_3] \) is included in

\[
\frac{1}{2} G_1(j) G_2^{0−1}(j, j′) G_2^0(j′, k′) G_1(k) = \frac{1}{2} G_1(j) G_2^{0−1}(j, j′) G_1(j′), \quad (C\cdot7)
\]

but is counted \( N(\text{art } l) \) times corresponding all possible choices of the articulation line in the diagram — Eq. (C\cdot7) does not represent correct \( iW[v_1, v_2, v_3] \) but each diagram is weighted by \( N(\text{art } l) \). In the same way, one finds that

\[
\kappa^{(l)}(G_1) \quad \text{or} \quad iv_1(j) G_1(j) \quad (C\cdot8), (C\cdot9)
\]

also produces all the diagrams of \( iW[v_1, v_2, v_3] \) but each diagram is counted \( N(\kappa^{(l)}) \)- or \( N(v_i) \)-times, respectively. Now from (C\cdot6), the set of connected 0-diagram \( iW \) in (3\cdot1\cdot1) (defined up to the irrelevant constant) is obtained in proper weight if we take the combination as follows,

\[
iW = -\frac{1}{2} G_1(j) G_2^{0−1}(j, j′) G_1(j′) + \kappa^{(l)}(G_1) + iv_1(j) G_1(j). \quad (C\cdot10)
\]

So we find from (C\cdot2a) that,

\[
F_1[G_1, v_2, v_3] = \frac{1}{2} G_1(j) i[G_2^0]^{−1}(j, j′) G_1(j′) - i\kappa^{(l)}(G_1) \quad (C\cdot11)
\]

or equivalently,

\[
I_1[G_1, J_2, J_3] \equiv v_1(j) G_1(j) + \frac{1}{2} G_1(j) iG_2^{0−1}(j, j′) G_1(j′) - i\kappa^{(l)}(G_1). \quad (C\cdot12)
\]

When external source is introduced only in one-body channel, \( i(G_2^0)^{−1}(i, j) \) in (C\cdot12) is given as \( v_2^0(i, j) \), i.e., \( G_2^0(i, j) \) becomes the original bare propagator.

For simplicity, let us examine \( \lambda \phi^4 \)-theory (or the case \( v_1^0=v_3^0=0 \)) by setting \( J_2=J_3=0 \). Let us classify \( \kappa^{(l)} \) according to the number of loops. If this is done we see the relation between the formula (C\cdot12) and the wide spread formula which uses the "shifted field". For this purpose the effective action (C\cdot12) is graphically written as in Fig. C.2, where the diagrams have been separated into three parts according to the number of loops. They can obviously be summarized into the following three terms, respectively,
\[ I'[\bar{\phi}] = I[\bar{\phi}] + \frac{i}{2} \text{Tr} \ln(iD^{-1}) \]
\[-i \left\{ \text{1PI vacuum diagrams with the action } I[\phi + \bar{\phi}] - I[\bar{\phi}] - \phi \frac{\partial I[\bar{\phi}]}{\partial \bar{\phi}} \big|_{\phi=\bar{\phi}} \right\}, \]
(C-13)

where \( \bar{\phi} \equiv G_4 \), \( I[\phi] \) is the action functional of the model, and \( D \) is the propagator defined by the quadratic part of \( I[\phi + \bar{\phi}] \) with respect to the field \( \phi \). Note that \( I_1 \) in Fig. C.2 is written in terms of the bare propagator. The correction of the mass term perturbatively appears in the figure, which can be summed up into the propagator \( D \) in (C-13). Equation (C-13) is the well-known expression of effective action given by Jackiw.2)

\[
\Gamma_1 = \frac{1}{2} G_4 e^{G_2^0} G_4 - i \left\{ \begin{array}{c}
\text{tree} \\
+ \text{one-loop} \\
+ \text{higher order loop}
\end{array} \right. \]

Fig. C.2. Effective action \( \Gamma_1 \) for \( J_3 = J_4 = 0 \) in the case of \( A\phi^4 \) theory. A solid line is \( G_{bare} = (G_2^0)_{bare} \) and a dotted line is \( G_4 \). A four-point vertex is given by the original vertex \( iv_4 = iv_4^\circ \) of the model.

C.2. Legendre transformation for two-body channel

Next we want to express \( v_2(\equiv \Gamma^{G_2^0} - 1) \) and \( F_2[\ldots, v_2, \ldots] \) as functionals of \( \tilde{G}_2 \). For this purpose, we further analyze the diagrams of \( \kappa^{(1)} \).

Consider a set of \( m \) internal lines included in a diagram of \( \kappa^{(1)} \). This set is called a cycle of lines (of multiplicity \( m \)), if the diagram is disconnected by cutting any two lines of the set. Removal of \( m \) lines of the cycle separates the diagram into \( m \) disconnected parts. A 1- and 2-particle irreducible (1, 2PI) diagram is then defined as a diagram of \( \kappa^{(1)} \) with no cycle of multiplicity \( m \geq 1 \). (A diagram with a cycle of multiplicity \( m = 1 \) takes a "tea cup"-like form whose handle is a line of the cycle.) The class of all 1, 2PI 0-diagram is denoted as \( \kappa^{(0)}(G_1, G_2^0) \). The class of 1, 2PI 2-diagram is obtained by opening one line in all possible ways in the diagrams of \( \kappa^{(2)}(G_1, G_2^0) \). Then the general connected 2-diagram or \( \tilde{G}_2(i, j) \) is expressed as follows,

\[
\tilde{G}_2(i, j) = G_2^0(i, j) + G_2^0(i, i') K_2(i', j'; G_2) \tilde{G}_2(j', j), \quad \text{(C-14)}
\]

where \( K_2 \) is the mass operator,
Now the diagrams of $\kappa^{(1)}$ are precisely classified. For this purpose, the following topological relation is used

$$N(c) - N(l) + N(\kappa^{(2)}) = 1,$$  \hspace{1cm} (C·16)

where $N(c)$ is the number of cycles of lines, $N(l)$ the number of lines, and $N(\kappa^{(2)})$ the number of 1, 2PI skeletons similarly introduced as in the previous case.

**Example of (C·16):** Consider the graph of Fig. C.3. In the graph, $N(l) = 30$, $N(c) = 25$, $N(\kappa^{(2)}) = 6$. Thus leading to (C·16). To get $N(c)$ here, we note the sets of lines $(l_1, l_2, n_1, n_2, k_1, k_2, k_3, k_4)$ for $m = 2, 2, 4$ cycles respectively. Since there are three sets they make $N(c) = 3$. Other lines constitute $m = 1$ cycles by itself therefore they contribute $N(c) = 22$. As for $N(\kappa^{(2)})$, the parts encircled by thin circles, A ~ F, are the skeleton parts so that $N(\kappa^{(2)}) = 6$.

General proof of (C·16) goes as follows. Let the number of $m$-cycle be $N(c, m)$ then we have

$$N(l) = N(c, 1) + 2N(c, 2) + \cdots + mN(c, m) + \cdots,$$

$$N(c) = N(c, 1) + N(c, 2) + \cdots + N(c, m) + \cdots.$$

Therefore

$$N(l) - N(c) = N(c, 2) + 2N(c, 3) + \cdots + (m-1)N(c, m) + \cdots,$$

which is equal to $N(\kappa^{(2)}) - 1$ as one can convince oneself by generalizing the example of Fig. C.3.

Consider now the sum of all distinct 0-diagrams where one cycle of lines is distinguished in all possible ways,

$$\frac{1}{2} \sum_{m=1}^{m} \frac{1}{m} [G_2^0 K_2]^m = -\frac{1}{2} \text{Tr} \ln [1 - G_2^0 K_2],$$  \hspace{1cm} (C·17)

which represents $\kappa^{(1)}$ but is weighted by $N(c)$. If we distinguish one line, the 0-diagrams are weighted by $N(l)$ and are represented by

$$\frac{1}{2} [G_2^0]^{-1}(i, i') \tilde{G}_2(i', j) [G_2^0]^{-1}(j, j') G_2(j', i) = \frac{1}{2} [G_2^0]^{-1}(i, i') \tilde{G}_2(i', i).$$  \hspace{1cm} (C·18)

In the same way, if we distinguish one 1, 2PI skeleton, we get

$$\kappa^{(2)}(G_1, \tilde{G}_2),$$  \hspace{1cm} (C·19)
\[ \Gamma_2 = \frac{1}{2} G_1 G_2^0 G_1 \]  
\[ - \frac{i}{2} \left[ \text{tree} \right] + \frac{i}{2} \left[ \text{one-loop} \right] + \frac{i}{2} \left[ \text{higher order loop} \right] \]

Fig. C.4. Effective action \( \Gamma_2 \) for \( J_5 = 0 \) in the case of \( \lambda \phi^4 \)-theory. Similar notations are employed as in Fig. C.2 except for a solid line, which represents \( \bar{G}_2 \) in this case. The graphically represented terms come from \( \kappa^{(2)} \)-part of the effective action (C.22). Note that \( K^{(0)} \) includes the tree term.

which is \( \kappa^{(1)} \) but is weighted by \( N(\kappa^{(0)}) \). Combining these expressions with (C.14) and (C.16), we then obtain

\[ \kappa^{(1)} = \frac{1}{2} \text{Tr} \left( \ln \tilde{G}_2 - \ln G_2^0 \right) - \frac{1}{2} \text{Tr} \left( [G_2^0]^{-1} \tilde{G}_2 \right) + \kappa^{(2)}(G_1, \tilde{G}_2), \tag{C.20} \]

which gives

\[ F_2[G_1, \tilde{G}_2, v_3] = F_1[G_1, v_2, v_3] - \frac{1}{2i} \text{Tr} \left( [G_2^0]^{-1} \tilde{G}_2 \right) \left( \tilde{G}_2(j, k) + G_2(j) G_2(k) \right) \]

\[ = - \frac{i}{2} \text{Tr} \ln \tilde{G}_2 - i \kappa^{(2)}(G_1, \tilde{G}_2). \tag{C.21} \]

Here irrelevant constant term has been omitted. From (C.3b), the effective action is now derived in the form,

\[ \Gamma_2[G_1, \tilde{G}_2, J_5] = v_3(j) G_1(j) G_2(j, k) \]

\[ - \frac{i}{2} \text{Tr} \ln \tilde{G}_2 - i \kappa^{(2)}(G_1, \tilde{G}_2). \tag{C.22} \]

For the case of the \( \lambda \phi^4 \)-theory, the result becomes as in Fig. C.4 by conveniently setting \( J_5 = 0 \). After a proper recombination of (C.22) as shown in Fig. C.4, we can write the result in the form,

\[ \Gamma[\phi, G] = I[\phi] + \left( \frac{i}{2} \text{Tr} \ln G^{-1} + \frac{i}{2} \text{Tr} D^{-1} G \right) \]

\[ - i(1, 2\Pi) \text{ vacuum diagrams constructed with propagator } G \]

\[ \text{and the vertices of } I[\phi + \bar{\phi}], \tag{C.23} \]

where \( \bar{\phi} = G_1, G = \tilde{G}_2, I \) is the action functional of the model, and \( D \) is the bare propagator given by the quadratic part of \( I[\phi + \bar{\phi}] \). Equation (C.23) is the rule of Cornwall-Jackiw-Tomboulis.\(^{35,40} \)

Note that \( \kappa^{(2)} \) in (C.22) includes the tree term.

C.3. Legendre transformation for three-body channel

We come next to the final step, where \( v_3 \) and \( F_3[\cdots, \cdots, v_3] \) are expressed as functionals of \( C_3 \) or the sum of all distinct amputated (connected) 3-diagrams.
Consider a set of three lines in a 1, 2PI 0-diagram (\(\kappa^{(3)}\)). This set is called an articulation triplet if the diagram is separated into two disconnected parts by cutting all three lines. If one and only of the disconnected parts is a single \(v_3\)-vertex, the articulation line is said to be trivial. A 1-, 2- and 3-particle irreducible (1, 2, 3PI) 0-diagram is defined as a diagram of \(\kappa^{(3)}\) having only trivial articulation triplet. Let us examine the class of all 1, 2, 3PI 0-diagram, which is similarly represented as \(\kappa^{(3)}(G_1, \tilde{G}_2, iv_3)\). By convention, \(\kappa^{(3)}\) does not include the contribution of 0-diagram built out of a single \(v_3\)-vertex. The 1, 2, 3PI 3-diagram \(K_3(i, j, k; iv_3)\) is defined correspondingly

\[
K_3(i', j', k'; iv_3)(\tilde{G}_2(i', i))\tilde{G}_2(j', j)(\tilde{G}_2(k', k)) = \frac{3!}{\delta(\tilde{G}_2(i', i) \tilde{G}_2(j', j) \tilde{G}_2(k', k))} \cdot \delta(G_1, \tilde{G}_2, iv_3) . \tag{C·24}
\]

Then we can write

\[
C_3(i, j, k) = iv_3(i, j, k) + K_3(i, j, k; C_3) , \tag{C·25}
\]

which iteratively generates the three-particle reducible diagrams written in terms of the original \(v_3\)-vertex.

To obtain \(F_3\) as a functional of \(C_3\), the topological method is employed again. The proper weight of 0-diagram belonging \(\kappa^{(3)}\) is constructed by the relation,

\[
-N(\text{art } l) + N(\kappa^{(3)}) + N(v_3) = 1 . \tag{C·26}
\]

\(N(\text{art } l)\) is the number of articulation triplet, \(N(\kappa^{(3)})\) is the number of 1, 2, 3PI skeletons, and \(N(v_3)\) is the number of \(v_3\)-vertices.

Example of (C·26): Consider Fig. C.5. The white circles in Fig. C.5 are 1, 2PI. Here \(N(\text{art } l) = 5, N(v_3) = 3, N(\kappa^{(3)}) = 3\), thus leading to (C·26). We have assumed that the shaded circle does not contain articulation triplet or \(v_3\).

The general proof goes through in a similar way as in (C·6). The diagrams of \(\kappa^{(3)}\) is then summed up in proper weight as follows,

\[
\kappa^{(3)} = -\frac{1}{2} \frac{1}{3!} C_3(i, j, k) \tilde{G}_2(i, i') \tilde{G}_2(j, j') \tilde{G}_2(k, k') C_3(i', j', k')
\]
\[ + \frac{i}{3!} v_3(i, j, k) G_3(i, j, k) + \kappa^{(3)}(G_1, \tilde{G}_2, C_3), \]  

where we have distinguished one articulation triplet, one 1, 2, 3PI skeleton, and one \( v_3 \)-vertex, respectively in constructing each term of (C·27). \( F_3 \) is now obtained as

\[
F_3[G_1, \tilde{G}_2, C_3] = F_3[G_1, \tilde{G}_2, v_3] - \frac{i}{3!} v_3(i, j, k) G_3(i, j, k)
= - \frac{i}{2} \text{Tr} \ln \tilde{G}_2 + \frac{i}{2} \frac{1}{3!} C_3(i, j, k) \tilde{G}_2(i, i') \tilde{G}_2(j, j') \tilde{G}_2(k, k') C_3(i', j', k')
- i \kappa^{(3)}(G_1, \tilde{G}_2, C_3).
\]

Combining with (C·3c), we get

\[
I_3[G_1, \tilde{G}_2, C_3] = v_1^g(j) G_1(j) + \frac{1}{2!} v_2^g(j, k) G_2(j, k) + \frac{1}{3!} v_3^g(j, k, l) C_3(j, k, l)
- \frac{i}{2} \text{Tr} \ln \tilde{G}_2 + \frac{i}{2} \frac{1}{3!} C_3(i, j, k) \tilde{G}_2(i, i') \tilde{G}_2(j, j') \tilde{G}_2(k, k') C_3(i', j', k')
- i \kappa^{(3)}(G_1, \tilde{G}_2, C_3).
\]

Effective action (C·29) defined with three-body operators is not familiar in particle physics. However, the result is important especially when one derives the QCD effective action to examine the basic three quark or anti-quark channels as is discussed in § 4.1. The formula is also used in three electron atomic system in § 8.1.

