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Unified time-path approach to the generating functional of the Brownian oscillator system: The bilinearly corrected Feynman rule for nonequilibrium processes

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We derive fully corrected propagators of a bilinearly interacting Brownian oscillator system by summing up an infinite number of Feynman diagrams. The generating functional of a nonequilibrium system is calculated in terms of the bilinearly corrected propagators thus obtained. The result offers the Feynman rule for systematically studying the effects of both anharmonicity of the potential and nonbilinear system-bath couplings on the Brownian oscillator system. The reduced density matrix, which is useful for investigating the dynamics of the system, is also calculated. The unified time path, which is powerful in calculating propagators, is introduced and used effectively throughout the work.

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I. INTRODUCTION

Feynman rule for a nonequilibrium quantum system has been widely used effectively in various fields. The temperature Green function was introduced, from which the information on the real-time process was pulled out by using a rather intricate method of analytical continuation [1–4]. On the other hand, the double-path method starts from the real-time instead of the imaginary time [5–8].

Recently the double-path formalism is extended to a formalism in which the propagator becomes a 3×3 matrix instead of a 2×2 of the double-path formalism [9,10]. Typical nonequilibrium processes are explicitly calculated through the Feynman rule in terms of the 3×3 propagators [11]. We introduce *the unified time path* from this formalism in the following section. The path integral is *directly* performed on this unified time path.

In this paper we consider a nonequilibrium process where the total system is initially in the equilibrium state and then the time-dependent external force (applied after the initial time) derives the total system towards a nonequilibrium state. In such a case the unified time-path approach gives a unified perspective to calculation and argument as we see below. The quantity explicitly derived below is the generating functional for this case of nonequilibrium process, from which the Feynman rule is readily known and thus all the physical quantities can be estimated by diagrams. The generating functional is here defined as a functional of the external force which is obtained from the density matrix by tracing over all degrees of freedom of the total system [see Eq. (2.11) below]. The generating functional of nonequilibrium system provides a convenient means for incorporating effects of dissipation in physical systems [12].

We intend to calculate the generating functional of the Brownian motion model. One of the most fruitful models of the Brownian motion is described by the system-bath Hamiltonian [13],

$$H_{\mathrm{SB}} = \frac{P^2}{2M} + \frac{M\Omega^2}{2}Q^2 + \sum_{i=1}^{N}\left(\frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2}{2}q_i^2\right) - Q\sum_{i=1}^{N}c_iq_i + V(Q,q,t). \tag{1.1}$$

Following the work by Caldeira and Leggett [14], there has been a renewed interest in the problem of Brownian motion. This model has been successfully used to study problems in chemical reaction [15,16], electron transportation in the semiconductor [17], and quantum optics [18]. Various techniques have been developed to include the effects of $V(Q,q,t)\neq 0$ both numerically and analytically [19–23].

Though many studies have been done by using this system-bath Hamiltonian in diverse fields, there were no systematic and analytical ways of calculating the effects of the anharmonicity of the potential and the nonbilinear coupling [i.e., the case of $V(Q,q,t)\neq 0$]. [Though the interaction $Q\sum_{i=1}^{N}c_iq_i$ is usually called linear, we call it bilinear or linear-linear in what follows since, if we view the system (1.1) as a special case of (2.1) with (2.2) below, it may be appropriate to call the term $\sum_{i,j=0}^{N}c_{ij}q_iq_j \to Q\sum_{i=1}^{N}c_iq_i$ *bilinear* interacting term.] This is partly because the Feynman rule in which propagators are fully corrected by the bilinear interaction has not been derived up to now. Needless to say, this line of study is important since the real mechanism of dissipation may be much more complex than the simple harmonic case.

In this paper we derive the bilinearly corrected 3×3 propagators for a general bilinear coupling term $\sum_{i,j=0}^{N}c_{ij}q_iq_j$ and obtain an expression for the generating functional in terms of these propagators [see Eq. (6.1) below]. This expression gives a Feynman rule for a nonequilibrium system where anharmonic interactions correspond to vertices. Note here that the bilinear interaction does not appear as vertices since it is fully taken into the propagator. Thus we can systematically study the nonequilibrium process of the total system not only for the case of anharmonic potential (both for the system and for the bath) but also for the case of general (nonbilinear) mechanism of the system-bath interactions. We also show that the reduced density matrix, which is useful for studying the dynamics of the system, can be calculated from the generating functional.

Finally we point out the close relation between [24] and the present work. In [24] they derived various correlation functions for the case of the harmonic system potential and the bilinear system-bath coupling. Some of their expressions can be regarded as elements of our 3×3 propagators for the special coupling case [see Eq. (4.19)] while they did not derive the other elements of the propagator even for this special coupling case. The general coupling case is not dealt with in [24] at all. In this sense the present work can be viewed as a generalization of [24]. We show explicitly, however, how these elements of propagators can be used as the basis for investigating the effect of the anharmonicity or nonbilinear coupling by using the Feynman diagrammatic technique. Especially, the nonbilinear coupling correction can be systematically examined in our forumlation.

II. THE UNIFIED TIME PATH

Let us consider a quantum system of $N+1$ degrees of freedom. The total Hamiltonian is expressed in a generalized form as

$$H_T(p,q) = \sum_{i=0}^{N} \left(\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2}{2} q_i^2 \right) + V_T(q,t), \quad (2.1)$$

$$V_T(q,t) = -\tfrac{1}{2} \sum_{\substack{i,j=0 \\ (i \neq j)}}^{N} c_{ij} q_i q_j + V(q,t), \quad (2.2)$$

where $V(q,t)$ is the nontrivial part of the interaction [for example, $V(q,t) = \lambda q_0^2 \sum_{i=1}^{N} q_i$]. The conventional system-bath Hamiltonian can always be cast into this form, if we set $(p_0, q_0, \omega_0, m_0) \equiv (P, Q, \Omega, M)$ and regard the other degrees of freedom as the heat bath. Strictly speaking, the bath degrees of freedom N should be taken to infinity at some stage in order to dissipate the energy of the system (P, Q) to the bath.

We are interested in the case where the total system is initially in equilibrium with the temperature $1/\beta$, and then the time-dependent external force is applied at some time, say $t = 0$. The external force brings the total system to a nonequilibrium state. In this context the total nontrivial interaction $V(q,t)$ is really time dependent while *initially* it is only a function of the coordinates, i.e., $V_I(q) \equiv V(q,0)$. In what follows we assume $c_{ij} (= c_{ji})$ time independent without loss of generality.

The experimental observable of the system is always expressed by the expectation value of various operators or correlation functions. Such quantities can be systematically investigated when the generating functional is introduced. To this end, we add artificial source terms to the original Hamiltonian,

$$\begin{aligned} H(t) \equiv H_T(p,q) &\to H^{J_\alpha}(t) \\ &= H(t) - \sum_i J_{\alpha,i}(t) q_i \quad (\alpha = 1,2). \end{aligned} \quad (2.3)$$

Then the time evolution operators from initial time to infinite future (and vice versa) of the total system with the source are given by

$$K^{J_1} = T e^{-\frac{i}{\hbar}\int_0^\infty dt H^{J_1}(t)}, \quad \tilde{K}^{J_2} = \tilde{T} e^{\frac{i}{\hbar}\int_0^\infty dt H^{J_2}(t)}, \quad (2.4)$$

where T and $\tilde{T}$ are the usual time ordering and antitime ordering operators, respectively. We introduce the generalized version of the unnormalized initial density matrix,

$$\sigma^{\tilde{J}_3} = T_\tau e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau H^{\tilde{J}_3}(\tau)}, \quad (2.5)$$

where T_τ is the τ-ordering operator and $H^{\tilde{J}_3}(\tau)$ is given by

$$H^{\tilde{J}_3}(\tau) = H(t=0) - \sum_i \tilde{J}_{3,i}(\tau) q_i. \quad (2.6)$$

Then the normalized initial equilibrium density matrix of the original system is expressed as

$$\rho_I = \left(\sigma^{\tilde{J}_3} / \mathrm{Tr}\sigma^{\tilde{J}_3} \right)_{\tilde{J}_3 = 0}. \quad (2.7)$$

Consider the generating functional for the correlation function Z_J or that for the connected correlation function W_J defined by

$$Z_J = e^{\frac{i}{\hbar}W_J} = \mathrm{Tr}\left(\sigma^{\tilde{J}_3} \tilde{K}^{J_2} K^{J_1} \right). \quad (2.8)$$

By using the generating functional, the expectation value of the coordinate of the system at t is given as

$$\langle q_i \rangle_t = \left. \frac{\partial W}{\partial J_{1,i}(t)} \right|_{J=0} = - \left. \frac{\partial W}{\partial J_{2,i}(t)} \right|_{J=0} \quad (t \geq 0), \quad (2.9)$$

$$\langle q_i \rangle_{t=0} = \frac{1}{i} \left. \frac{\partial W}{\partial J_{3,i}(\tau)} \right|_{J=0}. \quad (2.10)$$

Here, $J = 0$ implies $J_{1,i} = J_{2,i} = J_{3,i} = 0$ for all i. We can also obtain the expectation value of the momentum or the correlation function including both p_i and q_i [after replacing all $p_i(t)$ with $m_i \dot{q}_i(t)$] by taking derivatives of W with respect to J_i [10,25] [see also Eq. (5.20)].

At this point we introduce *the unified time path* $C = C_1 + C_2 + C_3$ in the complex time plane as in shown Fig. 1 (see Ref. [10]). Namely, it starts from the origin up to infinity along the real path (C_1), returns to the origin (C_2), and then goes to $-i\beta\hbar$ along the imaginary axis (C_3).

The step function $\theta_C(t,t')$ on C is naturally defined such that $\theta_C(t,t')$ takes the value unity if the time t is *later* than the time t'; otherwise $\theta_C(t,t') = 0$. The word *later* here means that the time t appears *later* than the

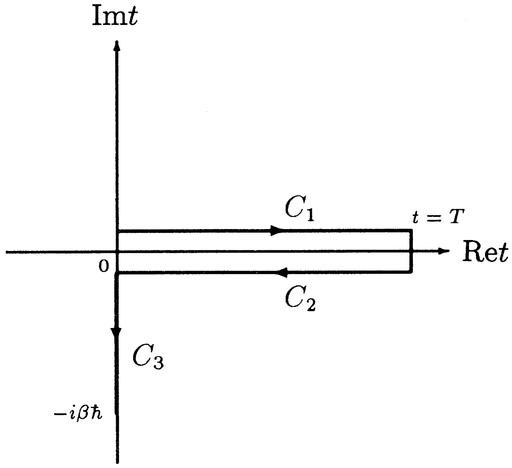


FIG. 1. The unified time path $C = C_1 + C_2 + C_3$ on the complex t plane. The actual paths C_1 and C_2 are on the real time axis and $T \to \infty$.

time t' when we go along the unified time path following the direction of the arrow in Fig. 1. The δ function $\delta_C(t,t')$ on C is also defined accordingly. Note here that

$$\theta_C(t_2,t_2') = \theta(t_2' - t_2), \theta_C(t_3,t_3') = \theta(it_3 - it_3'),$$
$$\delta_C(t_2,t_2') = -\delta(t_2 - t_2'),$$

etc. $(t_\alpha, t_\alpha' \in C_\alpha)$ while $\theta(t)$ and $\delta(t)$ are the usual step function and δ function, respectively.

Thanks to the unified time path the generating functions Z_J and W_J are now expressed in the compact form

$$Z_J = e^{\frac{i}{\hbar}W_J} = \mathrm{Tr} T_C e^{-\frac{i}{\hbar}\int_C dt H^J(t)}, \tag{2.11}$$

where T_C is the time-ordering operator on the unified time path defined through $\theta_C(t,t')$ and $H^J(t)$ should be interpreted as $H^J(t) = H^{J_\alpha}(t)$ $(t \in C_\alpha)$. Note that $H^{J_3}(t)$ is here defined by

$$H^{J_3}(t) = H(t=0) - \sum_i J_{3,i}(t) q_i$$

with $J_3(t) = \tilde{J}_3(-i\tau)$ while $H^{J_{1,2}}(t)$ are given in Eq. (2.3).

The path integral on the unified time path can be performed by a simple generalization of the usual one. The essential point is that we divide the unified time path into $N+1$ pieces $(t_0 = 0, t_1, \ldots, t_N, t_{N+1} = -i\beta\hbar)$ and introduce ϵ_i's; $\epsilon_i \equiv (\epsilon_0, \epsilon_1, \ldots, \epsilon_N)$ such that

$$t_i = \sum_{k=0}^{i-1} \epsilon_k, \quad t_i - t_j = \sum_{k=j}^{i-1} \epsilon_k \quad (i > j). \tag{2.12}$$

We should notice that ϵ_i is positive if t_i is on C_1, negative if t_i is on C_2, and pure imaginary if t_i is on C_3. Then the generalization of the familiar method follows naturally. The result is

$$Z_J = e^{\frac{i}{\hbar}W_J} = \int [q] e^{\frac{i}{\hbar}\int_C dt \mathcal{L}^J(t)}, \tag{2.13}$$

where $\int[q]$ implies the path integration on the unified time path and $\mathcal{L}^J(t)$ is the Lagrangian corresponding to $H^J(t)$ (see Appendix A). Now that all the quantities appearing in Z_J become the c number, we can pull out the interaction term by using the simple identity $e^{F(q)} e^{Jq} = e^{F(\frac{d}{dJ})} e^{Jq}$,

$$Z_J = e^{-\frac{i}{\hbar}\int_C dt V_T(\frac{\partial}{\partial J(t)})} \prod_{i=0}^{N} Z_{J,i}^{(0)}, \tag{2.14}$$

where

$$Z_{J,i}^{(0)} = \int [q_i] e^{\frac{i}{\hbar}\int_C dt\left[\frac{m_i}{2}\dot{q}_i^2(t) - \frac{m_i\omega_i^2}{2} q_i^2(t) + J_i(t) q_i(t)\right]}, \tag{2.15}$$

and $V_T(\frac{\partial}{\partial J(t)})$ implies $V_T(q,t)$ with q_i replaced by $\frac{\hbar}{i}\frac{\partial}{\partial J_i(t)}$.