The above results are also applicable when various fields are taken into account. In such cases, the subscript \( j \) of \( \phi_j \) in (3·1·1) denotes the species of the field as well as other degrees of freedom. If the Grassmann number fields \( \phi_1, \phi_2, \cdots \) are further considered besides the bosonic ones \( \phi_1, \phi_2, \cdots \), the field \( \phi \) in (3·1·1) is written as \( \phi = (\phi_1, \phi_2, \cdots, \phi_1, \phi_2, \cdots) \), or as the form of super vector. Starting with this type of field in general, \( \text{Tr} \ln \tilde{G}_2 \) in (C·22) or (C·29) is naturally replaced by \( \text{STr} \ln \tilde{G}_2 \) where \( \tilde{G}_2 \) is given in the form of supermatrix and \( \text{STr} \) represents the supertrace. With other additional sign factors required to obtain the correct vacuum diagrams, the corresponding effective actions for QCD and atomic system are explicitly written and discussed in Chapters IV and VIII respectively.

The Legendre transformation of four-body channel is rather complicated but the result is known.\(^1\),\(^6\) Up to now the formula for \( n \)-body (\( n \geq 5 \)) is unknown.

References

Appendix D

--- In-Field Out-Field Formalism ---

In this appendix, in or out-field formalism for non-relativistic case is explained. Originally it was invented for the scattering problem of relativistic field theory but actually it can be applied for non-relativistic case also. The formalism relates the scattering matrix element to the residue of the pole of the Green’s functions and is used in § 8.4. Below we discuss separately the case of Hermite and non-Hermite field and use the space-time notation \( x = (t, \mathbf{x}) = (x_0, \mathbf{x}) \). Let us start with the review of the field quantization.

D.1. Quantization formula — Hermite field case

The Hermite field, like phonon or photon field, is denoted by \( \phi(x) \) which satisfies \( \phi^\dagger(x) = \phi(x) \). Here \( \dagger \) implies the Hermite conjugation. The symbol \( \hat{\phi} \) to denote the operator is not used below since only the field operator appears in this appendix. The Lagrangian \( L \) of the system is written by the integral of the density \( \mathcal{L} \) which is the sum of free part and interacting part (we use in this appendix \( \mathcal{L} \) to denote the density),

\[
L = \int d^3x \mathcal{L} = \int d^3x (\mathcal{L}_0 + \mathcal{L}').
\]  (D.1)

The free and interacting part are written as follows,

\[
\mathcal{L}_0 = \frac{1}{2} \{ \phi(x)^2 - \phi(x)\omega^2(-\nabla^2)\phi(x) \},
\]  (D.2)

\[
\mathcal{L}' = \mathcal{L}'(\phi(x)),
\]  (D.3)

where \( \hat{\phi} = (\partial/\partial t)\phi = \partial_0 \phi \). The notation \( \omega(-\nabla^2) \) represents the dispersion relation of \( \phi \) field. The canonical momentum is defined to be

\[
\Pi(x, t) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x, t)}.
\]  (D.4)

At equal time, we have fundamental canonical commutation relations as follows,

\[
[\Pi(x, t), \phi(y, t)] = \frac{1}{i} \delta^3(x - y),
\]

\[
[\Pi(x, t), \Pi(y, t)] = [\phi(x, t), \phi(y, t)] = 0.
\]  (D.5)

Now the time evolution is governed by Euler-Lagrange equation of motion,

\[
\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)} - \frac{\partial \mathcal{L}}{\partial \phi(x)} = 0.
\]  (D.6)

In the case considered here it takes the form,
\[ (\partial^2 - \omega^2(-\nabla^2))\phi(x) - \frac{\partial L'}{\partial \phi(x)} = 0. \quad \text{(D\cdot7)} \]

**Free case:** For free case the equation of motion (D\cdot7) can be solved as follows,

\[ \phi(x) = \sum_k \frac{1}{\sqrt{2\sqrt{k_0}}} (a_k e^{-ikx} + a_k^* e^{ikx}), \quad \text{(D\cdot8)} \]

\[ \Pi(x) = \phi(x) = \sum_k \frac{-ik_0}{\sqrt{2\sqrt{k_0}}} (a_k e^{-ikx} - a_k^* e^{ikx}), \quad \text{(D\cdot9)} \]

where \( k = (k_0, k) \) with \( k_0 = \omega_k = \omega(k^2) \) and \( kx = k_0 x_0 - k \cdot x \). \( \sum_k \) implies the sum over \( k = (2\pi/L)(n_x, n_y, n_z) \) where \( V = L^3 \) and \( n_{x,y,z} = 0, \pm 1, \pm 2, \ldots \). By solving (D\cdot8) and (D\cdot9) for \( a_k \) or \( a_k^* \), we get

\[ [a_k, a_{k'}] = \delta_{k,k'}, \quad [a_k, a_k^*] = [a_k^*, a_k^*] = 0, \quad \text{(D\cdot10)} \]

\[ a_k = -\frac{i}{\sqrt{2\sqrt{k_0}}} \int d^3 x e^{ikx} \frac{\partial}{\partial \phi_0} \phi(x), \quad \text{(D\cdot11)} \]

where \( \delta_0 = \overline{\delta_0} = -\overline{\delta_0} \) with \( \overline{\delta_0(\delta_0)} \) indicating that the time derivative acts on the right (left). It is easy to check that the right-hand side of the formula (D\cdot11) is indeed time independent. We have of course similar equation as (D\cdot11) for \( a_k^* \). The Hamiltonian is calculated by using the standard formula,

\[ H = \int d^3 x \left\{ \frac{\partial L_0}{\partial \dot{\phi}_0} \phi(x) - L_0 \right\} = \sum_k \omega_k a_k^* a_k. \quad \text{(D\cdot12)} \]

**D.2. Quantization of field — non-Hermite case**

Let us write non-Hermite field, like electron or atoms, by \( \psi(x) \). The Bosonic and Fermionic case can be discussed simultaneously. Let us assume the Lagrangian of the form (D\cdot1) with

\[ L_0 = i\psi^*(x) \dot{\psi}(x) - \psi^*(x) \omega(-\nabla^2) \psi(x), \quad \text{(D\cdot13)} \]

\[ L' = L'('\psi(x), \phi^*(x)) \].

Instead of (D\cdot13) we can take explicitly Hermitian form for the term involving time derivative,

\[ \frac{i}{2} \psi^*(x) \overline{\delta_0} \phi(x), \quad \text{(D\cdot15)} \]

but this is equivalent to \( i\psi^*(x) \dot{\psi}(x) \) because both give the same equation of motion. Note here that the difference is written as a total time derivative which does not affect Euler-Lagrange equation. The canonical momentum is now given by

\[ \Pi(x) = \frac{\delta L'}{\delta \dot{\phi}(x)} = -i\kappa \psi^*(x), \quad \text{(D\cdot16)} \]

\[ [-i\kappa \psi^*(x, t), \psi(x, t)]_\epsilon = \frac{1}{\epsilon} \delta^3(x-y), \quad \text{(D\cdot17)} \]
\[ \{ \partial_\nu, -\partial^2 \}\phi(x) - \overline{\partial} \frac{\partial F}{\partial \overline{\phi}^\nu(x)} = 0. \]  \hfill (D.19)

**Free case:** The formulas for the case of the free field are summarized below,

\[ \phi(x) = \sum_k \frac{e^{-ikx}}{\sqrt{V}} b_k, \]  \hfill (D.20)

\[ [b_k, b_k^\dagger] = \delta_{k,k'}, \quad [b_k, b_{k'}] = [b_k^\dagger, b_{k'}] = 0, \]  \hfill (D.21)

\[ H = \int d^3x \phi^\dagger(x) \omega(-\partial^2) \phi(x) = \sum_k \omega_k b_k b_k^\dagger. \]  \hfill (D.22)

In particular, the following inverse formula of (D.20) becomes important in the discussion that follows,

\[ b_k = \int d^3x \frac{e^{ikx}}{\sqrt{V}} \phi(x), \]  \hfill (D.23)

and similarly for \( b_k^\dagger \).

**D.3. In-field or out-field formalism**

In the presence of interaction, field obeys Eq. (D.7) or (D.19) which cannot be solved in general. In the actual situation of the scattering experiment, however, incoming or outgoing particles are described by wave packets and are well separated in space from each other. In such a situation incoming particles, prepared at \( t = -\infty \), can be thought of as free particles that are annihilated or created by field operator which obeys free field equation. We call this operator as incoming field. Similarly we define outgoing field at \( t = +\infty \). Explicitly they are introduced as

\[ \phi(x) \rightarrow \begin{cases} \sqrt{Z} \phi_{\text{in}}(x), & (t \rightarrow -\infty) \\ \sqrt{Z} \phi_{\text{out}}(x), & (t \rightarrow +\infty) \end{cases} \]  \hfill (D.24)

\[ \phi(x) \rightarrow \begin{cases} \sqrt{Z'} \phi_{\text{in}}(x), & (t \rightarrow -\infty) \\ \sqrt{Z'} \phi_{\text{out}}(x), & (t \rightarrow +\infty) \end{cases} \]  \hfill (D.25)

Here \( Z, Z' \) represent the wave function renormalization factors. Since in or out-field satisfies the free field equation, it can be expanded as follows,

\[ \phi_{\text{in(out)}}(x) = \sum_k \frac{1}{\sqrt{2V}k_0} (a_k^{\text{in(out)}} e^{-ikx} + a_k^{\text{in(out)}} e^{ikx}), \]  \hfill (D.26)

\[ \phi_{\text{in(out)}}(x) = \sum_k \frac{e^{-ikx}}{\sqrt{V}} b_k^{\text{in(out)}}. \]  \hfill (D.27)
Here $k_0 = \omega_k$ and similar expression holds for $\phi^\dagger(x)$ of course. Creation or annihilation operators satisfy the usual commutation relations,

$$ [a_k^{\text{in}}, a_k^{\text{in}}] = \delta_{k,k'}, \quad [a_k^{\text{in}}, a_k^{\text{out}}] = [a_k^{\text{out}}, a_k^{\text{in}}] = 0 . \tag{D·28} $$

The same relations hold for out-field and also for $b_k$ with the replacement $[\ ,\ ]$ by $[\ ,\ ]_k$. The inversed relations are

$$ a_k^{\text{in(out)}} = \frac{i}{\sqrt{2Vk_0}} \int d^3 x e^{ikx} \frac{x}{\partial_0 \phi_{\text{in(out)}}(x)} , \tag{D·29} $$

$$ b_k^{\text{in(out)}} = \frac{1}{\sqrt{V}} \int d^3 x e^{ikx} \phi_{\text{in(out)}}(x) , \tag{D·30} $$

and the same expression for $a_k^{\text{in(out)}}$ or $b_k^{\text{in(out)}}$.

Now the state is defined. The vacuum (i.e., no-particle) state $|0\rangle$ is the state which is annihilated by both in and out annihilation operator,

$$ a_k^{\text{in(out)}} |0\rangle = 0 . \tag{D·31} $$

One particle state is the same state whether it is created by in or out operator, since there is no scattering if only one particle is present,

$$ |k\rangle = a_k^{\text{in}} |0\rangle = a_k^{\text{in(out)}} |0\rangle . \tag{D·32} $$

For multi-particle state we have to distinguish between in and out state,

$$ |k_1, k_2\cdots k_n; \text{in(out)}\rangle = a_k^{\text{in(out)}} a_k^{\text{in(out)}} \cdots a_k^{\text{in(out)}} |0\rangle . \tag{D·33} $$

In the case of non-Hermite field and also for the case where both Hermite and non-Hermite field are present, the definition of the state is given in a similar way. The scattering amplitude is the inner product of in and out states of (D·33).

D.4. Reduction formula — Hermite field

Let us start from the scattering matrix element,

$$ \langle p_1, p_2\cdots p_m; \text{out}|k_1, k_2\cdots k_n; \text{in} \rangle $$

$$ = \langle p_1, p_2\cdots p_m; \text{out}|a_k^{\text{in}}|k_2\cdots k_n; \text{in} \rangle $$

$$ = \langle p_1, p_2\cdots p_m; \text{out}|a_k^{\text{out}}|k_2\cdots k_n; \text{in} \rangle + \langle p_1\cdots p_m; \text{out}|(a_k^{\text{in}} - a_k^{\text{out}})|k_2\cdots k_n; \text{in} \rangle . \tag{D·34} $$

The first term on the right-hand side of (D·34) survives only when one of the momenta $p_1, p_2\cdots$ is equal to $k_1$. Diagrammatically it corresponds to a disconnected graph which is excluded in the following discussions. The second term is rewritten by using (D·29) as

$$ -i \frac{1}{\sqrt{2Vk_{10}}} \int d^3 x e^{-ik_1 x} \partial_0 \phi_{\text{in}}(x) - \phi_{\text{out}}(x) |k_2\cdots k_n; \text{in} \rangle $$

$$ = i \frac{1}{\sqrt{2ZVk_{10}}} \left( \lim_{t \to -\infty} - \lim_{t \to +\infty} \right) \int d^3 x e^{-k_1 x} \partial_0 \phi(x) |k_2\cdots k_n; \text{in} \rangle $$

$$ = i \frac{1}{\sqrt{2ZVk_{10}}} \left( \lim_{t \to -\infty} - \lim_{t \to +\infty} \right) \int d^3 x e^{-k_1 x} \partial_0 \phi(x) |k_2\cdots k_n; \text{in} \rangle $$
\[ = \frac{i}{\sqrt{2ZV\kappa_0}} \int d^4x \partial_\alpha e^{-i\kappa_1 x^\alpha} \partial_\alpha \langle p_1 \cdots p_m; \text{out}|\phi(x)|k_2 \cdots k_n; \text{in} \rangle \]

\[ = \frac{i}{\sqrt{2ZV\kappa_0}} \int d^4x e^{-i\kappa x} (\delta^2 + \kappa_0^2) \langle p_1, \cdots p_m; \text{out}|\phi(x)|k_2 \cdots k_n; \text{in} \rangle, \quad (D\cdot35) \]

where we have introduced the notation \( \int d^4x = \int dt \int d^3x \). This is one-particle reduction formula in which one particle is reduced to the operator \( \phi(x) \). The reduction of the second particle goes as follows,

\[ \langle p_1, p_2 \cdots p_m; \text{out}|\phi(x)|k_2, \cdots k_n; \text{in} \rangle \]

\[ = \langle p_2, \cdots p_m; \text{out}|a_{p_i}^{\text{out}} \phi(x)|k_2 \cdots k_n; \text{in} \rangle \]

\[ = \langle p_2 \cdots p_m; \text{out}|\phi(x) a_{p_i}^{\text{out}}|k_2 \cdots k_n; \text{in} \rangle \]

\[ + \langle p_2 \cdots p_m; \text{out}||a_{p_i}^{\text{out}} \phi(x) - \phi(x) a_{p_i}^{\text{out}}||k_2 \cdots k_n; \text{in} \rangle. \quad (D\cdot36) \]

The first term represents the disconnected piece and is neglected in the following. Now the second term is transformed with the help of \( (D\cdot29) \) as

\[ \frac{i}{\sqrt{2Vp_{10}}} \int d^3y e^{ip_{10} y} \delta_{y_0} \langle p_2 \cdots p_m; \text{out}|\phi(y) \phi(x) - \phi(x) \phi(y)||k_2 \cdots k_n; \text{in} \rangle. \]

\[ (D\cdot37) \]

Here we utilize the fact that formula \( (D\cdot29) \) is independent of time and the expression inside \( \{ \cdots \} \) can be rewritten as follows,

\[ \frac{1}{\sqrt{Z}} \left( \lim_{y_0 \to +\infty} \phi(y) \phi(x) - \lim_{y_0 \to -\infty} \phi(y) \phi(x) \right) = (\lim_{y_0 \to +\infty} - \lim_{y_0 \to -\infty}) T \phi(y) \phi(x). \]

\[ (D\cdot38) \]

We have introduced here the time-ordering operation

\[ T \phi(y) \phi(x) = \theta(y_0 - x_0) \phi(y) \phi(x) + \theta(x_0 - y_0) \phi(x) \phi(y). \]

\[ (D\cdot39) \]

Therefore Eq. \( (D\cdot37) \) is transformed into

\[ \frac{i}{\sqrt{2ZVp_{10}}} \int d^4y \partial_\alpha \left( e^{ip_{10} y} \delta_{y_0} \right) \langle p_2 \cdots p_m; \text{out}|T \phi(y) \phi(x)|k_2 \cdots k_n; \text{in} \rangle \]

\[ = \frac{i}{\sqrt{2ZVp_{10}}} \int d^4y e^{ip_{10} y} (\delta_{y_0} + \kappa_{10}) \langle p_2 \cdots p_m; \text{out}|T \phi(y) \phi(x)|k_2 \cdots k_n; \text{in} \rangle. \quad (D\cdot40) \]