Although the quantity $Z_{J,i}^{(0)}$ itself has been already obtained [24,10], we present a quick derivation based on the unified time path. For simplicity we drop the index i of q_i. The well-known result (see, for example, [26]) on the C_1 path,

$$\langle q'| T e^{-\frac{i}{\hbar}\int_0^T dt\left(\frac{p^2}{2m} + \frac{m\omega^2}{2} q^2(t) - J_1(t) q(t)\right)} |q\rangle = \left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{1/2} e^{\frac{i}{\hbar}S}, \tag{2.16}$$

$$S = \frac{m\omega}{2\sin\omega T}[(q^2 + q'^2)\cos\omega T - 2qq'] + \frac{1}{\sin\omega T}\int_0^T dt J_1(t)[q\sin\omega(T-t) + q'\sin\omega t] + \frac{1}{2}\int_0^T dt \int_0^T ds J_1(t) G_{11}(t-s) J_1(s), \tag{2.17}$$

$$G_{11}(t-s) = -\frac{1}{m\omega}\left[\theta(t-s)\frac{\sin\omega(T-t)\sin\omega s}{\sin\omega T} + (t \leftrightarrow s)\right], \tag{2.18}$$

is generalized on the unified path C as

$$\langle q'| T_C e^{-\frac{i}{\hbar}\int_C dt\left[\frac{p^2}{2m} + \frac{m\omega^2}{2} q^2(t) - J(t) q(t)\right]} |q\rangle = \left(\frac{m\omega}{2\pi\hbar \sinh\omega\beta\hbar}\right)^{1/2} e^{\frac{i}{\hbar}S_C}, \tag{2.19}$$

where S_C is given by S with the following replacements:

$$T \to -i\beta\hbar,$$
$$\int_0^T dt \to \int_C dt,$$
$$J_1(t) \to J(t) = J_\alpha(t) \quad (t \in C_\alpha),$$
$$\theta(t-s) \to \theta_C(t,s). \tag{2.20}$$

We emphasize the fact that, although these replacements may be almost self-evident, the above result can be directly obtained by natural extension of the known methods (see Appendix A). On the contrary, they first derive $\langle q|\sigma^{J_3}|q'\rangle$, $\langle q'|\tilde{K}^{J_2}|q''\rangle$, $\langle q''|K^{J_1}|q\rangle$ separately and then performed integration with respect to q, q', q'' to derive the quantity $\mathrm{Tr}\, \sigma^{J_3}\tilde{K}^{J_2}K^{J_1}$ in [24,10].

The generating functional $Z_J^{(0)}$ is obtained from Eq. (2.19) by tracing over the coordinate, i.e., by setting $q = q'$ and integrating over q. We thus get the known result,

$$Z_J^{(0)} = e^{\frac{i}{\hbar}W_J^{(0)}} = \frac{1}{2\sinh(\omega\beta\hbar/2)}e^{\Phi_J}, \tag{2.21}$$

$$\Phi_J = \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 \int_C dt \int_C ds J(t)D(t-s)J(s), \tag{2.22}$$

$$D(t-s) = \frac{\hbar}{2m\omega}\frac{1}{\sinh(\omega\beta\hbar/2)} \times [\theta_C(t-s)\cos\omega(t-s-i\beta\hbar/2) + (t \leftrightarrow s)]. \tag{2.23}$$

Thus the notion of the unified time path which was introduced in Ref. [10] can be extended in a useful way.

By recovering the index i of q_i, we arrive at the following expression for the generating functional for the total system:

$$Z_J = e^{-\frac{i}{\hbar}\int_C dt V(\frac{\partial}{\partial J(t)})} Z_J^L, \tag{2.24}$$

$$Z_J^L = e^{\frac{i}{\hbar}W_J^L} = e^{\frac{\hbar}{i}\int_C dt \sum_{i,j}\frac{\partial}{\partial J_i(t)}c_{ij}\frac{\partial}{\partial J_j(t)}} e^{\frac{1}{2}(\frac{i}{\hbar})^2\int_C dt\int_C ds \sum_i J_i(t)D_i(t-s)J_i(s)}, \tag{2.25}$$

where $D_i(t-s)$ is defined in Eq. (2.23) with m, ω replaced by m_i, ω_i, and $V(\frac{\partial}{\partial J(t)})$ implies $V(q,t)$ in Eq. (2.2) with q_i replaced by $\frac{\hbar}{i}\frac{\partial}{\partial J_i(t)}$.

By using the trivial identity (see Appendix B)

$$e^{-\frac{\partial}{\partial J_i}A_{ij}\frac{\partial}{\partial J_j}} e^{\frac{1}{2}J_i B_{ij}^{-1}J_j} = e^{\frac{1}{2}J_i(A+B)_{ij}^{-1}J_j} \times (\text{a factor independent of } J), \tag{2.26}$$

which holds for matrices A, B and the vector J, we see that Z_J^L can be *formally* cast into the following form:

$$Z_J^L = e^{\frac{i}{\hbar}W_J^L}, \tag{2.27}$$

$$\frac{i}{\hbar}W_J^L = \frac{1}{2}\left(\frac{i}{\hbar}\right)^2 \int_C dt \int_C ds \sum_{i,j} J_i(t)D_{ij}(t-s)J_j(s), \tag{2.28}$$

where

$$[D_{ij}(t-s)]^{-1} = [D_i(t-s)\delta_{ij}]^{-1} - \frac{i}{\hbar}c_{ij}\delta(t-s), \tag{2.29}$$

and δ_{ij} is Kronecker's delta. The inverse in the above expression is the inverse of the matrix when you consider $D_{ij}(t-s)$ as the matrix D_{ab} with $a = (i,t)$, $b = (j,s)$. Moreover note here that t, s is on the unified time path. In Sec. IV, we derive the explicit form of the bilinearly corrected propagator $D_{ij}(t-s)$ by noting the graphical meaning of Eq. (2.26), which will become clear as we go along. It should be emphasized that Eq. (2.24) with (2.27) and (2.28) gives the Feynman rule based on the bilinearly corrected propagator. This Feynman rule is a starting point of studying a nonequilibrium system subject to an anharmonic potential in addition to the linear-linear interaction.

III. THE LAPLACE-FOURIER REPRESENTATION

If we introduce variables $J^{(+)}$ and $J^{(-)}$ by

$$J^{(+)} = (J_1 + J_2)/2, \quad J^{(-)} = J_1 - J_2, \tag{3.1}$$

then the quantity Φ_J in Eq. (2.22) can be expressed as [24,10]

$$\Phi_J = \left(\frac{i}{\hbar}\right)^2 \int_0^\infty dt \int_0^\infty ds \left(J^{(-)}(t)D_0^{(-+)}(t-s)J^{(+)}(s) + \frac{1}{2}J^{(-)}(t)D_0^{(--)}(t-s)J^{(-)}(s)\right)$$
$$+\frac{i}{\hbar}\frac{1}{\hbar}\int_0^\infty dt \int_0^{\beta\hbar} d\tau J^{(-)}(t)D_0^{(-3)}(t+i\tau)J_3(\tau) + \frac{1}{2}\frac{1}{\hbar^2}\int_0^{\beta\hbar} d\tau \int_0^{\beta\hbar} d\tau' J_3(\tau)D_0^{(33)}(-i\tau+i\tau')J_3(\tau'), \tag{3.2}$$

where

$$\begin{aligned} D_0^{(-+)}(t) &= \frac{\hbar}{i}\theta(t)\frac{\sin\omega t}{m\omega}, \\ D_0^{(--)}(t) &= \hbar\frac{\coth(\omega\beta\hbar/2)}{2m\omega}\cos\omega t, \\ D_0^{(-3)}(t+i\tau) &= \hbar\frac{\cosh\omega(it-\tau+\beta\hbar/2)}{2m\omega\sinh(\omega\beta\hbar/2)}, \\ D_0^{(33)}(-i\tau) &= \hbar\theta(\tau)\frac{\cosh\omega(\tau+\beta\hbar/2)}{2m\omega\sinh(\omega\beta\hbar/2)} + (\tau\leftrightarrow-\tau). \end{aligned} \tag{3.3}$$

By noting that

$$D_0^{(-+)}(t-s) = \frac{\hbar}{i}\frac{\partial}{\partial J^{(-)}(t)}\frac{\partial}{\partial J^{(+)}(s)}W_J^{(0)}\bigg|_{J=0}, \tag{3.4}$$

with $W_J^{(0)}$ defined in Eq. (2.22), we have

$$D_0^{(-+)}(t-s) = \theta(t-s)[\langle q(t-s)q\rangle_0 - \langle qq(t-s)\rangle_0], \tag{3.5}$$

where $\langle X\rangle_0$ is the connected part of the average of X by the initial density matrix for the noninteracting system. The time evolution is also done by the noninteracting Hamiltonian. Explicitly,

$$\langle q(t)q\rangle_0 = (q(t)q)_0 - (q)_0^2, \tag{3.6}$$

where

$$(q(t)q)_0 = \mathrm{Tr}\left(e^{-\beta H}e^{iHt/\hbar}qe^{-iHt/\hbar}q\right)/\mathrm{Tr}e^{-\beta H}, \tag{3.7}$$

with $H = p^2/2m + m\omega^2q^2/2$. Similarly we have

$$D_0^{(--)}(t-s) = \frac{1}{2}\langle q(t-s)q + qq(t-s)\rangle_0. \tag{3.8}$$

Since $\langle q(t-s)q\rangle_0$ is the complex conjugate of $\langle qq(t-s)\rangle_0$, we can recast the above relation into

$$D_0^{(-+)}(t) = -2i\theta(t)\mathrm{Im}\langle qq(t)\rangle_0, \tag{3.9}$$

$$D_0^{(--)}(t) = \mathrm{Re}\langle qq(t)\rangle_0. \tag{3.10}$$

We also have

$$D_0^{(-3)}(t+i\tau) = \langle qq(t+i\tau)\rangle_0, \tag{3.11}$$

$$D_0^{(33)}(-i\tau) = \theta(\tau)\langle qq(-i\tau)\rangle_0 + (\tau\to-\tau). \tag{3.12}$$

Equations (3.9)–(3.12) imply the fact that once the quantity $D_0^{(-3)}(t+i\tau)$ is evaluated the others can be obtained as a special value of this quantity. For example, $D_0^{(33)}(-i\tau)$ is given by $D_0^{(-3)}(t+i\tau')$ evaluated at $t=0, \tau'=-\tau$ [see Eq. (3.3)] if $\tau>0$.

We note here that these equations also imply the well-known fact that one can obtain all the expressions by the analytic continuation of the Matsubara Green function $D_0^{(33)}(-i\tau)$.

By introducing the Laplace-Fourier transform

$$X(z,n) \equiv \int_0^{\beta\hbar} d\tau e^{-i\nu_n\tau}\int_0^{\infty} dt e^{-zt}X(t,\tau) \qquad (0<t, 0<\tau<\beta\hbar), \tag{3.13}$$

we have

$$D_0^{(-+)}(t) = \int_{C_z}\frac{dz}{2\pi i}e^{zt}D_0^{(-+)}(z) \quad (t>0), \tag{3.14}$$

$$D_0^{(--)}(t) = \int_{C_z}\frac{dz}{2\pi i}[\theta(t)e^{zt} + \theta(-t)e^{-zt}]D_0^{(--)}(z), \tag{3.15}$$

$$D_0^{(-3)}(t+i\tau) = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty} e^{i\nu_n\tau}\int_{C_z}\frac{dz}{2\pi i}e^{zt}D_0^{(-3)}(z,n) \qquad (t>0), \tag{3.16}$$

$$D_0^{(33)}(-i\tau) = \frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty} e^{i\nu_n\tau}D_0^{(33)}(n) \qquad (0<\tau<\beta\hbar), \tag{3.17}$$

where

$$D_0^{(-+)}(z) = \frac{\hbar}{i}f(z), \tag{3.18}$$

$$D_0^{(--)}(z) = \frac{-\hbar}{\beta\hbar}\sum_{n=-\infty}^{\infty}\frac{z}{z^2-\nu_n^2}[f(z)-f(\nu_n)], \tag{3.19}$$

$$D_0^{(-3)}(z,n) = -\hbar\frac{z+\nu_n}{z^2-\nu_n^2}[f(z)-f(\nu_n)], \tag{3.20}$$

$$D_0^{(33)}(n) = \hbar f(\nu_n). \tag{3.21}$$

Here, ν_n is the Matsubara frequency defined by

$$\nu_n = 2\pi n/\beta\hbar, \tag{3.22}$$

and the function $f(x)$ by

$$f(x) = \frac{1}{m}\frac{1}{\omega^2+x^2}. \tag{3.23}$$

The contour C_z on the complex z plane runs parallel to the imaginary axis where the real part is chosen so that there are no poles on the left side of the path. Note that $D_0^{(--)}(z)$ cannot be denoted as the summation of $D_0^{(-3)}(z,n)$ since the term $\frac{\nu_n}{z^2-\nu_n^2}$, though odd in terms of n, is singular in the sense that it behaves like $1/n$ as $n\to\infty$.

Equations (3.14)–(3.17) with (3.18)–(3.21) may be easily checked if we use $(0<\tau<\beta\hbar)$

$$\frac{\cosh\omega(\tau-\beta\hbar/2)}{2\sinh(\omega\beta\hbar/2)}=\frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}\frac{\omega e^{i\nu_n\tau}}{\omega^2+\nu_n^2}, \tag{3.24}$$

$$\frac{\sinh\omega(\tau-\beta\hbar/2)}{2\sinh(\omega\beta\hbar/2)}=\frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}\frac{i\nu_n e^{i\nu_n\tau}}{\omega^2+\nu_n^2}, \tag{3.25}$$

and

$$\frac{1}{z^2-\nu_n^2}[f(z)-f(\nu_n)]=-mf(z)f(\nu_n). \tag{3.26}$$

Note that the summand in the right-hand side of Eq. (3.25) is singular implying jumps at $\tau=0,\beta\hbar$. This fact leads to the following relation to be used later:

$$\lim_{\tau\to 0^\pm}\frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}{}'\frac{e^{i\nu_n\tau}}{i\nu_n}=\pm\frac{1}{2}. \tag{3.27}$$

The prime means that the summation excludes the contribution from $n=0$.