The final formula for two-particle reduction is, apart from disconnected diagrams,

\[ \langle p_1, p_2 \cdots p_m; \text{out}|k_1, k_2 \cdots k_n; \text{in} \rangle \]

\[ = \frac{i^2}{\sqrt{2ZV\kappa_0} \sqrt{2ZVp_{10}}} \int d^4x \int d^4y e^{-i\kappa x} e^{ip_{10} y} \]

\[ \times (\delta^2 + \kappa_{10}^2)(\delta_{y_0} + \kappa_{10}) \langle p_2 \cdots p_m; \text{out}|T \phi(y) \phi(x)|k_2 \cdots k_n; \text{in} \rangle. \quad (D\cdot41) \]

It is straightforward to generalize the formula to the one where all the particles are reduced, which is the reduction formula we are looking for.
\[ \langle p_1, p_2 \cdots p_m; \text{out}|k_1, k_2 \cdots k_n; \text{in} \rangle = \prod_{i=1}^{n} \prod_{j=1}^{m} \int \frac{i d^4 x_i}{\sqrt{2 Z V k_{i0}}} \int \frac{i d^4 y_j}{\sqrt{2 Z V p_{j0}}} e^{-i k_i x_i} e^{i p_j y_j} \left( \partial_{x_{i0}}^2 + k_{i0}^2 \right) \left( \partial_{y_{j0}}^2 + p_{j0}^2 \right) \]
\[ \times \langle 0|T \phi(y_1) \phi(y_2) \cdots \phi(y_m) \phi(x_1) \phi(x_2) \cdots \phi(x_n)|0 \rangle. \] (D.42)

D.5. Reduction formula — non-Hermite field

The case of non-Hermite field can similarly be discussed and only the final formula is given below,

\[ \langle p_1, p_2 \cdots p_m; \text{out}|k_1, k_2 \cdots k_n; \text{in} \rangle = \left( \frac{i}{\sqrt{2 Z V}} \right)^{n+m} \prod_{i=1}^{n} \prod_{j=1}^{m} \int d^4 x_i \int d^4 y_j e^{-i k_i x_i} e^{i p_j y_j} \left( i \partial_{x_{i0}} + k_{i0} \right) \left( -i \partial_{y_{j0}} + p_{j0} \right) \]
\[ \times \langle 0|T \phi(y_m) \phi(y_{m-1}) \cdots \phi(y_1) \phi^*(x_1) \phi^*(x_2) \cdots \phi^*(x_n)|0 \rangle. \] (D.43)

The order of field operator inside \{\cdots\} is important for fermionic case. It will not be necessary to write down the formula here in the case where both Hermite and non-Hermite field are present.

D.6. Reduction formula in terms of Green's functions

Let us write (D.42) in terms of Green's functions only. For this purpose we introduce the wave function

\[ \phi(x) \equiv \langle 0|\phi(x)|k \rangle = \sqrt{Z} \langle 0|\phi_{\text{in(out)}}(x)|k \rangle = \sqrt{Z} \frac{-i}{2 V k_0} e^{-i k x}, \] (D.44)

and its complex conjugate. The propagator is defined as

\[ W^{(2)}(x, y) = \langle 0|T \phi(x) \phi(y)|0 \rangle. \] (D.45)

The pole part of \( W^{(2)} \) comes from the contribution of the one particle state, and has the form,

\[ W^{(2)}(x, y) \sim Z \langle 0|T \phi_{\text{in(out)}}(x) \phi_{\text{in(out)}}(y)|0 \rangle = Z \frac{i}{V} \sum_k \int d k_0 \frac{e^{i k (x-y)}}{2 \pi k_0^2 - \omega_k^2}. \] (D.46)

Its inverse

\[ (W^{(2)})^{-1}(x, y) = \frac{i}{Z} \left( \partial_{x_0}^2 + \omega_k^2 \right) \delta^4(x-y) \] (D.47)

is inserted into (D.42) in place of \( (\partial_{x_0}^2 + \omega_k^2) \). This is allowed because, owing to the presence of the on-shell wave function \( e^{-i k x} \), only the pole part of \( W^{(2)}(x, y) \) shown in (D.46) gives contribution to (D.42). Thus we get, the factor \( Z \) and \( i \) being cancelled
\[ \langle \rho_1, \rho_2 \cdots \rho_m ; \text{out} | k_1, k_2 \cdots k_n ; \text{in} \rangle = \prod_{i=1}^{n} \prod_{j=1}^{m} \int \cdots \int d^4x_i d^4x_j d^4y_i d^4y_j \Phi_{k_i}(x_i) \Phi_{p_j}(y_j) \]
\[ \times (W^{(2)})^{-1}(x_i, x_j)(W^{(2)})^{-1}(y_i, y_j) W^{(n+m)}(x_1, x_2 \cdots x_n ; y_1, y_2 \cdots y_m) , \]  

(D.48)

where we have introduced

\[ W^{(n+m)}(x_1, x_2 \cdots ; y_1, y_2 \cdots) = \langle 0 | T \phi(x_1) \phi(x_2) \cdots \phi(x_n) \phi(y_1) \phi(y_2) \cdots \phi(y_m) | 0 \rangle . \]  

(D.49)

For non-Hermite field similar formula holds. In terms of Green’s function, it can be written as follows. Let us introduce

\[ \Psi_k(x) = \langle 0 | \psi(x) | k \rangle = \sqrt{Z} \langle 0 | \psi_{in}(x) | k \rangle = \sqrt{Z} \frac{1}{\sqrt{V}} e^{-i k x}, \]  

(D.50)

\[ W^{(2)}(x, y) = \langle 0 | T \phi(x) \phi^\dagger(y) | 0 \rangle , \]  

(D.51)

\[ W^{(n+m)}(y_m, y_{m-1} \cdots ; x_1, x_2 \cdots x_n) = \langle 0 | T \phi(y_m) \phi(y_{m-1}) \cdots \phi(y_1) \phi^\dagger(x_1) \phi^\dagger(x_2) \cdots \phi^\dagger(x_n) | 0 \rangle . \]  

(D.52)

Then the reduction formula in this case is

\[ \langle \rho_1, \rho_2 \cdots ; \text{out} | k_1, k_2 \cdots ; \text{in} \rangle = \prod_{i=1}^{n} \prod_{j=1}^{m} \int \cdots \int d^4x_i d^4x_j d^4y_i d^4y_j \Psi_k(x_i) \Psi_{p_j}(y_j) \]
\[ \times (W^{(2)})^{-1}(y_i, y_j)(W^{(2)})^{-1}(x_i, x_j) W^{(n+m)}(y_1, y_2 \cdots ; x_1, x_2 \cdots x_n) . \]  

(D.53)

Here we have used the following representation for the pole part of \( W^{(2)} \) and its inverse \( (W^{(2)})^{-1} \),

\[ W^{(2)}(x, y) \sim Z' \frac{i}{V} \sum_k \int \frac{dk_0}{2\pi} \frac{e^{-i k x}}{k_0 - \omega_k} , \]  

(D.54)

\[ (W^{(2)})^{-1}(x, y) \sim \frac{i}{Z} (-i \partial_{x_0} + \omega(-\nabla^2)) \delta^4(x-y) . \]  

(D.55)

Note the order of field operator for Fermi case which is in accordance with the state definition of (D.33) with \( a_k^\dagger \) replaced by \( b_k^\dagger \).

D.7. **Multicomponent field and composite bound state**

In case the particle has extra degrees of freedom other than the space-time variable \( x \), spin for example, the field becomes multicomponent which is written as \( \phi_j(x) \) or \( \phi_j(x) \). The index \( j \) does not necessarily coincide with the index \( l \) which specifies the correct \( l \)-th mode and we have to perform a rotation from \( \phi_j(x) \) or \( \phi_j(x) \) to the field of eigen-channel \( \phi^{(i)}(x) \) or \( \phi^{(i)}(x) \),
\[ \phi_j(x) = O_{jl} \phi^{(l)}(x), \quad (D\cdot56) \]
\[ \phi_j(x) = U_{jl} \phi^{(l)}(x). \quad (D\cdot57) \]

The sum has to be taken here over mode index \( l \). Both \( \phi_j \) or \( \phi \) and \( \phi^{(l)} \) or \( \phi^{(l)} \) are required to satisfy the canonical (anti-) commutation relations at equal time,

\[ [\phi_j(x, t), \phi_k(y, t)]_\epsilon = [\phi^{(l)}(x, t), \phi^{(m)}(y, t)]_\epsilon = \frac{1}{i} \delta^3(x - y) \delta_{jk}, \quad (D\cdot58) \]
\[ [\phi^{(l)}(x, t), \phi^{(m)}(y, t)]_\epsilon = [\phi^{(l)}(x, t), \phi^{(m)}(y, t)]_\epsilon = \frac{1}{i} \delta^3(x - y) \delta_{lm}. \quad (D\cdot59) \]

These relations imply that \( U_{jl} \) is a unitary matrix and, because of the Hermiticity of \( \phi \) field, \( O_{jl} \) is an orthogonal matrix.

The multicomponent system includes an important case of the composite bound state, which is seen as follows. Let us write, for instance, the two-particle composite field \( \phi(x) \phi(y) \) in the following way,

\[ \phi(x) \phi(y) = \phi_j(X). \quad (D\cdot60) \]

Here we have introduced the space-time centre coordinate \( X = (x + y)/2 \) and the relative space-time coordinate \( j = x - y \). The identification of the relative coordinate with the index \( j \) is particularly convenient for our discussions. The same arguments hold for non-Hermite field and also for \( N \)-particle composite field. In this case the index \( j \) signifies all the possible relative coordinates of \( N \)-particle system. Now the channel operator \( \phi^{(l)} \) or \( \phi^{(l)} \) approaches directly to in or out-field of the corresponding channel as \( t \to \pm \infty \),

\[ \phi^{(l)}(x) \to \begin{cases} \sqrt{Z_l} \phi^{(l)}_\text{in}(x), & (t \to -\infty) \\ \sqrt{Z_l} \phi^{(l)}_\text{out}(x), & (t \to \infty) \end{cases} \quad (D\cdot61) \]
\[ \phi^{(l)}(x) \to \begin{cases} \sqrt{Z_l} \phi^{(l)}_\text{in}(x), & (t \to -\infty) \\ \sqrt{Z_l} \phi^{(l)}_\text{out}(x), & (t \to \infty) \end{cases} \quad (D\cdot62) \]

The similar expression holds for \( \phi^\dagger \) of course. Now in or out channel-field has the expansion,

\[ \phi^{(l)}_\text{in/\text{out}}(x) = \sum_k \frac{1}{\sqrt{2V\epsilon_k^{(l)}}} \left\{ a_k^{(l)\text{in/\text{out}}} e^{-ik^{\text{out}}x} + a_k^{(l)\text{in/\text{out}}} e^{ik^{\text{out}}x} \right\}, \quad (D\cdot63) \]
\[ \phi^{(l)}_\text{in/\text{out}}(x) = \sum_k \frac{e^{-ik^{\text{out}}x}}{\sqrt{V}} b_k^{(l)\text{in/\text{out}}}. \quad (D\cdot64) \]

We have introduced the notation \( k^{(l)} = k_0^{(l)} t - \mathbf{k} \cdot \mathbf{x}, \quad k_0^{(l)} = \omega^{(l)}(\mathbf{k}^2) \). The dispersion relation \( \omega^{(l)}(\mathbf{k}^2) \) is the energy of \( l \)-th mode with \( \mathbf{k} \) denoting the momentum of center of mass and it includes the binding energy. The inverted relations (D\cdot29) and (D\cdot30) hold if we understand \( a_k^{(l)\text{in/\text{out}}}, b_k^{(l)\text{in/\text{out}}}, \phi^{\text{in/\text{out}}}(x), \phi^{\text{in/\text{out}}}(x) \) and \( k \) as referring to a specific channel \( l \); we have only to attach superscript \( (l) \). We use below the follow-
ing relation written in terms of the original field,
\[
\phi_j(x) \longrightarrow U_{ij} \sqrt{Z_i} \phi_{in}^{(i)} , \quad (t \to -\infty)
\]
and so forth. If we introduce one particle state as
\[
|k^{(i)}\rangle = a_k^{(i)\text{in}} |0\rangle = a_k^{(i)\text{out}} |0\rangle
\]
(likewise for non-Hermite case), then we have
\[
\langle 0 | \phi_{\text{in(out)}}^{(m)}(x) |k^{(i)}\rangle = \delta_i^m \frac{1}{\sqrt{2V_{k_0}^{(i)}}} e^{-ik_0x} ,
\]
(similarly for non-Hermite case with the replacement $\sqrt{2V_{k_0}} \to \sqrt{V}$). The pole part of the inverse of the propagator,
\[
W_{lm}^{(2)}(x, y) = \langle 0 | T \phi^{(i)}(x) \phi^{(m)}(y) |0\rangle
\]
is given by
\[
(W_{lm}^{(2)})^{-1} (x, y) \sim \delta_i^m - \frac{i}{Z_i} (\partial_x^2 + \omega^{(i)}(-\nabla^2)^2) \delta^4(x-y)
\]
The reduction formula in this case is directly written down if we use the channel operator having the index \(l\),
\[
\langle p^{(1)}, p^{(2)}, \ldots | \text{out} | k^{(m_1)} \ldots k^{(m_m)} ; \text{in} \rangle
= \prod_{i=1}^N \frac{1}{\sqrt{2Z_i} V_{k_0}^{(m_i)}} \prod_{i=1}^N \frac{1}{\sqrt{2Z_i} V_{p_0}^{(i)}} \int \cdots \int d^4x_1 d^4y_1 d^4x_2 d^4y_2 e^{-ik_0x_1} e^{ip_0y_1}
\times \frac{1}{Z_{m_1}} (W_{m_1})^{-1}_{m_1 m_1}(x_1, x_1) \frac{1}{Z_{m_2}} (W_{m_2})^{-1}_{m_2 m_2}(y_2, y_2)
\times W_{l_1, \ldots l_m : m_1 \ldots m_m}(y_1, x_1, y_2, x_2, \ldots),
\]
where the summation over \(l_1, l_2, \ldots l_m, m_1, m_2, \ldots m_m\) is implied. We have introduced the notation
\[
W_{l, m_1 \ldots m_m : m_1 \ldots m_m}(y_1, y_2, \ldots x_1, x_2, \ldots)
= \langle 0 | T \phi^{(l_1)}(y_1) \phi^{(l_2)}(y_2) \ldots \phi^{(m_1)}(x_1) \phi^{(m_2)}(x_2) \ldots |0\rangle .
\]
The final form is given which is written by the original field \(\phi_j(x)\). As in the previous case, all the factors \(Z_i\) and orthogonal matrix \(O_{il}\) cancel out. Let us define
\[
\Phi^{(i)}(x) = \langle 0 | \phi_j(x) |k^{(i)}\rangle
= \sum_l O_{il} \langle 0 | \phi^{(l)}(x) |k^{(i)}\rangle
= O_{il} \langle 0 | \phi^{(l)}(x) |k^{(i)}\rangle
= \sqrt{Z_i} O_{il} \langle 0 | \phi^{(l)\text{in(out)}}(x) |k^{(i)}\rangle
\]
In the fourth line of the above equations we have used the fact that for one particle state the operator $\Phi^{(i)}(x)$ can be replaced by $\Phi^{(i)(\text{in-out})}(x)$. In this way we arrive at

$$\langle \Phi^{(i)}(\Phi^{(i)} \cdots \Phi^{(i)}; \text{out} | \mathbf{k}^{(m_1)} \cdots \mathbf{k}^{(m_n)} ; \text{in} \rangle$$

$$= \int \cdots \int dx_1 dx_2 \cdots dy_1 dy_2 \cdots \Phi^{(m_1)}(x_1) \Phi^{(m_2)}(x_2) \cdots \Phi^{(i)}(y_1) \Phi^{(i)}(y_2) \cdots$$

$$\times (W^{(2)})^{-1}_{i' i}(x_1, x_1) \cdots (W^{(2)})^{-1}_{i' i}(y_1, y_1) \cdots W^{(N+M)}_{i' i' \cdots j' j' \cdots} (x_1', x_2', \cdots y_1', y_2', \cdots). \quad (D\cdot73)$$

The definition of $W^{(N+M)}$ here will be obvious and the summation over $i, i' \cdots j, j' \cdots$ is understood. Equation (D\cdot73) is our formula. For non-Hermite field similar formula as (D\cdot53) holds. All we have to do is to replace $\Psi_n(x_i)$ in (D\cdot53) by

$$\Psi^{(i)}(x_i) = \langle 0 | \phi_j(x_i) | \Phi^{(i)} \rangle$$

$$= U_{ji} \sqrt{\frac{Z_i}{2V_{k_0}}} e^{-i\omega_{x_i} x_i} \quad (D\cdot74)$$

and to append necessary indices $i, i' \cdots j, j' \cdots$ to $(W^{(2)})^{-1}$ and $W^{(N+M)}$.