By virtue of Eqs. (3.9)–(3.12), once one knows $D_0^{(-3)}(z,n)$, one can derive the other propagators. Though the process is trivial, it is useful when we derive the bilinearly corrected propagators so that we examine this process. Let us start from

$$D_0^{(-3)}(t+i\tau)=\frac{-\hbar}{\beta\hbar}\sum_{n=-\infty}^{\infty}e^{i\nu_n\tau}\int_{C_z}\frac{dz}{2\pi i}\times e^{zt}\frac{z+\nu_n}{z^2-\nu_n^2}[f(z)-f(\nu_n)]. \tag{3.28}$$

If we use

$$\int_{C_z}\frac{dz}{2\pi i}e^{zt}\frac{z+\nu_n}{z^2-\nu_n^2}[f(z)-f(\nu_n)]\to -f(\nu_n)\quad (t\to 0^+), \tag{3.29}$$

which is clear from the initial value theorem of the Laplace transformation, we get the following result by setting $t=0$ in Eq. (3.28):

$$D_0^{(33)}(-i\tau)=\frac{\hbar}{\beta\hbar}\sum_{n=-\infty}^{\infty}e^{i\nu_n\tau}f(\nu_n). \tag{3.30}$$

Thus we obtain $D_0^{(33)}(n)=\hbar f(\nu_n)$ as desired. Next, by noting a simple relation (for $n\neq 0$)

$$\frac{z+\nu_n}{z^2-\nu_n^2}=\frac{z}{z^2-\nu_n^2}+\frac{1}{\nu_n}\frac{z^2}{z^2-\nu_n^2}-\frac{1}{\nu_n}, \tag{3.31}$$

we have

$$\frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}e^{i\nu_n\tau}\frac{z+\nu_n}{z^2-\nu_n^2}[f(z)-f(\nu_n)] \tag{3.32}$$

$$\to\frac{1}{\beta\hbar}\sum_{n=-\infty}^{\infty}\frac{z}{z^2-\nu_n^2}[f(z)-f(\nu_n)]-\frac{i}{2}f(z)\quad(\tau\to 0^+). \tag{3.33}$$

We have used Eq. (3.27) and the fact that nonsingular terms, which are odd in terms of n, are summed up to zero. If we set $\tau=0^+$ in Eq. (3.28), the left-hand side becomes $\langle qq(t)\rangle$. Since $D_0^{(-+)}$ and $D_0^{(--)}$ are the imaginary and real part of $\langle qq(t)\rangle$, respectively, we get Eqs. (3.18) and (3.19) as desired.

IV. DERIVATION OF THE BILINEARLY CORRECTED PROPAGATORS

With the $J^{(\pm)}$ representation, we can recast Eq. (2.25) into the following form:

$$Z_J^L=e^{\frac{i}{\hbar}W_J^L}=e^{\sum_{i,j}\Psi_{ij}(\frac{\partial}{\partial J})}e^{\sum_i\Phi_{J,i}}\equiv e^{\Phi^{+-}}, \tag{4.1}$$

where

$$\Psi_{ij}\left(\frac{\partial}{\partial J}\right)=\frac{i}{\hbar}\left(\frac{\hbar}{i}\right)^2 c_{ij}\int_0^\infty dt\left(\frac{\partial}{\partial J_i^{(+)}(t)}\frac{\partial}{\partial J_j^{(-)}(t)}+\frac{\partial}{\partial J_i^{(-)}(t)}\frac{\partial}{\partial J_j^{(+)}(t)}\right)+\frac{1}{\hbar}\left(\frac{\hbar}{i}\right)^2 c_{ij}\int_0^{\beta\hbar}d\tau\frac{\partial}{\partial J_{3,i}(t)}\frac{\partial}{\partial J_{3,j}(t)}, \tag{4.2}$$

and $\Phi_{J,i}$, Φ^{+-} are given by making the following replacement in Eq. (3.2) [see also Eq. (6.2)].

Replacements with respect to $\Phi_{J,i}$:

$$(J^{(-)},J^{(+)},J_3)\to(J_i^{(-)},J_i^{(+)},J_{3,i}), \tag{4.3}$$

$$(D_0^{(-+)},D_0^{(--)},D_0^{(-3)},D_0^{(33)})\to(D_{0,i}^{(-+)},D_{0,i}^{(--)},D_{0,i}^{(-3)},D_{0,i}^{(33)}), \tag{4.4}$$

where $D_{0,i}^{(lm)}$ $(l,m=+,-,3)$ is given by the replacement:

$$(m,\omega)\to(m_i,\omega_i) \tag{4.5}$$

in Eq. (3.3). In the Laplace-Fourier representations in Eqs. (3.18)–(3.21), $D_{0,i}^{(lm)}$ is given through the following replacement:

$$f(x)=\frac{1}{m}\frac{1}{\omega^2+x^2}\to f_i(x)=\frac{1}{m_i}\frac{1}{\omega_i^2+x^2}. \tag{4.6}$$

Replacements with respect to Φ^{+-} [see (6.2)]:

$$(J^{(-)},J^{(+)},J_3)\to(J_i^{(-)},J_i^{(+)},J_{3,i}), \tag{4.7}$$

$$(D_0^{(-+)},D_0^{(--)},D_0^{(-3)},D_0^{(33)})\to(D_{ij}^{(-+)},D_{ij}^{(--)},D_{ij}^{(-3)},D_{ij}^{(33)}). \tag{4.8}$$

These quantities $D_{ij}^{(lm)}$ are the bilinearly corrected propagators we aim at deriving in what follows.

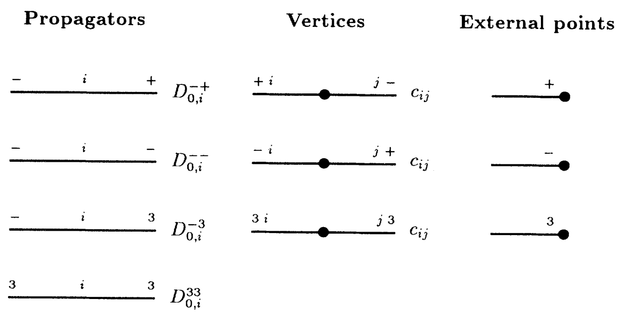
Let us begin with the derivation of $D_{ij}^{(-+)}$. This quantity is expressed as

$$D_{ij}^{(-+)}(t) = \frac{\hbar}{i}\theta(t)\frac{\partial}{\partial J_i^{(-)}(t)}\frac{\partial}{\partial J_j^{(+)}(0)}W_J^L$$
$$= \theta(t)\langle q_i(t)q_j - q_j q_i(t)\rangle, \tag{4.9}$$

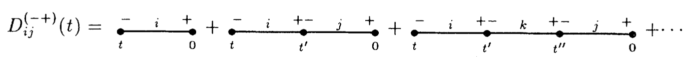
where $\langle X\rangle$ is the average of X by the initial bilinearly corrected density matrix whose dynamics is governed by the bilinearly corrected Hamiltonian. For example, $\langle q_i(t)q_j\rangle$ is given by Eq. (3.6) with Eq. (3.7) under the replacement

$$q \to q_i, \quad H \to \sum_i \left(\frac{q_i^2}{2m_i} + \frac{m_i\omega_i^2}{2}q_i^2\right) - \sum_{i,j} q_i c_{ij} q_j. \tag{4.10}$$

Thus we can calculate $D_{ij}^{(-+)}(t)$ by using the following Feynman rule. Note that this rule is immediately obtained from the third expression in Eq. (4.1).



By using the fact that $D_{0,i}^{(-+)}(t)$ is causal, we easily find the following graphical expression:



(4.11)

Let us consider the third graph explicitly. The algebraic expression of this quantity is given by

$$\left(\frac{i}{\hbar}\right)^3 \int_0^t dt' \int_0^t dt'' D_{0,i}^{(-+)}(t-t')c_{ik}D_{0,k}^{(-+)}(t'-t'')c_{kj}D_{0,j}^{(-+)}(t'') \tag{4.12}$$

$$= \frac{\hbar}{i}\int_{C_z}\frac{dz}{2\pi i}f_i(z)c_{ik}f_k(z)c_{kj}f_j(z). \tag{4.13}$$

Thus if we define matrices

$$[F_d(z)]_{ij} = f_i(z)\delta_{ij},$$
$$[F(z)]_{ij} = C_{ij}, \tag{4.14}$$

we have

$$D_{ij}^{(-+)}(z) = \frac{\hbar}{i}[F_d(z) + F_d(z)F(z)F_d(z)$$
$$+F_d(z)F(z)F_d(z)F(z)F_d(z) + \cdots]_{ij}, \tag{4.15}$$

which leads to the final expression,

$$D_{ij}^{(-+)}(z) = \frac{\hbar}{i}\tilde{F}_{ij}(z). \tag{4.16}$$

Here we have introduced the matrix $\tilde{F}(z)$ by

$$[\tilde{F}(z)]^{-1} = [F_d(z)]^{-1} - F(z), \tag{4.17}$$

where the inverse implies the one regarding (i,j) as the indices of the matrices.

We can calculate $D_{ij}^{(--)}(t)$ in a similar way. The graphs at the second order in c_i is given in Fig. 2. Due to the causality the number of graphs is considerably re-

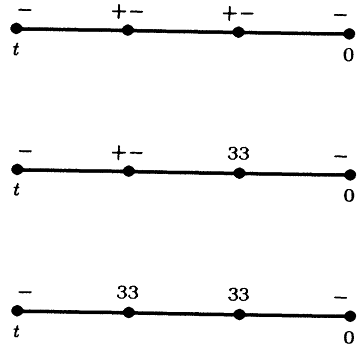


FIG. 2. The second-order graphs of $D^{(--)}(t)$.

duced by setting the time of the right end of graphs to $t = 0$. The estimation of these graphs is again done by the Laplace-Fourier transform. After many terms are canceled with one another, we arrive at the following simple expression:

$$D_{ij}^{(--)}(z) = -\frac{\hbar}{\beta\hbar}\sum_n \frac{z}{z^2-\nu_n^2}\Big\{[F_d(z) - F_d(\nu_n)] + [F_d(z)F(z)F_d(z) - F_d(\nu_n)F(\nu_n)F_d(\nu_n)] + \cdots\Big\}_{ij} .$$

The higher-order contributions are summed up to the following final result:

$$D^{(--)}(z) = -\frac{\hbar}{\beta\hbar}\sum_n \frac{z}{z^2-\nu_n^2}[\tilde{F}(z) - \tilde{F}(\nu_n)]. \qquad (4.18)$$

By a similar analysis we obtain $D^{(-3)}(z)$ and $D^{(33)}(z)$. The second-order graphs needed for calculation are written in Figs. 3 and 4. The results are given [see (6.3) below] if we replace $f(x)$ with the matrix $\tilde{F}(x)$ in Eqs. (3.18)–(3.21).

We would have been able to obtain all the elements of the bilinearly corrected propagators starting from $D^{(-3)}(z,n)$ just as before [see below (3.27)] and, in principle, we could have started from $D^{(33)}(\tau)$ by using the analytic continuation.

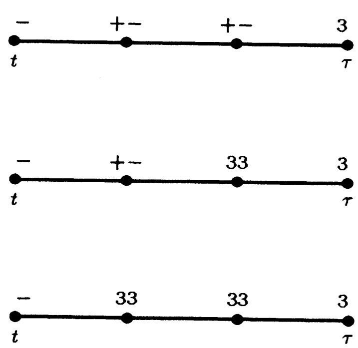


FIG. 3. The second-order graphs of $D^{(-3)}(t+i\tau)$.

FIG. 4. The second-order graphs of $D^{(33)}(-i\tau)$.

For the case where the linear-linear coupling matrix c_{ij} takes a nonzero value only when

$$c_{0j} = c_{j0} \equiv c_j \quad (j \neq 0), \qquad (4.19)$$

the expressions of the diagonal elements $D_{00}^{(-+)}(z)$ and $D_{00}^{(--)}(z)$ have been obtained in Ref. [24] [expressed as $2i\hat{A}(z)$ and $\hat{S}(z)$, respectively]. In this case the matrix $\tilde{F}(x)$ is replaced by a mere number $[1/f_0(x) - f_B(x)]^{-1}$ with $f_B(x) = \sum_{i=1}^N c_i^2 f_i(x)$. Their $\hat{\gamma}(x)$ and μ satisfy $Mx\hat{\gamma}(x) = \mu - f_B(x)$ with $M \equiv m_0$. If we recall that they started from the system Hamiltonian $H^{GSI} = P^2/2M + (M\Omega^2 + \mu)Q^2/2$ with $(P, Q, \Omega, M) \equiv (p_0, q_0, \omega_0, m_0)$, we find that our results reduce to theirs.

The Fourier transformation for the real-time variables instead of the Laplace transformation (the Fourier-Fourier representation) is easily obtained if we make the replacement

$$\int_{C_z} \frac{dz}{2\pi i} \to \int_{-\infty}^{\infty} \frac{dk}{2\pi}, \quad e^{zt} \to e^{ikt} \qquad (4.20)$$

in Eqs. (3.14)–(3.17) and

$$z \to i(k - i0^+) \qquad (4.21)$$

in Eqs. (3.18)–(3.21), etc. In this representation we can also show easily that our results reduce to those in Ref. [24] for the above special case of Eq. (4.19).

V. THE REDUCED DENSITY MATRIX

The coordinate representation of the reduced density matrix $\rho_J(Q', Q, t)$ can be obtained by using the method similar to the one used in deriving the generating functional. In this section we regard the 0th coordinate and momentum as the system degrees of freedom, i.e., $(p_0, q_0) = (P, Q)$. The reduced density matrix with the source $J = J_{\alpha,i}$ ($\alpha = 1,2,3; i = 1, \ldots, N$) is given by

$$\rho_J(t) = \frac{\mathrm{Tr}_B \sigma_J(t)}{\mathrm{Tr}\sigma_J(t)}, \qquad (5.1)$$

where

$$\sigma_J(t) = T_C e^{-\frac{i}{\hbar}\int_C dt' H^J(t')}, \qquad (5.2)$$

and Tr_B (Tr) implies the trace over all degrees of freedom of the bath (the total system). The time $t = T$ of

$\sigma_J(t)$ is the final (initial) time of C_1 (C_2) (see Fig. 1) and $t = T$ is assumed to be finite in this section. Though the actual reduced density matrix is obtained as $\rho_J(t)$ at $J = 0$, we introduce the source terms for later convenience. In the coordinate representation the unrenormalized reduced density matrix $\mathrm{Tr}_B\sigma_J(t)$ is expressed as

$$\sigma_J(Q',Q,t) \equiv \langle Q'|\mathrm{Tr}_B\sigma_J(t)|Q\rangle \tag{5.3}$$

$$= e^{-\frac{i}{\hbar}\int_C dt' V(\frac{\partial}{\partial J(t')})}\sigma_J^L(Q',Q,t), \tag{5.4}$$

where V in the above expression is the nonbilinear interaction of the total system and $\sigma_J^L(Q',Q,t)$ is given by

$$\sigma_J^L(Q',Q,t) = e^{-\frac{i}{\hbar}\int_C dt' \sum_{ij}\frac{\partial}{\partial J_i(t')}c_{ij}\frac{\partial}{\partial J_j(t')}} \times \langle Q'|T_C e^{-\frac{i}{\hbar}\int_C dt' H_S^J(t')}|Q\rangle \times \prod_{i=1}^{N} e^{\Phi_{J,i}}. \tag{5.5}$$