**Appendix E**

---

**Calculation of $W_0[J_1, J_2]$ of Harmonic Oscillator** ---

We show here the calculation of $W_0[J_1, J_2]$, which is the non-interacting case of $W[J_1, J_2]$. The Hamiltonian is (12\cdot4\cdot5) with $\hat{H}$ replaced by $\hat{H}_0$ (i.e., $V(\bar{q})=0$) of (12\cdot4\cdot2). We use the time evolution operator $\hat{R}_0^{J_i} (i=1, 2)$ of this problem and $W_0$ is written as follows,

$$e^{(i\hbar)W_0[J_1, J_2]} = \text{Tr} \{ \hat{R}_0^{J_2} \hat{\rho}_1 (\hat{R}_0^{J_2})' \} \quad (E\cdot1)$$

$$= \int d^Nq_1 d^Nq_2 \rho_0^N(q_1, q_2) \langle q_2 | (\hat{R}_0^{J_2})' \hat{R}_0^{J_1} | q_1 \rangle \quad (E\cdot2)$$

$$= \int d^Nq^+ d^Nq^- \rho_0^N(q_1, q_2) \prod_{k=1}^{N} [ \langle q^+ k | (\hat{R}_0^{J_2})' \hat{R}_0^{J_1} | q^+ k \rangle ], \quad (E\cdot3)$$

because $\hat{R}_0^{J_i}$ is factorized into the products of $\hat{R}_0^{J_k}$ which is the time evolution kernel of the $k$-th harmonic oscillator. The purpose of this appendix is to show the following formula,

$$\langle q^+ k | (\hat{R}_0^{J_2})' \hat{R}_0^{J_1} | q^+ \rangle$$

$$= \delta \left( q^+ - \int_{t_1}^{t_2} dt J_k^-(t) \frac{\sin \omega_k(t-t_1)}{m_k \omega_k} \right)$$

$$\times \exp \left[ \frac{i}{\hbar} \int_{t_1}^{t_2} dt J_k^+ (t) \left( q^+ k \cos \omega_k(t-t_1) \right. \right.$$
where $q^{(-)} = q_1 - q_2$, $q^{(+)} = (q_1 + q_2)/2$ and $J_k^{(-)} = J_{k1} - J_{k2}$, $J_k^{(+)} = (J_{k1} + J_{k2})/2$. $\Delta^k(t-s)$ is the retarded Green's function which serves as the propagator in perturbative expansion, and is given by using the step function $\theta(t-s)$ as

$$
\Delta^k(t,s) = \theta(t-s) \frac{\sin \omega_k (t-s)}{m_k \omega_k}. \quad (k = 1, \cdots, N)
$$

(E·5)

The $\delta$-function in (E·4) is expressed in the integral form,

$$
\delta\left(q^{(-)} - \int_{t_1}^{t_f} dt J_k^{(-)}(t) \frac{\sin \omega_k (t-t_i)}{m_k \omega_k}\right)
= \int_{-\infty}^{\infty} \frac{dp_k}{2\pi \hbar} \exp\left\{-i \frac{p_k}{\hbar} \left(q^{(-)} - \int_{t_1}^{t_f} dt J_k^{(-)}(t) \frac{\sin \omega_k (t-t_i)}{m_k \omega_k}\right) \right\}.
$$

(E·6)

In this form the integral $\int d\theta^{(-)}$ in (E·3) naturally leads us to use the Wigner representation $\tilde{\rho}^N$ defined as

$$
\rho^N(q, \dot{q}) = \int \frac{d^Np}{(2\pi \hbar)^N} e^{i(q, p - q, \dot{q})} \tilde{\rho}^N(p, q).
$$

(E·7)

We use the following notation for the phase space average of an arbitrary function $A(p, q)$ with the weight $\tilde{\rho}^N(p, q)$

$$
\langle A(p, q) \rangle_{\tilde{\rho}^N} = \int \frac{d^Np d^Nq}{(2\pi \hbar)^N} \tilde{\rho}^N(p, q) A(p, q).
$$

(E·8)

By substituting (E·4) into (E·3), $W_0[J_1, J_2]$ is expressed as

$$
e^{i(\hbar) W_0[J_1, J_2]} = \int d^Nq^{(+)} d^Nq^{(-)} \left\{ \int \frac{d^Np d^Nq}{(2\pi \hbar)^N} \delta(q - q^{(+)}) e^{i(\hbar) p \cdot q^{(-)}} \tilde{\rho}^N(p, q) \right\}
\times \left[ \prod_{k=1}^N \delta\left(q^{(-)} - \int_{t_1}^{t_f} dt J_k^{(-)}(t) \frac{\sin \omega_k (t-t_i)}{m_k \omega_k}\right) \right]
\times \exp\left\{ i \frac{\hbar}{\sum_{k=1}^{\infty}} \int_{t_1}^{t_f} dt J_k^{(-)}(t) \left\{ q^{(+)} \omega_k (t-t_i) + \int_{t_1}^{t_f} ds \Delta^k(t-s) J_k^{(+)}(s) \right\} \right\}
\times \exp\left\{ \frac{\hbar}{m_k \omega_k} \sin \omega_k (t-t_i) + \int_{t_1}^{t_f} ds \Delta^k(t-s) J_k^{(+)}(s) \right\}
\times \left\langle \exp\left\{ i \frac{\hbar}{\sum_{k=1}^{\infty}} \int_{t_1}^{t_f} dt J_k^{(-)}(t) \left\{ q_0(t, p_k, q_k) + \int_{t_1}^{t_f} ds \Delta^k(t-s) J_k^{(+)}(s) \right\} \right\} \right\}_{\tilde{\rho}^N},
$$

(E·9)

(E·10)

(E·11)

where $\langle \rangle_{\tilde{\rho}^N}$ is defined in (E·8) and $q_0(t, p_k, q_k)$ is the classical solution of the coordinate of $k$-th harmonic oscillator with the initial position $(q_k, p_k)$ in phase space. It is written explicitly as
\[ q_0(t, p_h, q_h) = q_h \cos \omega_h (t - t_i) + \frac{p_h}{m_h \omega_h} \sin \omega_h (t - t_i). \quad (k = 1, \ldots, N) \quad \text{(E·12)} \]

We now prove (E·4) by dropping the index \( k \) for simplicity. Before calculation, let us define various quantities as follows,

\[ J^{(-)} = J_1 - J_2, \quad J^{(+)} = \frac{1}{2} (J_1 + J_2), \quad \text{(E·13)} \]

\[ N = \sqrt{\frac{m \omega}{2 \pi \hbar \sin \omega T}}, \quad T = t_f - t_i, \quad \text{(E·14)} \]

\[ a = \frac{i}{\hbar} \frac{m \omega \cos \omega T}{\sin \omega T}, \quad b = -\frac{i}{\hbar} \frac{m \omega}{\sin \omega T}, \quad \text{(E·15)} \]

\[ v_1(t) = \frac{i}{\hbar} \frac{\sin \omega (t - t_i)}{\sin \omega T}, \quad v_2(t) = \frac{i}{\hbar} \frac{\sin \omega (t_f - t)}{\sin \omega T}, \quad \text{(E·16)} \]

\[ G(t, s) = -\frac{1}{b} \{ \theta(t - s) v_2(t) v_1(s) + \theta(s - t) v_1(t) v_2(s) \}. \quad \text{(E·17)} \]

The function \( G(t, s) \) is the propagator of the finite time interval which is symmetric under the exchange of \( t \) and \( s \). The explicit form of the evolution kernel of the harmonic oscillator \( \widehat{K}_0^{(t)} \) is well known\(^2\) and is written by using the above notations as

\[ \langle x | \hat{\mathcal{K}}_0^{(t)} | q_1 \rangle = N \exp (A), \]

\[ \{A\} = a(x^2 + q_1^2) + bxq_1 + \int_{t_i}^{t_f} dt \{ v_1(t)x + v_2(t)q_1 \} J_1(t) \]

\[ -\frac{1}{2} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} ds J_1(t) G(t, s) J_1(s), \quad \text{(E·18)} \]

\[ \langle x | \hat{\mathcal{K}}_0^{(t)} | q_2 \rangle^* = N^* \exp (B), \]

\[ \{B\} = -a(x^2 + q_2^2) - bxq_2 - \int_{t_i}^{t_f} dt \{ v_1(t)x + v_2(t)q_2 \} J_2(t) \]

\[ +\frac{1}{2} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} ds J_2(t) G(t, s) J_2(s). \quad \text{(E·19)} \]

These are inserted into the left-hand side of (E·4) and the relation \( q_1 J_1 - q_2 J_2 = q^{(-)} J^{(-)} + q^{(+)} J^{(+)} \) is used. Then we obtain

\[
\int dx \langle x | \hat{\mathcal{K}}_0^{(t)} | q_1 \rangle \langle x | \hat{\mathcal{K}}_0^{(t)} | q_2 \rangle^* \]

\[ = |N|^2 \int dx \exp \left[ x \left( b q^{(-)} + \int v_1 J^{(-)} \right) + q^{(+)} \int v_2 J^{(-)} \right. \]

\[ + \left. \left( 2a q^{(+)} + \int v_2 J^{(+)} \right) q^{(-)} - \frac{1}{2} \iint (J_1 G J_1 - J_2 G J_2) \right] \]

\[ = \frac{(-2\pi i)}{b} |N|^2 \delta \left( q^{(-)} + \frac{1}{b} \int v_1 J^{(-)} \right) \]

\[ (E·20) \]
\[ \exp \left[ q^{(+)T} \int v_2 J^{(-)} + \left(2aq^{(+)T} + \int v_2 J^{(+)T} \right) \left( -\frac{1}{b} \int v_1 J^{(-)} - \int J^{(-)}GJ^{(+)T} \right) \right] \]  
\[ = \delta \left( q^{(-)} + \frac{1}{b} \int v_1 J^{(-)} \right) \times \exp \left[ q^{(+)T} \int \left( v_2 - \frac{2a}{b} v_1 \right) J^{(-)} - \int J^{(-)} \left( G + \frac{1}{b} v_1 v_2 \right) J^{(+)T} \right]. \]  
(E\22)

Here we have used, \((-2\pi\hbar |N|^2/b = 1\). By putting the value of \(a, b, v_1, v_2, G\) defined in (E\15) \sim (E\17) into the factors contained in the above equation, we get

\[ \frac{1}{b} \int_{t_i}^{t_f} dt J^{(+)T}(t) v_1(t) = -\int_{t_i}^{t_f} dt J^{(-)}(t) \frac{\sin \omega (t-t_i)}{m \omega}, \]  
(E\23)

\[ -\frac{2a}{b} v_1(t) + v_2(t) = \frac{i}{\hbar} \cos \omega (t-t_i), \]  
(E\24)

\[ G(t, s) + \frac{1}{b} v_1(t) v_2(s) = -\frac{i}{\hbar} \Delta (t-s). \]  
(E\25)

Again by putting these factors back into (E\22), we finally obtain

\[ \langle q_2 | \hat{K}_0^{(+)T} \hat{K}_0^{(+)} | q_1 \rangle \]

\[ = \delta \left( q^{(-)} - \int_{t_i}^{t_f} dt J^{(-)}(t) \frac{\sin \omega (t-t_i)}{m \omega} \right) \]

\[ \times \exp \left[ \frac{i}{\hbar} \int_{t_i}^{t_f} dt J^{(+)T}(t) \cos \omega (t-t_i) + \frac{i}{\hbar} \int_{t_i}^{t_f} dt \int_{t_i}^{t_f} ds J^{(-)}(t) \Delta (t-s) J^{(+)T}(s) \right]. \]  
(E\26)

Equation (E\4) is proved through recovering the index \(k\) in (E\26).

References


Appendix F

Diagrammatical Rule of \(W[J_1, J_2]\) with Arbitrary Initial Distribution

In Appendix E, \(W_0\) has been calculated in the form of (E\11). Here the interaction is included thus establishing the Feynman rule of \(W\) for arbitrary initial density matrix. In order to apply our inversion method to practical problems, we need diagrammatical expansion of \(W[J_1, J_2]\).

Let us start from the definition (12\4\3) taking the Hamiltonian (12\4\1). We write it in path integral form by taking the coordinate representation,

\[ e^{i(1/W[J_1, J_2])} = \int d^N x d^N q_1 d^N q_2 \rho_0(q_1, q_2) \langle x | \hat{R}^{(+)T} | q_1 \rangle \langle x | \hat{R}^{(+)} | q_2 \rangle^* \]  
(F\1)
\[= \int_\beta [d\phi_1 d\phi_2] \rho_0^N(\phi_1', \phi_2') \exp \frac{i}{\hbar} (S^k[\phi_1] - S^k[\phi_2]). \]  

Here the path integration variable is denoted by \( \phi_i \) and * denotes the complex conjugation and \( \rho_0^N(\phi_1', \phi_2') = \langle \phi_1'| \rho_0^N | \phi_2' \rangle \). We have defined \( S^k[\phi_i] \) as the action of the system given by

\[S^k[\phi_1] = S_0[\phi_1] + \int_{t_t}^{t_F} dt \sum_{k=1}^N \int_{t_t}^{t_F} dt \left[ \frac{m_k}{2} \dot{\phi}_k^i(t)^2 - \frac{1}{2} m_k \omega_k^2 \phi_k^i(t)^2 \right], \quad (i=1, 2) \]  

where \( \phi_i = d \phi_i / dt \). The path integral \( \int_\beta [d\phi_1 d\phi_2] \) is performed for \( t_t \leq t \leq t_F \) with the condition \( \phi_i(t_F) = \phi_i(t_F) \). The following notation has also been introduced

\[\int_\beta [d\phi_1 d\phi_2] = \int_\beta \prod_{k=1}^N [d\phi_k^i(t)] d\phi_k^i(t) d\phi_k^i(t) \times \delta(\phi_k^i(t_F) - \phi_k^i(t_F)) \int_\beta [d\phi_1] [d\phi_2], \]  

where in the last two path integrals on the right-hand side, \( \phi_k^i(t_F) \) and \( \phi_k^i(t_F) \) \( (i=1, 2) \) are fixed and are equal to the value \( \phi_k^i(t_F) \) and \( \phi_k^i(t_F) \) respectively. These are also equal to \( \phi_1', \phi_2' \) appearing in the matrix element \( \langle \phi_1'| \rho_0^N | \phi_2' \rangle \).

In order to proceed further the interaction \( V(q) \) is assumed to be

\[V(q) = \sum_{n=3}^{\infty} \sum_{k_1, \ldots, k_n=1}^N \lambda^{(n)}_{k_1 \cdots k_n} q_{k_1} q_{k_2} \cdots q_{k_n}. \]  

By multiplying unity

\[\exp \left[ \frac{i}{\hbar} \int_{t_t}^{t_F} dt \left[ J_1(t) \phi_1(t) - J_2(t) \phi_2(t) \right] \right] \bigg|_{J_1=J_2=0} = 1 \]  

at the end on the right-hand side of (F·2), we get the following expression of \( W[J_1, J_2] \),

\[e^{(i/\hbar) W[J_1, J_2]} = \exp \left[ - \frac{i}{\hbar} \int_{t_t}^{t_F} dt \left[ V\left( \frac{\hbar}{i} \frac{\delta}{\delta J_1(t)} \right) - V\left( - \frac{\hbar}{i} \frac{\delta}{\delta J_2(t)} \right) \right] \right] \exp \left[ \frac{i}{\hbar} W_0[J_1, J_2] \right], \]  

where \( \delta/\delta J \equiv (\delta/\delta J_1^1, \delta/\delta J_1^2, \cdots, \delta/\delta J_1^n) \) \( (i=1, 2) \) and \( W_0[J_1, J_2] \) is the generating functional of the system of harmonic oscillators, i.e., \( V(q) = 0 \), in the presence of linearly coupled source term averaged over the initial distribution \( \rho_0^N(q_1, q_2) \).