Here, $\Phi_{J,i}$ is given in Eq. (4.1) and the second element in the product on the right-hand side is given by Eq. (2.19) with (q',q,p,m,ω,J,T) replaced by (Q',Q,P,M,Ω,J_0,t). The exponent of the second element in Eq. (5.5) is bilinear in terms of the vector (Q',Q,J_0) [see Eq. (2.19)]. The functional $\Phi_{J,i}$ is also bilinear in terms of the vector $(J_1,\ldots,J_N)$. Thus, we can write Eq. (5.5) in the following form:

$$\sigma_J^L(Q',Q,t) = e^{-\frac{i}{\hbar}\int_C dt' \sum_{ij}\frac{\partial}{\partial J_i(t')}c_{ij}\frac{\partial}{\partial J_j(t')}} e^{\tilde{\mathbf{J}}\cdot M\tilde{\mathbf{J}}} \times (\text{a factor independent of } Q',Q,J), \tag{5.6}$$

where $\tilde{\mathbf{J}} = (Q',Q,J_0,\ldots,J_N)$ and M is a matrix independent of $\tilde{\mathbf{J}}$. From the identity (2.26), we know that $\sigma_J^L(Q',Q,t)$ takes the following form:

$$\sigma_J^L(Q',Q,t) = \tilde{\sigma}_J^L(r,x,t)$$
$$= N(t)e^{-\frac{1}{2}Ar^2-\frac{1}{2}Bx^2+Crx+Er+Fx+\mathbf{J}\cdot D\mathbf{J}}, \tag{5.7}$$

where A,B,C are independent of $J_0,\ldots,J_N$ while E,F are linear combinations of $J_0,\ldots,J_N$, and $N(t)$ is independent of $r,x,J_0,\ldots,J_N$. Here we have introduced r and x by

$$r = \frac{Q'+Q}{2}, \quad x = Q'-Q, \tag{5.8}$$

and $\mathbf{J}\cdot D\mathbf{J}$ is a symbolic notation for

$$\mathbf{J}\cdot D\mathbf{J} \equiv \left(\frac{i}{\hbar}\right)^2 \sum_{ij}\int_C dt\int_C ds J_i(t)D_{ij}(t-s)J_j(s)$$
$$= \frac{i}{\hbar}W_J^L, \tag{5.9}$$

where D_{ij} is the bilinearly corrected propagator. In order to identify D_{ij} with the bilinearly corrected operator we have used the fact that $Z_J^L = \int dr\tilde{\sigma}_J^L(r,0,t)$. The coordinate representation of the reduced density matrix is now expressed as

$$\rho_J(Q',Q,t) \equiv \langle Q'|\rho_J(t)|Q\rangle$$
$$= \frac{e^{-\frac{i}{\hbar}\int_C dt' V(\frac{\partial}{\partial J(t')})}\tilde{\sigma}_J^L(r,x,t)}{e^{-\frac{i}{\hbar}\int_C dt' V(\frac{\partial}{\partial J(t')})}\int dr\tilde{\sigma}_J^L(r,0,t)}. \tag{5.10}$$

We are now in a position to connect A,B,C,E,F with various expectation values or correlation functions. Let us start from the expectation value of Q;

$$\langle Q\rangle_t \equiv \mathrm{Tr}Q\rho_J^L(t) = \int dQQ\rho_J^L(Q,Q,t)$$
$$= \frac{\partial}{\partial E}\ln\int dQe^{-\frac{1}{2}AQ^2+EQ+\frac{1}{2}\mathbf{J}\cdot D\mathbf{J}} = \frac{E}{A}, \tag{5.11}$$

where $\rho_J^L(t)$ is $\rho_J(t)$ with nonbilinear interaction V set to zero, or

$$\rho_J^L(Q',Q,t) \equiv \langle Q'|\rho_J^L(t)|Q\rangle = \frac{\tilde{\sigma}_J^L(r,x,t)}{\int dr\tilde{\sigma}_J^L(r,0,t)}. \tag{5.12}$$

The connected part of the equal-time autocorrelation function of Q (variance of Q) can be connected with A in the following manner:

$$\langle Q^2\rangle \equiv \mathrm{Tr}Q^2\rho_J^L(t) - (\mathrm{Tr}Q\rho_J^L(t))^2$$
$$= \frac{\partial}{\partial E^2}\ln\int dQe^{-\frac{1}{2}AQ^2+EQ+\frac{1}{2}\mathbf{J}\cdot D\mathbf{J}} = \frac{1}{A}. \tag{5.13}$$

The expectation value of the momentum P is identified with F as follows:

$$\langle P\rangle_t \equiv \mathrm{Tr}P\rho_J^L(t)$$
$$= \int dPdQ'dQPe^{\frac{i}{\hbar}P(Q-Q')}\rho_J^L(Q',Q,t)$$
$$= \frac{\hbar}{i}\int dr\left.\frac{\partial\tilde{\rho}_J^L(r,x)}{\partial x}\right|_{x=0} = \frac{\hbar}{i}F. \tag{5.14}$$

We can show that $C = 0$ by considering the following symmetric correlation function;

$$\left\langle\frac{PQ+QP}{2}\right\rangle \equiv \mathrm{Tr}\left[\frac{PQ+QP}{2}\rho_J^L(t)\right]$$
$$= \int dPdQ'dQP\frac{Q'+Q}{2}e^{\frac{i}{\hbar}P(Q-Q')}$$
$$\times\rho_J^L(Q',Q,t)$$
$$= \frac{\hbar}{i}\int drr\left.\frac{\partial\tilde{\rho}_J^L(r,x,t)}{\partial x}\right|_{x=0} = \frac{\hbar}{i}\frac{C}{A}. \tag{5.15}$$

If we note that

$$\left.\begin{array}{l}\langle PQ\rangle\\ \langle QP\rangle\end{array}\right\} = \int drdx\left(-\frac{\hbar}{i}\frac{\partial\delta(x)}{\partial x}\right)\left(r\pm\frac{x}{2}\right)\tilde{\rho}_J^L(r,x,t)$$
$$=\pm\frac{\hbar}{2i}\int dr\tilde{\rho}_J^L(r,0,t) \tag{5.16}$$

we arrive at the result $C=0$.