Now the result (E·11) of Appendix E can be written in a compact form as follows,

\[e^{(i/\hbar) W_0[J_1, J_2]} = \left\{ \exp \left[ \frac{i}{\hbar} \int_{t_t}^{t_F} dt d\mathbf{J}^{(-)}(t) \left\{ q_0(t) + \int_{t_t}^{t_F} ds \mathbf{A}(t, s) \mathbf{J}^{(+)}(s) \right\} \right] \right\}_{\partial^N}, \]  

where

\[\mathbf{J}^{(-)} = \frac{1}{2} (\mathbf{J}_1 + \mathbf{J}_2), \quad \mathbf{J}^{(+)} = \frac{1}{2} (\mathbf{J}_1 - \mathbf{J}_2), \]  

\[\mathbf{J}_1 = \mathbf{J}^{(+)} + \frac{1}{2} \mathbf{J}^{(-)}, \quad \mathbf{J}_2 = \mathbf{J}^{(+)} - \frac{1}{2} \mathbf{J}^{(-)}. \]  

Note that the physical condition \( \mathbf{J}_1 = \mathbf{J}_2 \) is \( \mathbf{J}^{(-)} = 0 \) but \( \mathbf{J}^{(+)} \) is always physically realizable source. Here \( q_0(t, p_k, q_k) \) is given in (E·12) and all the dependence of \( A(p, q) \) on the initial state, i.e., the dependence on \( p \) and \( q \), are contained in \( q_0 \). As
we will see shortly, in diagrammatic terminology, the dependence on the initial state appears as external lines of the Feynman graphs.

Apart from the term \( q_0(t, p, q) \) we have only one type of the propagator, i.e., the retarded Green's function. This is a consequence of using the variables \( J^{(-)} \) or \( J^{(+)} \) and the Wigner representation (E·7). It implies that the signal of the disturbance caused by the interaction potential \( V(q) \) propagates toward the future with respect to the interaction point. This is the non-relativistic causality, as pointed out in Refs. 1) \( \sim 3 \).

Note that \( q_0(t)+\int_{t'}^t dsA(t-s)J^{(+)}(s) \) in the exponent of (F·9) is the classical solution of the harmonic oscillators in the presence of the external force \( J^{(+)} \). In the limit \( \hbar \to 0 \), \( \tilde{\rho} \) goes to the classical distribution \( \rho_c \) so that we can easily imagine the classical limit of the generating functional from this compact form. This will be discussed in detail in § 12.4.

Now let us multiply again unity

\[
\exp\left[\frac{i}{\hbar} \int_{t'}^{t} dt \{J_1(t)\phi_1(t)-J_2(t)\phi_2(t)\}\right]_{\phi_1=\phi_2=0}
\]

\[
=\exp\left[\frac{i}{\hbar} \int_{t'}^{t} dt \{J^{(+)}(t)\phi^{(-)}(t)+J^{(-)}(t)\phi^{(+)}(t)\}\right]_{\phi^{(-)}=\phi^{(+)}=0}
\]

to the right-hand side of (F·8) where \( \phi^{(+)}=(1/2)(\phi_1+\phi_2), \phi^{(-)}=\phi_1-\phi_2 \). (Here \( \phi \) has nothing to do with the path integral variable \( \phi \) of (F·2).) \( W[J_1, J_2] \) now is written in \( \phi \) representation as

\[
e^{(i/\hbar)\mathcal{W}[J_1, J_2]}
\]

\[
=\exp\left[i\int_{t'}^{t} dt \left\{\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, -\frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right\}\right] \exp\left[-\frac{i}{\hbar} \int_{t'}^{t} dt \{V(\phi_1)-V(\phi_2)\}\right]_{\phi_1=\phi_2=0}
\]

\[
=\left\langle \exp\left[i\int_{t'}^{t} dt \left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right] \right\rangle_{\tilde{\rho}^{n}}
\]

\[
\times \left\{q_0(t)+\int_{t'}^{t} dsA(t-s)\left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right\}\right\}_{\tilde{\rho}^{n}}
\]

\[
\times \exp\left[-\frac{i}{\hbar} \int_{t'}^{t} dt \{V(\phi_1(t))-V(\phi_2(t))\}\right]_{\phi_1=\phi_2=0}
\]

\[
=\left\langle \exp\left[i\int_{t'}^{t} dt \left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right] \right\rangle_{\tilde{\rho}^{n}}
\]

\[
\times \exp\left[i\int_{t'}^{t} dt \left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right] \exp\left[i\int_{t'}^{t} dt \left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right]_{\tilde{\rho}^{n}}
\]

\[
\times \exp\left[i\int_{t'}^{t} dt \left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right] \exp\left[i\int_{t'}^{t} dt \left(\frac{\hbar}{i} \frac{\delta}{\delta \phi_1}, \frac{\hbar}{i} \frac{\delta}{\delta \phi_2}\right)\right]_{\tilde{\rho}^{n}}
\]

\[
\times \exp\left[-\frac{i}{\hbar} \int \left\{V\left(\phi^{(+)}+\frac{1}{2} \phi^{(-)}\right)-V\left(\phi^{(+)}-\frac{1}{2} \phi^{(-)}\right)\right\}\right]_{\phi^{(+)}=\phi^{(-)}=0},
\]

(F·13)
where we have introduced
\[
\frac{\delta}{\delta \phi^{(+)}_1} - \frac{\delta}{\delta \phi^{(-)}_1} + \frac{\delta}{\delta \phi^{(+)}_2} - \frac{\delta}{\delta \phi^{(-)}_2} = \frac{1}{2} \left( \frac{\delta}{\delta \phi^{(+)}} - \frac{\delta}{\delta \phi^{(-)}} \right),
\]  

and \((\cdots)|_0\) implies that \((\cdots)\) is evaluated at \(\phi^{(-)} = \phi^{(+)} = 0\). We have also used the relation
\[
\exp \left( A \frac{\delta}{\delta \phi} \right) \exp(B\phi) = \exp(B\phi) \exp \left( A \frac{\delta}{\delta \phi} \right) \exp(AB).
\]

The diagrammatical rule of evaluating \(W[J_1, J_2]\) is readily obtained by (F·13). The operation of the average carried out by \(\bar{\rho}^N\) acts only on \(q_0(t)\).

There are several interesting features specific to our diagrammatic theory but the essential points are the followings.

(i) The double path vertex \(V(\phi_1) - V(\phi_2)\) is written in terms of \(\phi^{(-)}, \phi^{(+)}\) as
\[
V(\phi_1) - V(\phi_2) = \sum_{k=1}^{N} \phi^{(-)}_k f_k(\phi^{(+)}_1, \phi^{(-)}_2, \phi^{(+)}_2, \lambda),
\]
where \(f_k\) is some function determined from \(V(q)\). The arguments of \(f_k\) show that the double path vertex always has odd number of \(\phi^{(-)}\).

(ii) The operator \(i\int(\delta/\delta \phi^{(+)}(s))\Delta(\delta/\delta \phi^{(-)}(t))\) is called the contraction operator and replaces one-pair \(\phi^{(+)}_k(t)\phi^{(-)}_k(s)\) by \(\Delta^k(t, s)\). The rule of the diagram is to assign the line with an arrow \(t \rightarrow s\) for \(\Delta^k(t, s)\) since \(\Delta^k\) contains the step function \(\theta(t-s)\).

(iii) The factor \(\exp[\{i\hbar/(\delta/\delta \phi^{(+)}(s))\Delta(\delta/\delta \phi^{(-)}(t))\}]\) applied to \(\exp[-(i\hbar)/(V(\phi_1) - V(\phi_2))]\) produces the expression \(\exp[\tilde{G}_{\text{conn}}]\) where \([\tilde{G}_{\text{conn}}]\) is the sum of connected diagrams with external lines representing \(\phi^{(+)}_k\) or \(\phi^{(-)}_k\) which remains after contraction. They are constructed by the propagator \(\Delta^k\) and the vertices \(\lambda = \{\lambda^{(n)}\}\) determined by \(V(q)\), see (F·6).

(iv) The operation \(\exp[i\int(\delta/\delta \phi^{(+)})(\phi_0 + \Delta J^{(+)}))]\) or \(\exp[i\int(\delta/\delta \phi^{(-)})(\phi_0 + \Delta J^{(-)}))]\) in (F·13) then replaces the external factor \(\phi^{(+)}_k\) or \(\phi^{(-)}_k\) by \(\phi^{(+)}_k + \Delta^k J^{(+)}_k\) or \(\phi^{(-)}_k + \Delta^k J^{(-)}_k\) respectively.

(v) If a diagram has \(L\) loops of \(\Delta^k (k = 1 \sim N)\) then the factor \((\hbar/i)^L\) is assigned for this diagram. This can be proved using a similar technique of power counting in field theoretical Feynman diagram expansion. We write explicitly the \(\hbar\) dependence of \(\tilde{G}_{\text{conn}}\) by \(\tilde{G}_{\text{conn}}(\lambda, \hbar)\).

Now combining all the above observations, we get finally
\[
\exp \left\{ \frac{i}{\hbar} W[J_1, J_2] \right\}
= \left\langle \exp \left\{ \frac{i}{\hbar} \int J^{(-)}(q_0 + \Delta J^{(+))})
+ \frac{i}{\hbar} \sum_{m=1}^{N} \sum_{n=0}^{\infty} [J^{(-)} \Delta]^m \cdot \left[ \tilde{G}_{\text{conn}}^{(m+n)}(\lambda, \hbar) \right] \cdot [q_0 + \Delta J^{(+)}]^n \right\} \right\}_{\bar{\rho}^N},
\]

where we have defined
\[ [A]^n \cdot \tilde{G}_{\text{conn}}^{(n+m)} \cdot [B]^n \]
\[ \equiv \int_{t_i}^{t_f} dt_1 \cdots dt_m \int_{t_i}^{t_f} ds_1 \cdots ds_n \sum_{k_1=1}^{N} \sum_{k_m=1}^{N} A_{k_1}(t_1) \cdots A_{k_m}(t_m) \]
\[ \times (\tilde{G}_{\text{conn}}^{(n+m)})(t_1, \cdots, t_m, s_1, \cdots, s_n)^{k_1, \cdots, k_m, t_1, \cdots, t_m} B_{i_1}(s_1) \cdots B_{i_n}(s_n). \]  
(F·17)

Here \( \tilde{G}_{\text{conn}}^{(n+m)} \) is the interaction part (starting from the linear term in the potential \( V \)) of the sum of connected graphs having \( m \)-external lines, each having a factor \( J^{-1} \mathcal{A} \) and \( n \)-external lines, having \( q_0 + \Delta J^{(+)} \). Note that the initial distribution of the system is arbitrary in (F·17). For the use of these rules to a model system see Ref. 4).

References


Appendix G

--- Feynman Rule with Initial Equilibrium ---

The rule of the Feynman diagram is derived assuming that the initial density matrix is that of equilibrium distribution\(^*\) under the Hamiltonian \( H_I \). It is brought into the non-equilibrium state by the time dependent Hamiltonian \( H(t) \) starting from some time \( t = t_i \). Both \( H_I \) and \( H(t) \) contain the same interaction part inherent in the system and it is required to discuss both Hamiltonians on the same footing. We take this attitude in this section and study the Feynman rule of the non-equilibrium process by expanding both \( H_I \) and \( H(t) \) in powers of the unharmonicity. This type of formalism enables us to discuss the equilibrium and the non-equilibrium phenomenon in a unified way.

We will see that the propagator of the diagram becomes \( 3 \times 3 \) matrix and that off-diagonal elements referring to the third row or column depend explicitly on \( t_i \). Conventional approach takes \( t_i = -\infty \) and neglects these off-diagonal terms thus the propagator matrix becoming \( 2 \times 2 \). Also the time integration appearing in our Feynman rule starts from \( t_i \), not from \( -\infty \).

Let us take a quantum mechanical system whose Hamiltonian is given by \( H(p, q) \). In order to make our formula as simple as possible, we first consider a system of one degree of freedom, \( q \) or \( p \) denoting the coordinate or the canonical momentum respectively. The Hamiltonian is initially assumed to be time independent with the unharmonic potential part \( V_I(q) \) (the initial correlation),

\[ H_I = \frac{p^2}{2m} + \frac{m \omega^2}{2} q^2 + V_I(q). \]  
(G·1)

Here \( m \) is the mass of the particle and we assume \( \omega > 0 \). It is straightforward to generalize the following discussions to the case where the potential \( V_I \) includes the
momentum variable $p$.

Initially the system is supposed to be in the equilibrium with the temperature $T$ and the time dependent external force is applied at some time $t = t_f$ which brings the system to the non-equilibrium state. The Hamiltonian for $t \geq t_f$ is therefore written as

$$H(t) = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 + V(q, t). \quad (G \cdot 2)$$

It is not necessary that the relation $V(t) = V(q, t_f)$ or $H(t) = H(t_f)$ holds but instead the potential part may have a jump at $t = t_f$ by the application of some external force. Following discussions do not rely on this equality. The initial density matrix is now,

$$\rho_i = \exp(-\beta H_i) / \text{Tr} \exp(-\beta H_i), \quad (G \cdot 3)$$

$$\beta = 1/T. \quad (G \cdot 4)$$

We add as usual the source term to the Hamiltonian which couples linearly to the coordinate $q$:

$$H_i \rightarrow H_i(\tau) = H_i - j(\tau)q, \quad (G \cdot 5)$$

$$H(t) \rightarrow H(t)^\prime = H(t) - j(t)q. \quad (G \cdot 6)$$

Note here that the source term $j(\tau)$ is introduced, besides $j(t)$, in the imaginary time domain. Introducing independent sources in $K, K^\dagger$ and $\rho_i$, the following expression is the object of the following discussions:

$$\exp \frac{i}{\hbar} W[j_1, j_2, j_3] = \text{Tr}(\rho^a K^{a_1} K^{a_2}). \quad (G \cdot 7)$$

Here $K^{a_1, a_2}$ is the time ordered product from $t_r$ to $t_f$ where $t_r$ is taken to be sufficiently large,

$$K^{a_1, a_2} = \text{Tr} \left\{ -\frac{i}{\hbar} \int_{t_r}^{t_f} d\tau H(\tau)^{a_1, a_2} \right\}. \quad (G \cdot 8)$$

We consider the range $t_r \leq t \leq t_f$. $\rho^a$ is given by

$$\rho^a = \text{Tr} \exp \left\{ -\frac{1}{\hbar} \int_{t_r}^{t_f} d\tau H^a(\tau) \right\}, \quad (G \cdot 9)$$

In (G \cdot 9), $T_\tau$ is the $\tau$-ordering operator. Recall that the results depend only on the difference $\tau_f - \tau_r$ for $j_3(\tau) = 0$.

$W$ is the generating functional in the following sense ($j = 0$ implies $j_1 = j_2 = j_3 = 0$),

$$\left. \frac{\delta W}{\delta j_1(\tau)} \right|_{j_1 = 0} = - \frac{\delta W}{\delta j_2(\tau)} \bigg|_{j_2 = 0}, \quad (t_r \leq t \leq t_f) \quad (G \cdot 10)$$

$$\left. \frac{\delta W}{\delta j_3(\tau)} \right|_{j_3 = 0} = \langle q | \tau = t_r, \quad (G \cdot 11)$$

Note that in (G \cdot 10), the parts of $K^{a_1, a_2}$ and $K^{a_2}$ corresponding to the region from $t$ to $t_f$ cancel each other. The right-hand side of (G \cdot 11) is independent of $\tau$. General
correlation functions of $q$ are obtained by further differentiations with respect to $j$.

Now we evaluate (G·7) as follows,

$$\exp \frac{i}{\hbar} W[j_i, j_s, j_s] = \int dq \int dq' \langle q | \rho^h | q' \rangle \langle q' | K^{*h} K^{ih} | q \rangle.$$  \hfill (G·12)

We write first as before

$$\langle q' | K^{*h} K^{ih} | q \rangle = \int dq'' \langle q' | K^{*h} K^{ih} | q'' \rangle \langle q'' | K^{ih} | q \rangle,$$  \hfill (G·13)

where

$$\langle q'' | K^{ih} | q \rangle = \exp \left( -\frac{i}{\hbar} \int_{t_i}^{t_f} dt V \left( \frac{\hbar}{i} \frac{\partial}{\partial j^i(t)} \right) \right) \times \langle q'' | K_0 j^i | q \rangle,$$  \hfill (G·14)

and similar expression for $\langle q' | K^{*h} | q'' \rangle$. We here use the result of (E·26),

$$\langle q' | K_0^{*h} K_0^{ih} | q \rangle = \delta(q'(-) - \int_{t_i}^{t_f} dt \Delta_k(t-t_i) j^i(t) dt) \left[ \exp \left( i \int_{t_i}^{t_f} dt \Delta_k(t-s)(j^i(s) \Delta_k(t-s) - j^i(t) \Delta_k(t-s)) \right) \right],$$  \hfill (G·15)

where $\delta (\cdots)$ is the Dirac $\delta$-function and $\Delta_k$ is the usual retarded function given by

$$\Delta_k(t-s) = \frac{\sin \omega (t-s)}{m \omega}.$$  \hfill (G·16)

We notice here that (G·16) becomes $\delta (q'(-))$ when $j^i(-) = 0$ as it should.

The expression for $\langle q | \rho^h | q' \rangle$ in (G·12) is easily obtained by replacing $t \rightarrow -i \tau$, $T \rightarrow -i \beta \hbar$ in the formulas (G·4)~(G·7). For definiteness we cite the explicit form,

$$\langle q | \rho^h | q' \rangle = \exp \left( -\frac{1}{\hbar} \int_{t_i}^{t_f} V_I \left( \frac{\hbar}{i} \frac{\partial}{\partial j^i(\tau)} \right) d\tau \right) \times \sqrt{\frac{m \omega}{2 \pi \hbar \sin \omega \beta \hbar}} \exp \frac{S_3}{\hbar},$$  \hfill (G·18)

$$S_3 = \frac{m \omega}{2 \sinh \omega \beta \hbar} \left[ -(q^2 + q'^2) \cosh \omega \beta \hbar + 2qq' \right]$$

$$+ \frac{1}{\sinh \omega \beta \hbar} \int_{t_i}^{t_f} \{ q \sinh \omega(\tau - \tau_i) + q \sinh \omega(\tau - \tau_i) \} \Delta_k(\tau) d\tau$$

$$+ \frac{1}{2} \int_{t_i}^{t_f} dt d\tau' \Delta_k(\tau) G(\tau, \tau') \Delta_k(\tau'), \hfill (G·19)$$

$$G(\tau, \tau') = \frac{1}{m \omega} \left\{ \theta (\tau - \tau') \frac{\sinh \omega(\tau - \tau') \sinh \omega(\tau' - \tau_i)}{\sinh \omega \beta \hbar} + (\tau \leftrightarrow \tau') \right\}.$$  \hfill (G·20)

The remaining integration $\int dq \int dq' = \int dq^{(+)} \int dq^{(-)}$ has to be done. The integration over $q^{(-)}$ is trivial because of the $\delta$-function in (G·16) while $q^{(+)}$ integration is Gaussian. The final expression is written in $\varphi$-representation instead of the formula involving $j$. It is obtained by multiplying the following identity to the above expres-
sion of \( \exp(i/\hbar)W \),
\[
1 = \exp\left\{ \frac{1}{\hbar} \left( \int_{t_1}^{t_2} dt \delta_3(t) \varphi_3(t) + i \int_{t_1}^{t_2} dt (j_1(t) \varphi_1(t) - j_2(t) \varphi_2(t)) \right) \right\}_{\varphi = 0}.
\] (G·21)

In the presence of this factor we can replace
\[
(j_1(t), j_2(t), j_3(t)) \equiv \mathbf{j}(t) \quad \rightarrow \quad \left( \frac{\hbar}{i} \frac{\delta}{\delta \varphi_1(t)}, \frac{\hbar}{i} \frac{\delta}{\delta \varphi_2(t)}, \hbar \frac{\delta}{\delta \varphi_3(t)} \right),
\]
\[
\left( \frac{\hbar}{i} \frac{\delta}{\delta j_1(t)}, \frac{\hbar}{i} \frac{\delta}{\delta j_2(t)}, \hbar \frac{\delta}{\delta j_3(t)} \right) \quad \rightarrow \quad (\varphi_1(t), \varphi_2(t), \varphi_3(t)) \equiv \varphi(t).
\]

Now we present the result in several forms. They all have the form
\[
\exp\left( \frac{i}{\hbar} W[j_1, j_2, j_3] \right) = \frac{1}{2 \sinh \frac{\omega \beta \hbar}{2}} \exp\left( S \right) \exp\left[ -\frac{1}{\hbar} \int_{t_1}^{t_2} V_1(\varphi_3(t)) dt - \frac{i}{\hbar} \int_{t_1}^{t_2} \{ V(\varphi_1(t), t) - V(\varphi_2(t), t) \} dt \right]_{\varphi = 0}.
\] (G·22)

Here \( S \) is a functional of \( \mathbf{j} \) and \( \delta/\delta \varphi \). We have to differentiate with respect to \( j_1 \) (or equivalently \( j_2 \)) in order to extract the desired operator \( O(t) \) whose expectation value is to be taken at the time \( t \) and then we set \( j = 0 \). The essential point is the presence of \( j^{(-)} \). Since \( (\delta/\delta j_1)|_{j=0} = (\delta/\delta j^{(-)})|_{j=0} \), the differentiation by \( j_1 \) can be taken in terms of \( j^{(-)} \). We can set \( j^{(+)} = 0 \) from the start but if the physical Hamiltonian contains the linear term \( -J(t)q \), \( j^{(+)}(t) \) is fixed to be \( J(t) \). Including this case, let us consider
\[
W[j^{(-)}] \equiv W\left[ j_1 = J + \frac{j^{(-)}}{2}, j_2 = J - \frac{j^{(-)}}{2}, j_3 = 0 \right]
\] (G·23)
as the generating functional without loss of generality. We use \( W[j^{(-)}] \) below instead of \( W[j_1, j_2, j_3] \).

In the following various expressions of \( W[j^{(-)}] \) are given. The different representations have different forms of the propagators which are the coefficients of the quadratic term of \( \delta/\delta \varphi \) appearing in \( S \). This operator has the same effect in Wick's contraction theorem.

I. \( \varphi^{(z)} \) representation

The most convenient form for the calculational purpose is the one written in terms of \( \varphi^{(z)} \) and \( \varphi_3 \). We use the notation \( \varphi_3 \equiv \varphi \) and
\[
\frac{\delta}{\delta \varphi^{(z)}} \equiv \frac{\delta}{\delta \varphi_1} + \frac{\delta}{\delta \varphi_2}, \quad \frac{1}{2} \left( \frac{\delta}{\delta \varphi_1} - \frac{\delta}{\delta \varphi_2} \right).
\] (G·24)
$S$ has four different propagators and is given, instead of explicit $3 \times 3$ matrix form, as follows,

\begin{align}
S &= i \int \! dt ds \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(s)}}(t) + j^{(-)}(t) \right) \Delta \kappa(t - s) \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(-)}}(s) + J(s) \right) \tag{G·25} \\
&+ \frac{1}{2} \int \! dt ds \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(s)}}(t) + j^{(-)}(t) \right) \overline{A}(t - s) \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(-)}}(s) + j^{(-)}(s) \right) \tag{G·26} \\
&+ \int \! dt \! dr \left( \frac{\hbar}{i} \frac{\delta}{\delta \phi^{(r)}}(t) + j^{(-)}(t) \right) \overline{G}(t, \tau) \hbar \frac{\delta}{\delta \phi^{(r)}} \tag{G·27} \\
&+ \frac{1}{2} \int \! dt \! dr \! r' \hbar \frac{\delta}{\delta \phi^{(r)}} G(\tau, \tau') \hbar \frac{\delta}{\delta \phi^{(r')}}. \tag{G·28}
\end{align}

Here the integration regions are $t_1 \leq t, s \leq t_F, \tau_1 \leq \tau, \tau' \leq t_F$ and $\Delta \kappa$ is given in (G·17). Other propagators are as follows,

\begin{align}
\overline{A}(t - s) &= - \frac{\coth \omega \beta \hbar}{2m \omega} \cos \omega (t - s), \tag{G·29} \\
\overline{G}(t, \tau) &= \frac{1}{2m \omega \sinh \omega \beta \hbar} \left\{ \sin \omega (t - t_1) \sinh \omega \left( \tau - \frac{\tau_1 + t_F}{2} \right) \right. \tag{G·30} \\
&\left. + \mathrm{i} \cos \omega (t - t_1) \cosh \omega \left( \tau - \frac{\tau_1 + t_F}{2} \right) \right\}, \tag{G·31} \\
G(\tau, \tau') &= \frac{1}{2m \omega \sinh \omega \beta \hbar} \left\{ \theta(\tau' - \tau) \cosh \omega \left( \tau - \tau' + \frac{\beta \hbar}{2} \right) + (\tau' \leftrightarrow \tau) \right\}. \tag{G·32}
\end{align}

The diagrammatic expansion is given by the above propagators and by the vertices determined by $V_i(\phi(\tau))$ and $V(\phi_i(t), t) - V(\phi_i(t), t)$ which is odd in $\phi^{(-)}$. We have not discussed the denominator of $\rho$ given in (G·3). It has the following effects in the diagrammatic expansion of $W[j_1, j_2, j_3]$ given in (G·22):

- eliminate the factor $\left(2 \sinh \frac{\omega \beta \hbar}{2}\right)^{-1}$
- eliminate all the diagrams having $V_i(\phi(\tau))$ vertices only

These exhaust our Feynman rule. Note that $G(\tau, \tau')$ is of course the Matsubara imaginary time Green's function.3)

The characteristic feature of the finite time interval theory is the appearance of the mixed propagator $\overline{G}$ which explicitly involves the initial time $t_1$. In the conventional approach of the infinite time interval, $t_1$ is taken to be $-\infty$ and $\overline{G}$ is neglected. If this is done our expression coincides with the existing formula. This is clearly seen in the $\phi_1^2 \phi_2^2 \phi_3^2$ representation which is discussed next.

II. $\phi_i$ representation

It is straightforward to rewrite $S$ in the original variables $\phi_i \ (i=1, 2, 3)$. The
result is given in the $3 \times 3$ matrix form. For the off-diagonal terms, there are various ways of writing them but we choose those which agree with the conventional expressions. With $j=(j_1, -j_2, j_3)=(J+(j^+)^{-1}/2), -J+(j^-)^{-1}/2, 0)$, $S/\hbar$ is given by

$$S/\hbar = \frac{1}{2} \int \int \left( \frac{\delta}{\delta \varphi(t)} + \frac{i}{\hbar} j(t) \right) \cdot G(t, s) \left( \frac{\delta}{\delta \varphi(s)} + \frac{i}{\hbar} j(s) \right) dt ds,$$

(G·33)

where $\delta \varphi = (\delta \varphi_1, \delta \varphi_2, \delta \varphi_3)$ and

$$G_{11}(t, s) = \Delta_F(t, s), \quad G_{22}(t, s) = \Delta_F(t, s),$$

(G·34)

$$G_{12}(t, s) = \Delta^{(+)}(t, s), \quad G_{21}(t, s) = \Delta^{(-)}(t, s) = \Delta^{(+)}(s, t),$$

(G·35)

$$G_{20}(\tau, \tau') = \hbar G(\tau, \tau'),$$

(G·36)

$$G_{10}(t, \tau) = G_{20}(t, \tau) = \frac{\hbar}{i} \tilde{G}(t, \tau),$$

$$G_{01}(\tau, t) = G_{20}(\tau, t) = \frac{\hbar}{i} \tilde{G}(\tau, t).$$

(G·37)

We have used in (G·33) the same notation $t$ or $s$ for $\tau$ or $\tau'$; if $t$ or $s$ corresponds to the index 3, it refers to $\tau$ or $\tau'$. The functions $\Delta_F, \Delta_F$ and $\Delta^{(\pm)}$ are the usual free propagators given by

$$\Delta^{(+)}(t, s) = \text{Tr} \rho_0 q(t)q(s)$$

$$= \frac{\hbar}{2m\omega} \left[ -i \sin \omega (t-s) + \coth \frac{\omega \beta \hbar}{2} \cos \omega (t-s) \right]$$

$$= \frac{\hbar}{2m\omega \sinh \frac{\omega \beta \hbar}{2} \cos \omega \left( t-s + i \frac{\beta \hbar}{2} \right)},$$

(G·38)

$$\Delta^{(-)}(t, s) = \Delta^{(+)}(s, t),$$

$$\Delta_F(t, s) = \theta(t-s) \Delta^{(+)}(t, s) + \theta(s-t) \Delta^{(-)}(t, s) = \text{Tr} \rho_0 Tq(t)q(s),$$

$$\Delta_F(t, s) = \theta(t-s) \Delta^{(-)}(t, s) + \theta(s-t) \Delta^{(+)}(t, s) = \text{Tr} \rho_0 \tilde{T}q(t)q(s),$$

(G·39)

where $\rho_0$ is the harmonic density matrix and $\tilde{T}$ is the anti-time ordering operator. Thus the small matrix $G_{ik}$ where $i, j=1, 2$ agrees with the conventional one. The remaining propagators have the following representations:

$$G_{10}(t, \tau) = \frac{\hbar}{2m\omega \sinh \frac{\omega \beta \hbar}{2}} \cos \omega \left( t-t_1 + i \left( \tau - \frac{\tau + \tau_1}{2} \right) \right),$$

(G·40)

$$G_{20}(\tau, \tau') = \frac{\hbar}{2m\omega \sinh \frac{\omega \beta \hbar}{2}} \left\{ \theta(\tau' - \tau) \cos \omega \left( \tau' - \tau + \frac{\beta \hbar}{2} \right) + (\tau' \leftrightarrow \tau') \right\}$$

$$= \text{Tr} \rho_0 Tq(\tau)q(\tau').$$

(G·41)

Equations (G·38)~(G·41) suggest that $S$ can be written by a single cosine propagator
in a complex $t$-plane. In Ref. 1) this has been shown by introducing the contour integral.

References


Appendix H

—— Fermion Path Integral and Feynman Rule for Hubbard Model ——

In this appendix we derive the path-integral formula for the fermion coherent state and then derive the Feynman rule in two different ways. In order to clarify the notations, we first enumerate some formulas for the fermionic coherent state in the case of single mode. The generalization to multi-mode is straightforward. For the anti-commuting operator $a$, $a^\dagger$ like (10·1·2), the coherent state is defined as

$$a|z\rangle = z|z\rangle, \quad \langle z|a^\dagger = \langle z|z^\ast, \quad \text{(H·1)}$$

where $z$ and $z^\ast$ are Grassmann numbers. Then inner product of the two states becomes

$$\langle z|z'\rangle = e^{z^\ast z'}, \quad \text{(H·2)}$$

which means that the coherent state is neither normalized nor orthogonalized. The matrix element in the coherent state is

$$\langle z|O(a^\dagger, a)|z'\rangle = O(z^\ast, z')e^{z^\ast z'}, \quad \text{(H·3)}$$

where $O$ is a normal-ordered operator. The over-completeness is expressed as

$$\int dz^\ast dze^{-z^\ast z}|z\rangle\langle z| = 1. \quad \text{(H·4)}$$

The trace of a normal-ordered operator becomes

$$\text{Tr} O(a^\dagger, a) = \int dz^\ast dze^{-z^\ast z} \langle -z|O(a^\dagger, a)|z\rangle. \quad \text{(H·5)}$$

Our first work is to derive the path-integral formula for the thermodynamic potential,

$$e^{-\beta} = \text{Tr} e^{-\int_{\tau}^\infty \mathcal{H} d\tau} \mathcal{U}, \quad \text{(H·6)}$$

where

$$\mathcal{H}[J] = \sum_{r, \sigma} t_{r\sigma} a^\dagger_r a_r + U \sum_{r} n_{r\uparrow} n_{r\downarrow} - \sum_{r, \sigma} J_\sigma(r\tau) n_{r\sigma}$$

$$= t_{ee} a^\dagger_e a_e - U a^\dagger_e a_e a_\uparrow a_\downarrow - J_\sigma(r\tau) a_\sigma a_\tau a_\uparrow a_\downarrow. \quad \text{(H·7)}$$

Here the source has $r$, $\tau$ dependence and $T_\tau$ is the $\tau$-ordering operator. The case in
which $J_r$ is independent of $r$ and $r$ can be dealt with in the same manner as the following.

In order to derive the path-integral formula for $Q$, we first estimate

$$\langle z_r | T_r \exp \left[ - \int d\tau (t_{a\beta} a_{\alpha}^\dagger a_{\beta} + CV(a_{\alpha}^\dagger a_{\alpha}) ) \right] | z_l \rangle e^{-\frac{1}{\epsilon}z_\beta z_\alpha}.$$  \hspace{1cm} (H.8)

Here $CV$ represents the on-site Coulomb term plus the source term appearing in (H.7) and $CV(a_{\alpha}^\dagger a_{\alpha})$, $z_l$ and $z_r$ are abbreviations of $CV(\{a_{\alpha}^\dagger\}, \{a_{\alpha}\})$, $\{z_l\}$ and $\{z_r\}$ respectively. $\{X_a\}$ represents the set of elements $X_a$ with allowed value of $a$. As usual we divide the exponential into $N+1$ pieces and insert $N$ multi-mode complete sets like (H.4).

We get

$$\left( \prod_{l=1}^{N} \prod_{a} \int dz_{l,a} dz_{l,a} \right) \exp \left( - \sum_{l=1}^{N+1} z_{l,a}^* z_{l,a} \right) \exp \left( \sum_{l=1}^{N+1} z_{l,a}^* z_{l-1,a} \right) \times \exp \left[ - \epsilon \sum_{l=1}^{N+1} \left( t_{a\beta}^\dagger a_{\alpha}^\dagger z_{l-1,a} + CV(z_{l,a}^* z_{l-1,a}) \right) \right],$$  \hspace{1cm} (H.9)

where $\epsilon = \beta/(N+1)$, $z_{0,a} = z_{l,a}$, $z_{N+1,a} = z_{r,a}$ and we have assumed $CV$ is normal-ordered. The first two exponential can be formally written as

$$\exp \left( - \epsilon \sum_{l=1}^{N+1} z_{l,a}^* (z_{l,a} - z_{l-1,a}) / \epsilon \right) \longrightarrow \exp \left( - \int_0^\beta dt z_{l,a}^* (t) z_{l,a}(t) \right).$$  \hspace{1cm} (H.10)

In what follows, we only use formal continuous expression instead of original discrete one for simplicity. If some ambiguity occurs we have to go back to the original discrete version. In this way, through the trace formula (H.5), we obtain the path-integral representation of (H.6),

$$e^{-a} = \int_{z_\alpha = -z_\beta} z_{\alpha}^* D z_{\alpha} \exp \left( - z_{\alpha}^* z_{\beta} - t_{a\beta} z_{\alpha}^* z_{\beta} + U z_{\alpha}^* \sum_{a} z_{\alpha}^* z_{\alpha} + J_{a\beta} z_{\alpha} \right),$$  \hspace{1cm} (H.11)

where the path integration is done under anti-periodic condition $z_\alpha(0) = -z_\alpha(\beta)$ and $z_{\alpha}^*(0) = -z_{\alpha}^*(\beta)$ while the exponent of the exponential of the right-hand side stands for

$$S[z_{\alpha}^*, z, J] = - \sum_{x} z_{x,0}^* G_{x,0} z_{x,0}^* \right) - U \sum_{x} z_{x,0}^* z_{x,0} + \sum_{x} J_{a\beta} z_{x,0}^* z_{x,0} \right) = - \sum_{x} z_{x,0}^* G_{x,0}^{-1} z_{x,0} - U z_{x,0}^* z_{x,0} + J_{a\beta} z_{x,0}^* z_{x,0},$$  \hspace{1cm} (H.12)

$$G_{x,0}^{-1} = \delta_{rr} \left( \frac{\partial}{\partial z_{r,0}} t_{rr} \right),$$  \hspace{1cm} (H.13)

where $x$ and $x'$ denote the sets $(rr)$ and $(r'r')$ respectively. Inserting

$$1 = \exp(\eta^* z + z^* \eta)|_{\eta = \eta^* = 0} = \exp \left( \sum_{x'} (\eta_{x,0}^* z_{x,0} + z_{x,0}^* \eta_{x,0}) \right)|_{\eta = 0}$$  \hspace{1cm} (H.14)

into Eq. (H.11), and moving the interaction term $CV(z_{\alpha}^*, z) = U z_{\alpha}^* z_{\alpha} z_{\alpha} - J z_{\alpha}^* z_{\alpha}$ outside of the path-integration, we obtain

$$e^{-a} = \exp \left( - \int_0^\beta d\tau CV \left( - \frac{\delta}{\delta z_{\alpha}(\tau)}, \frac{\delta}{\delta z_{\alpha}^*(\tau)} \right) \right),$$
\begin{equation}
\times \int_{z_{0} = -z_{a}} \mathcal{D}z^{*} \mathcal{D}z \exp\left\{ -\int_{0}^{\delta} dt (z^{*}_{a}(t) \dot{z}_{a}(\tau) + t_{ab} z_{a}^{*}(t) \dot{z}_{b}(\tau) - \eta^{*}_{a}(\tau) z_{a}(\tau) - z_{a}^{*}(\tau) \eta_{a}(\tau)) \right\} \bigg|_{\eta = 0}, \tag{H.15}
\end{equation}

where the path integration is done under the anti-periodic condition as before. Now we change the integration variables in the path integral as

\begin{align}
z_{a}(\tau) & \longrightarrow z_{a}^{0}(\tau) + z_{a}(\tau), \quad z_{a}^{*}(\tau) \longrightarrow z_{a}^{0*}(\tau) + z_{a}^{*}(\tau), \tag{H.16}
\end{align}

where \( z_{a}^{0}(\tau) \) and \( z_{a}^{0*}(\tau) \) are the solution of the following equations:

\begin{align}
\dot{z}_{a}^{0}(\tau) + t_{ab} z_{b}^{0}(\tau) = \eta_{a}(\tau), \quad -\dot{z}_{a}^{0*}(\tau) + t_{ab} z_{b}^{0*}(\tau) = \eta_{a}^{*}(\tau) \tag{H.17}
\end{align}

with the boundary conditions

\begin{align}
z_{a}^{0}(0) = -z_{a}^{0}(\beta), \quad z_{a}^{0*}(0) = -z_{a}^{0*}(\beta). \tag{H.18}
\end{align}

The new variables also satisfy the same anti-periodic boundary condition. The exponent of the last exponential of (H.15) becomes (in a symbolic notation where \( T \) stands for the matrix \( t_{ab} \))

\begin{align}
z^{*} \dot{z} + z^{*} T \dot{z} - \eta^{*} z - z^{*} \eta \\
\longrightarrow (z^{*} + z^{0*})(\dot{z}^{0} + T \dot{z}^{0} - \eta) + z^{0*} \dot{z} + (z^{0*} T - \eta^{*}) z - \eta^{*} \dot{z}^{0} + \dot{z}^{*} z + T \dot{z}^{*} \\
= -\eta^{*} \dot{z}^{0} + \dot{z}^{*} + z^{*} T \dot{z}. \tag{H.19}
\end{align}

The differential equations (H.17) are solved through the Green's functions. For example

\begin{align}
z_{a}^{0}(\tau) = \int_{0}^{\delta} dt' G_{ab}(\tau, \tau') \eta_{b}(\tau'), \tag{H.21}
\end{align}

where \( G_{ab}(\tau, \tau') \) should be solved through

\begin{align}
\left( \delta_{ab} \frac{\partial}{\partial \tau} + t_{ab} \right) G_{br}(\tau, \tau') = \delta_{br} \delta(\tau, \tau') \tag{H.22}
\end{align}

with the boundary condition

\begin{align}
G(0, \tau) = -G(\beta, \tau), \tag{H.23}
\end{align}

where \( \delta(\tau, \tau') \) is defined by

\begin{align}
\int_{0}^{\delta} d\tau \delta(\tau, \tau') \eta_{a}(\tau') = \eta_{a}(\tau). \tag{H.24}
\end{align}

Then the formula for the thermodynamic potential \( \Omega \) is

\begin{align}
e^{-\Omega} = & \exp\left\{ -\int_{0}^{\delta} d\tau CV \left( \frac{\delta}{\delta \eta(\tau)}, \frac{\delta}{\delta \eta^{*}(\tau)} \right) \right\} \\
\times & \exp\left\{ \int_{0}^{\delta} d\tau \int_{0}^{\delta} d\tau' \eta_{a}(\tau) G_{ab}(\tau, \tau') \eta_{b}(\tau') \right\} \bigg|_{\eta = 0} e^{-\Omega_{0}}, \tag{H.25}
\end{align}
where
\[ e^{-\Omega_0} = \int_{z_0 = -z_s} \mathcal{D} z^* \mathcal{D} z \exp \left[ - \int_0^\beta d\tau (z^*_a(\tau) z^*_a(\tau) + z^*_a(\tau) t_{ab} z_a(\tau)) \right], \] (H·26)
that is, \( \Omega_0 \) is the thermodynamic potential for the system with \( CV = 0 \) or no-interaction (see (H·15)). \( e^{-\Omega_0} \) can be determined through differential equations,
\[ \frac{\partial e^{-\Omega_0}}{\partial t_{ab}} = \int_0^\beta d\tau G_{ab}(\tau, \tau) e^{-\Omega_0} \] (H·27)

or
\[ \frac{\partial \Omega_0}{\partial t_{ab}} = -\beta G_{ab}(0, 0). \] (H·28)

From (H·25) the Feynman rule can be derived easily, although in the following we show another way to derive the Feynman rule. It is rather formal but quick. First, let us go back to (H·11) to (H·13) or, in a symbolic notation,
\[ e^{-\varphi} = \int_{z_0 = -z_s} \mathcal{D} z^* \mathcal{D} z \exp(-z^* G^{-1} z - U z^* z + J z^* z) \] (H·29)
\[ = e^{-CV(\partial/\partial \varphi), (\partial/\partial \varphi^*)} \int_{z_0 = -z_s} \mathcal{D} z^* \mathcal{D} z \exp(-z^* G^{-1} z + \eta^* z + z^* \eta) \bigg|_{\eta = 0} \] (H·30)
\[ = e^{-CV(\partial/\partial \varphi), (\partial/\partial \varphi^*)} \int_{z_0 = -z_s} \mathcal{D} z^* \mathcal{D} z \exp(-z^* G^{-1} z - G \eta) \bigg|_{\eta = 0}, \] (H·31)

where we have inserted (H·14) as when we get (H·15) from (H·11). Now the path integration can be carried out by changing the integration variables \( z^* \rightarrow z^* - \eta^* G \) and \( z \rightarrow z - G \eta \) and then by using the formula for Grassmann variables,
\[ \int \mathcal{D} z^* \mathcal{D} z \ e^{-z^* A z} \equiv \left( \prod_i \int dz_i^* \right) e^{-z^* A z} \left. = \det A \right). \] (H·32)

In this way we get
\[ e^{-\varphi} = \det G^{-1} e^{-CV(\partial/\partial \varphi), (\partial/\partial \varphi^*)} e^{(\eta^* G \eta)} \bigg|_{\eta = 0}. \] (H·33)

Notice that the anti-periodic condition of the path integral requires both \( z^* - \eta^* G \) and \( z - G \eta \) satisfy the same condition. Thus \( G \) satisfies (H·23). We again insert unity
\[ 1 = e^{\eta^* z + z^* \eta} \bigg|_{z = 0}, \] (H·34)

where \( z^* \) and \( z \) are new Grassmann variables which have nothing to do with the previous path-integration variables. Then we get
\[ e^{-\varphi} = \det G^{-1} e^{\eta^* z + z^* \eta} e^{-((\partial/\partial z) - \eta^* G((\partial/\partial \varphi^*) + \eta)} e^{-CV(z^* z)} \bigg|_{\eta = 0}. \] (H·35)

Setting \( \eta = \eta^* = 0 \) in the last expression we get
\[ Q = -\text{Tr} \ln G^{-1} - \sum_{\text{conn}} \left. \left. e^{(-U z^* z + J z^* z)} \right|_{z = 0}, \] (H·36)

from which the Feynman graph rule is obtained as follows. Here the superscript
conn implies that we should keep only the connected graphs.

Rule 1) In one specific way (as one likes), assign \(n\) labels \(x_1, \cdots, x_n\) (internal points) to all the 4-point vertices where \(n\) is the total number of vertices.

Rule 2) Associate \(y \longrightarrow x\) and \(y \cdots \cdots \longrightarrow x\) with \([G_1]_{x_2}\) and \([G_2]_{x_2}\) respectively and the factor \(U\) is assigned to the 4-point vertex. In addition the factor \(J_{\gamma}\) is assigned to the 2-point vertex although the 2-point vertex can be fully or partly absorbed in the propagator. No factor is required to the external point.

Rule 3) Associate a factor \((-1)^{V+1}(-1)^{L_\gamma}\) for each diagram where \(V\) is the number of the factors \(U\) in the graph and \(L_\gamma\) is the number of fermion loops.

Rule 4) Associate the inverse of the symmetry factor \(1/S\) for the diagram.

Rule 5) Sum (Integrate) the product of all factors in 2) to 4) over the space and imaginary time indices \(x_1, \cdots, x_n\).

As is well known, the symmetry factor \(S\) for each graph is given by the product of the line symmetry factor and the vertex symmetry factor. The line symmetry factor is 1 in this theory and the rule for the vertex symmetry factor \(S_{\gamma}\) is the following.

Rule \(S_{\gamma}\) Assign \(n\) labels \(1, \cdots, n\) to \(n\) vertices in one specific but an arbitrary way. Count the number of all possible other ways of assigning \(n\) labels that give the same topological structure as the first specific one. The number thus obtained plus 1 is \(S_{\gamma}\). Note that we have to distinguish the spin-up and spin-down propagators and the directions of the arrows when we consider the topological equivalence.

For definiteness we give some examples; the graph in (10·1·16) or (10·1·17) has \(S=1\) and three graphs in (10·1·18) have \(S=1, 2,\) and 1 respectively.

References


Appendix I

—— Inversion Formulas of Many Variables ——

Let us consider the case where we have \(M\) sources \(J_i\) and corresponding \(M\) order parameters \(\phi_i (i=1, 2, \cdots, M)\). We are going to generalize the inversion formulas to this case. The original and inverted series ((7·2·2) and (7·2·3)) are written as follows,

\[
\phi_i = \phi_i[g, J] = \phi_i^{(0)}[J] + g\phi_i^{(1)}[J] + g^2\phi_i^{(2)}[J] + \cdots,
\]  
(I·1)
\[ J_i = J_i[\phi, \phi] = J_i^{(0)}[\phi] + \frac{\partial J_i^{(1)}[\phi]}{\partial J_i^{(0)}} + \cdots. \tag{1.2} \]

We have defined \( \phi_i^{(0)}, \phi_i^{(1)} \cdots \) and \( J_i^{(0)}, J_i^{(1)} \cdots \) in place of \( h_i^{(0)}, h_i^{(1)} \cdots \) and \( f_i^{(0)}, f_i^{(1)} \cdots \). (There are slight differences in the notation here compared with those of § 7.2.) Now expand \( \phi_i[J] \) around \( J_i^{(0)} \),

\[
\phi_i = \sum_{n=0}^{\infty} g^n \phi_i^{(n)}[J^{(0)} + \Delta J] \\
= \sum_{n=0}^{\infty} g^n \sum_{m_1, m_2, \cdots} \frac{1}{m_1! m_2! \cdots} \left( \frac{\partial^{m_1 + m_2 + \cdots}}{\partial J_i^{(0)m_1}\partial J_j^{(0)m_2}\cdots} \phi_i^{(n)}[J^{(0)}] \right) \left( \Delta J \right)^{m_1} \left( \Delta J \right)^{m_2} \cdots \\
= \phi_i^{(0)}[J^{(0)}] + g \phi_i^{(0)}[J^{(0)}] J_i^{(1)} + \phi_i^{(1)}[J^{(0)}] \\
+ g^2 \left[ \frac{1}{2} \phi_i^{(0)}[J^{(0)}] J_j^{(1)} \phi_i^{(1)}[J^{(0)}] J_j^{(1)} + \phi_i^{(0)}[J^{(0)}] J_j^{(2)} + \phi_i^{(2)}[J^{(0)}] \right] + \cdots, \tag{1.3} \]

where the following notation has been used

\[ \phi_i^{(0)}[J^{(0)}] = \frac{\partial \phi_i^{(0)}[J^{(0)}]}{\partial J_i^{(0)}}. \tag{1.4} \]

The summation over \( 1 \sim M \) by the repeated index \( j, k \cdots \) is implied. Thus we get order by order

\[
\phi_i = \phi_i^{(0)}[J^{(0)}], \tag{1.5} \\
0 = \phi_i^{(0)}[J^{(0)}] J_i^{(1)} + \phi_i^{(1)}[J^{(0)}], \tag{1.6} \\
0 = \frac{1}{2} \phi_i^{(0)}[J^{(0)}] J_j^{(1)} \phi_i^{(1)}[J^{(0)}] J_j^{(1)} + \phi_i^{(0)}[J^{(0)}] J_j^{(2)} + \phi_i^{(2)}[J^{(0)}], \tag{1.7} \\
\cdots.
\]

Note that we have to invert (1.5) and express \( J_1, J_2 \cdots \) in terms of \( \phi_1, \phi_2 \cdots \). Thus we can get \( J^{(n)} \) successively from these equations. Recall here that in inversion method, fixed variable is not external field \( J_i \) but order parameter \( \phi_i \), therefore \( J^{(0)} = \phi_i^{(0)}[\phi] \) (in vector notation) plays a role of order parameter rather than external field.

In case \( \phi \) is obtained from some function \( W \) by a differentiation like

\[ W[J] = \sum_{n=0}^{\infty} g^n W^{(n)}[J], \quad \phi_i^{(n)}[J] = \frac{\partial W^{(n)}[J]}{\partial J_i}, \tag{1.8} \]

\( W^{(n)}[J] \) is also expanded in the same way as the expansion of \( \phi_i[J] \),

\[ W^{(n)}[J] = \sum_{m_1, m_2, \cdots} \frac{1}{m_1! m_2! \cdots} \left( \frac{\partial^{m_1 + m_2 + \cdots}}{\partial J_i^{(0)m_1}\partial J_j^{(0)m_2}\cdots} W^{(n)}[J^{(0)}] \right) (\Delta J)^{m_1} (\Delta J)^{m_2} \cdots. \tag{1.9} \]

Here we introduce \( \Gamma[\phi] \) as the Legendre transformation of \( W[J] \) by

\[ \Gamma[\phi] = W[J] - J \phi. \tag{1.10} \]

It satisfies
\[
\frac{\partial \Gamma[\phi]}{\partial \phi_i} = -J^i. \tag{I\cdot 11}
\]

Then from (I\cdot 8), (I\cdot 5) and (I\cdot 9), Eq. (I\cdot 10) becomes

\[
\Gamma[\phi] = \sum_{n=0}^{\infty} g^n W^{(n)}[J] - \{J^{(0)}_i + (\Delta J)_i\} \phi^{(0)}_i[J^{(0)}]
\]
\[
= \sum_{n=0}^{\infty} g^n \left[ W^{(n)}[J^{(0)}] + g \frac{\partial W^{(n+1)}[J^{(0)}]}{\partial J^{(0)}_i}(\Delta J)_i \right.
\]
\[
+ \sum_{m_1 + m_2 + \ldots \geq 2} \frac{1}{m_1! m_2! \ldots} \left( \frac{\partial^{m_1+m_2+\ldots}}{\partial J^{(0)}_1^m \partial J^{(0)}_2^m \partial \ldots} W^{(n)}[J^{(0)}] \right)(\Delta J)_1^{m_1}(\Delta J)_2^{m_2} \ldots \right]
\]
\[- J^{(0)}_i \phi_i. \tag{I\cdot 12}
\]

Note that the first derivative of \( W^{(n)}[J^{(0)}] \) does not appear in \( \Gamma \). Thus, we get \( \Gamma[\phi] = \sum_{n=0}^{\infty} g^n \Gamma^{(n)}[\phi] \) perturbatively as a function(al) of \( J^{(0)} \),

\[
\Gamma^{(0)}[\phi] = W^{(0)}[J^{(0)}] - J^{(0)}_i \phi_i, \tag{I\cdot 13}
\]

\[
\Gamma^{(1)}[\phi] = W^{(1)}[J^{(0)}], \tag{I\cdot 14}
\]

\[
\Gamma^{(2)}[\phi] = W^{(2)} + W^{(1)}_i J^{(1)}_i + \frac{1}{2} W^{(0)}_i J^{(1)}_i J^{(1)}_j
\]
\[
= W^{(2)} + \frac{1}{2} W^{(1)}_i J^{(1)}_i, \tag{I\cdot 15}
\]

\[
\Gamma^{(3)}[\phi] = W^{(3)} + W^{(2)}_i J^{(1)}_i + W^{(1)}_i J^{(2)}_j + \frac{1}{2} \left( W^{(0)}_i J^{(1)}_i J^{(1)}_j + W^{(1)}_i J^{(1)}_j J^{(1)}_k \right)
\]
\[
+ \frac{1}{3!} W^{(0)}_i J^{(1)}_i J^{(1)}_j J^{(1)}_k
\]
\[
= W^{(3)} + \frac{3}{2} W^{(2)}_i J^{(1)}_i + W^{(1)}_i J^{(1)}_j J^{(1)}_j + \frac{5}{12} W^{(0)}_i J^{(1)}_i J^{(1)}_j J^{(1)}_k, \tag{I\cdot 16}
\]

\[
\ldots
\]

Here, \( W^{(n)}_{\delta k} \) appearing in the above equations are function(al)s of \( J^{(0)} \) and are defined by

\[
W^{(n)}_{\delta k} = - \frac{\partial W^{(n)}[J^{(0)}]}{\partial J^{(0)}_i \partial J^{(0)}_j \partial J_k^{(0)}}. \tag{I\cdot 17}
\]

Appendix J

—— Loop Expansion of \( \Gamma \) and Propagators for Superfluid \(^4\)He ——

In this appendix, using the notation \((14\cdot 1\cdot 2)\), the Feynman rule necessary for the loop expansion of \( \Gamma[\phi] \) in the case of superfluid \(^4\)He is summarized using the contour integration. It is the graphical rule for \( \Gamma \) in the presence of the condensation and the
explicit form of the propagator is also derived. The Hamiltonian is given in (14·1·1).

Let us start from the action derived from (14·1·1) taking δ-function interaction for simplicity,

\[
I[\tilde{\phi}^i] = \int_c dt \int d^3 x \left\{ i\hbar \tilde{\phi}^i(t, x) \dot{\phi}(t, x) + \tilde{\phi}^i(t, x) \left( \frac{\hbar^2}{2m} \nabla^2 + \mu \right) \dot{\phi}(t, x) + \frac{1}{2} U_0 \tilde{\phi}^i(t, x) \tilde{\phi}^i(t, x) \tilde{\phi}^i(t, x) \right\}.
\]

(J·1)

The rule of the Legendre transformation is known to be given as follows; write \( \tilde{\phi}^i(t, x) = \phi^i(t, x) + \tilde{\phi}''^i(t, x) \) with \( \tilde{\phi}''^i(t, x) \) representing the fluctuating part. Then calculate the vacuum diagrams regarding \( \phi^i(t, x) \) as a given c-number field. In this process the following two conditions, which are the consequences of the Legendre transformation, have to be imposed, see Appendix C for details; (1) discard the linear term in \( \tilde{\phi}''^i \) appearing in (J·1), (2) among the vacuum diagrams higher than two loops, keep only the one-particle irreducible (1PI) graphs. Here 1PI diagram is a graph which is not separated into two disconnected graphs if any one of the propagators of \( \tilde{\phi}''^i(t, x) \) is cut. In this way \( \Gamma \) is given as \( \Gamma = \Gamma_{\text{tree}} + \Gamma_{\text{-loop}} + \Gamma_{\text{higher-loops}} \). \( \Gamma_{\text{tree}} \) has the same form as the starting action \( I[\phi^i] \) corresponding to (14·1·1),

\[
\Gamma_{\text{tree}}[\phi^i] = (I[\phi^i])_{\phi=\phi^0}
\]

\[
= \int_c dt \int d^3 x \left\{ \phi^i(x) \left( i\hbar \partial_t + \frac{\hbar^2}{2m} \nabla^2 + \mu \right) \phi(x) \right. \\
\left. - \frac{1}{2} U_0 \phi^i(x) \phi^i(x) \phi(x) \phi(x) \right\}.
\]

(J·2)

In order to write \( \Gamma_{\text{-loop}} \), so called trace-log term, in a compact way, define

\[
I^{(2)}(x, y) = \left( \frac{\delta^2 I[\phi]}{\delta \phi^i(x) \delta \phi^j(y)} \right)_{\phi=\phi^0}.
\]

(J·3)

The above \( I^{(2)}(x, y) \) is nothing but the inverse of the propagator matrix \( D \) which has to be used in the diagrammatic expansion of higher orders of \( \Gamma \),

\[
iD^{-1}[\phi^i]^j(x, y) = I^{(2)}(x, y)
\]

\[(J·4)\]

\[
=(iD^{0(-1)})^{j}(x, y) + V^{ji}(x, y),
\]

(J·5)

where \( D^0 \) is the free part independent of \( U_0 \) and \( V \) is the interacting part,

\[
V^{ji}(x, y) = \int_c dt d^3 z \tilde{V}^{ji}(z; x, y).
\]

(J·6)

The explicit expression of the matrix \( \tilde{V} \) is, for example,

\[
\tilde{V}^{ji}(z; x, y) = -2 U_0 \delta^4(x-z) \delta^4(y-z) \phi^j(z) \phi(z).
\]

(J·7)

Now \( \Gamma_{\text{-loop}} \) is given by

\[
\Gamma_{\text{-loop}}[\phi^i] = \frac{1}{2} i\hbar Tr c \ln I^{(2)}(x, y),
\]

(J·8)
where the trace is taken over the matrix $\ln I^{(a)}$ with the matrix index $(i, x)$ and $(j, y)$ and $\text{Tr}_c$ implies that when we take the trace over the time, it is the contour integral $\int_{\text{c}} dt$. For ease of reference we show the explicit form of $I^{(a)ij}(x, y)$,

$$I^{(a)ij}(x, y) = \begin{pmatrix} -i\hbar \partial_t + \frac{\hbar^2}{2m} \partial_x^2 + \mu - 2\phi^*(x)\phi(x)U_0 & -U_0\phi^*(x)\phi^* \left( x \right) \\ -U_0\phi(x)\phi(x) & i\hbar \partial_t + \frac{\hbar^2}{2m} \partial_x^2 + \mu - 2\phi^*(x)\phi(x)U_0 \end{pmatrix} \times \delta^i(x-y), \quad (J\cdot9)$$

$I_{\text{higher-loops}}$ consists of the vacuum diagrams with more than two loops. In this calculation we use the propagator $D$ (explicit form is given below) and the vertices, which are read from $(14\cdot1\cdot1)$. There are two types of vertices; $\bar{\phi}^i \bar{\phi}^j \bar{\phi}^k \phi^l$ and $\bar{\phi}^i \bar{\phi}^j \bar{\phi}^k \phi^l$.

The propagators are given by the inverse of $I^{(a)}$ as is shown in $(J\cdot9)$. Below we assume constant $\phi$ and for this $\phi$ the inverse can be calculated and the propagators are obtained. Let us solve

$$\begin{pmatrix} -i\hbar \partial_t - \varepsilon_k^0 + \mu - 2U_0\phi^* \phi, & -U_0\phi^* \phi^* \\ -U_0\phi \phi & i\hbar \partial_t - \varepsilon_k^0 + \mu - 2U_0\phi^* \phi \end{pmatrix} \times \begin{pmatrix} D_{11}(t, t'; k), & D_{12}(t, t'; k) \\ D_{21}(t, t'; k), & D_{22}(t, t'; k) \end{pmatrix} = \delta_c(t-t') \begin{pmatrix} 1, & 0 \\ 0, & 1 \end{pmatrix} \quad (J\cdot10)$$

here $\delta_c(t-t')$ is the contour $\delta$-function. The boundary condition plays an essential role. Using the contour $\theta$-function, we can write $D$, which is a function of $t-t'$, and its boundary condition as

$$D(t-t') = D^>(t-t')\theta_c(t-t') + D^<(t-t')\theta_c(t'-t), \quad (J\cdot11)$$

$$D^>(t-t' - i\beta\hbar) = D^<(t-t'). \quad (J\cdot12)$$

In the following, $t = -i\hbar\tau + t_l$ when we consider the third path $C_3$ and $t_l$ is taken to be $-\infty$ for simplicity.

Consider first the case where both $t$ and $t'$ are on the first path $C_1$. Therefore $\alpha = \beta = 1$. Then the factor $\delta_c(t-t')$ in $(J\cdot10)$ is replaced by the usual $\delta$-function $\delta(t-t')$. A solution to $(J\cdot10)$ is easily found to be

$$\begin{pmatrix} D_{11}(t, k) \\ D_{21}(t, k) \\ D_{12}(t, k) \\ D_{22}(t, k) \end{pmatrix} = -\frac{i}{\hbar} \theta(t)e^{-(i/\hbar)E_k^t} \begin{pmatrix} \psi_k \\ u_k \\ \bar{u}_k \end{pmatrix} - \frac{i}{\hbar} \theta(-t)e^{-(i/\hbar)E_k^t} \begin{pmatrix} \psi_k \\ u_k \end{pmatrix}. \quad (J\cdot13)$$

Here various quantities have been defined and will be used in what follows,

$$E_k = (\varepsilon_k^0 - \mu + 2U_0\phi^* \phi)^2 - (U_0\phi^* \phi)^2 \right)^{1/2}, \quad (J\cdot14)$$
\[
\begin{align*}
\begin{pmatrix}
u_k \\
v_k
\end{pmatrix} &= \frac{1}{2} \left[ \frac{(e^0_k - \mu + 2U_0 \phi \phi')}{E_k} \right] \pm 1, \\
C_k &= \frac{U_0 \phi \phi}{2E_k}, \quad C_k^* = (C_k)^*, \\
n_0 &= \phi^* \phi, \quad f_0(k) = \frac{1}{e^{E_k} + 1}.
\end{align*}
\] (J·15)

The general solution to (J·10) is the sum of (J·13) and the general solution to the homogeneous equation which is obtained by setting the right-hand side of (J·10) to be zero. Such a solution has four undetermined constants which should be fixed by the boundary condition (J·12). Since this part of calculation is straightforward, only the result is shown below. Writing \( t \) for \( t' \), it is given by

\[
\begin{pmatrix}
D_{11}^1(t, k) \\
D_{22}^2(t, k) \\
D_{12}^1(t, k) \\
D_{21}^2(t, k)
\end{pmatrix} = -\frac{i}{\hbar} \left\{ \theta(t) + f_0(k) \right\} e^{-iE_k t} \begin{pmatrix}
u_k \\
C_k
\end{pmatrix} - \frac{i}{\hbar} \left\{ \theta(-t) + f_0(k) \right\} e^{iE_k t} \begin{pmatrix}
u_k \\
C_k
\end{pmatrix}.
\] (J·18)

For the case where \( t \) or \( t' \) is on the path \( C_2 \) or \( C_3 \), we can similarly discuss and it turns out that the total formula can be obtained by simply replacing \( \theta(t-t') \) or \( \theta(t'-t) \) in the above formula (J·18) by the contour \( \theta_0(t-t') \) or \( \theta_0(t'-t) \). The final result of the propagator is thus

\[
\begin{align*}
\begin{pmatrix}
D_{11}^{11}(t, t'; k) \\
D_{22}^{22}(t, t'; k) \\
D_{12}^{12}(t, t'; k) \\
D_{21}^{21}(t, t'; k)
\end{pmatrix} &= -\frac{i}{\hbar} \left\{ \theta_0(t-t') + f_0(k) \right\} e^{-iE_k t} \begin{pmatrix}
u_k \\
C_k
\end{pmatrix} \\
&\quad -\frac{i}{\hbar} \left\{ \theta_0(t'-t) + f_0(k) \right\} e^{iE_k t} \begin{pmatrix}
u_k \\
C_k
\end{pmatrix}.
\end{align*}
\] (J·19)