The equal-time autocorrelation of P becomes

$$\mathrm{Tr}P^2\rho_J^L(t) = -\hbar^2\int dr\left.\frac{\partial^2\tilde{\rho}_J^L(r,x,t)}{\partial x^2}\right|_{x=0}$$
$$= -\hbar^2(-B+F^2). \tag{5.17}$$

Thus the variance of P is expressed as

$$\langle P^2\rangle \equiv \mathrm{Tr}P^2\rho_J^L(t) - \langle P\rangle_{L,t}^2 = \hbar^2 B. \tag{5.18}$$

Thereby we have the result

$$\tilde{\sigma}_J^L(r,x,t) = \sqrt{\frac{1}{2\pi\langle Q^2\rangle}}\; e^{-\frac{(r-\langle Q\rangle_t)^2}{2\langle Q^2\rangle}-\frac{\langle P^2\rangle}{2\hbar^2}x^2+\frac{i}{\hbar}\langle P\rangle_t x+\mathbf{J}\cdot D\mathbf{J}}, \tag{5.19}$$

where $\mathbf{J}\cdot D\mathbf{J}$ is given in Eq. (5.9). The quantities $\langle Q\rangle_t$, $\langle P\rangle_t$, $\langle Q^2\rangle$, $\langle P^2\rangle$ are easily obtained through the generating functional and are given explicitly in terms of the bilinearly corrected propagators as follows.

$$\langle Q\rangle_t = \frac{\partial W_J^L}{\partial J^{(-)}(t)} = \frac{i}{\hbar}\int_0^t ds\sum_j\left[D_{0j}^{(-+)}(t-s)J_j^{(+)}(s)+D_{0j}^{(--)}(t-s)J_j^{(-)}(s)\right]$$
$$+\frac{1}{\hbar}\int_0^{\beta\hbar}d\tau\sum_j D_{0j}^{(-3)}(t+i\tau)J_{3,j}(\tau),$$
$$\langle P\rangle_t = M\frac{\partial}{\partial t}\frac{\partial W_J^L}{\partial J^{(-)}(t)} = M\frac{\partial}{\partial t}\langle Q\rangle_t,$$
$$\langle Q^2\rangle = \frac{\hbar}{i}\frac{\partial}{\partial J_0^{(-)}(t)}\frac{\partial}{\partial J_0^{(-)}(t')}W_J^L\bigg|_{t=t'=0} = D_{00}^{(--)}(0),$$
$$\langle P^2\rangle = M^2\frac{\partial}{\partial t}\frac{\partial}{\partial t'}\frac{\hbar}{i}\frac{\partial}{\partial J_0^{(-)}(t)}\frac{\partial}{\partial J_0^{(-)}(t')}W_J^L\bigg|_{t=t'=0} = -M^2\ddot{D}_{00}^{(--)}(0). \tag{5.20}$$

The above results generalize the expression for the density-matrix element given in Ref. [12] with considerably easier calculation. Namely, the external forces were restricted to $F(t)$ and $f(t)$ only [which correspond to $J^-(t)$ and $J^+(t)$, respectively] in Ref. [12], while the three external forces $J^-(t)$, $J^+(t)$, and $J_3(t)$ are introduced in the present work. As a result, we can investigate anharmonicity and nonbilinear effects not only on the C_1+C_2 path but also on the C_3 path. The density-matrix element enables us to study the differences between quantum and classical dynamics, particularly if we introduce the Wigner representation [12,24].

VI. CONCLUSION

We have derived the bilinearly corrected propagator by using a graphical technique. Thereby we have succeeded in taking the inverse in (i,t) space with t on the unified time path [see below (2.29)]. The results are summarized as follows. The generating functional defined in (2.8) is given by

$$Z_J = e^{-\frac{i}{\hbar}\int_C dtV\left(\frac{\partial}{\partial J(t)}\right)}e^{\frac{i}{\hbar}W_J^L}, \tag{6.1}$$

where the generating functional for the connected correlation function $\frac{i}{\hbar}W_J^L$ given in Eq. (2.28) can be rewritten as

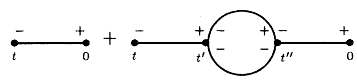
$$\Phi^{+-} = \left(\frac{i}{\hbar}\right)^2\int_0^\infty dt\int_0^\infty ds\left(J_i^{(-)}(t)D_{ij}^{(-+)}(t-s)J_j^{(+)}(s)+\frac{1}{2}J_i^{(-)}(t)D_{ij}^{(--)}(t-s)J_j^{(-)}(s)\right)$$
$$+\frac{i}{\hbar}\frac{1}{\hbar}\int_0^\infty dt\int_0^{\beta\hbar}d\tau J_i^{(-)}(t)D_{ij}^{(-3)}(t+i\tau)J_{3,j}(\tau)+\frac{1}{2}\frac{1}{\hbar^2}\int_0^{\beta\hbar}d\tau\int_0^{\beta\hbar}d\tau' J_{3,i}(\tau)D_{ij}^{(33)}(-i\tau+i\tau')J_{3,j}(\tau'), \tag{6.2}$$

where the Fourier-Laplace representations of the propagators are the following:

$$
\begin{aligned}
D_{ij}^{(-+)}(t) &= \int_{C_z} \frac{dz}{2\pi i} e^{zt} \frac{\hbar}{i} \tilde{F}_{ij}(z), \\
D_{ij}^{(--)}(t) &= \int_{C_z} \frac{dz}{2\pi i} [\theta(t)e^{zt} + \theta(-t)e^{-zt}] \frac{-\hbar}{\beta\hbar} \sum_n \frac{z}{z^2 - \nu_n^2} [\tilde{F}(z) - \tilde{F}(\nu_n)]_{ij}, \\
D_{ij}^{(-3)}(t + i\tau) &= \frac{1}{\beta\hbar} \sum_{n=-\infty}^{\infty} e^{i\nu_n \tau} \int_{C_z} \frac{dz}{2\pi i} e^{zt} \frac{-\hbar}{z - \nu_n} [\tilde{F}(z) - \tilde{F}(\nu_n)]_{ij}, \\
D_{ij}^{(33)}(-i\tau) &= \frac{1}{\beta\hbar} \sum_{n=-\infty}^{\infty} e^{i\nu_n \tau} \hbar \tilde{F}_{ij}(\nu_n),
\end{aligned}
\tag{6.3}
$$

where the matrix $\tilde{F}(\nu_n)$ is given in Eq. (4.17). As mentioned at the end of the fourth section, if we set $z = i(k - i0^+)$ in the above expressions, we readily obtain the Fourier-Fourier representation of the propagators. From the expression (6.1) it is trivial to construct the Feynman rule. It is emphasized here that the vertex $V(\partial/\partial J(t))$ comes from the anharmonic interaction since the linear-linear interactions are fully taken into the above propagators.

As a simple illustration of the Feynman rule, we consider the system-bath Hamiltonian with the anharmonic interaction $V(q,t) = gQ^3/3!$ where the system is represented by $(p_0, q_0, m_0, \omega_0) = (P, Q, M, \Omega)$. The Feynman rule for this system is given through the bilinearly corrected propagators $D_{ij}^{(lm)}(t - s)$ and the three-point vertices illustrated in Fig. 5. By this rule we have the following expression for the first-order correlation function of Q:

$-2i\mathrm{Im}\langle QQ(t)\rangle_g =$  $+ \cdots,$ (6.4)

where the lines represent not $D_i^{(lm)}$ but $D_{00}^{(lm)}$. $\langle X\rangle_g$ is the connected part of the average of X by the initial density matrix for the full Hamiltonian including the interacting term gQ^3. The time evolution on the left-hand side of (6.4) is done also by the full Hamiltonian. Explicitly the leading correction term becomes

$$
\begin{aligned}
&\left(-\frac{ig}{\hbar}\right)^2 \int_0^\infty dt' \int_0^\infty dt'' D_{00}^{(-+)}(t - t') D_{00}^{(--)}(t' - t'') D_{00}^{(-+)}(t' - t'') D_{00}^{(-+)}(t'') \\
&\qquad = \left(-\frac{ig}{\hbar}\right)^2 \int_{C_z} \frac{dz}{2\pi i} e^{zt} D_{00}^{(-+)}(z) \Sigma_{00}(z) D_{00}^{(-+)}(z),
\end{aligned}
\tag{6.5}
$$

where

$$
\Sigma_{ij}(z) = \int_0^\infty dt e^{-zt} D_{ij}^{(--)}(t) D_{ij}^{(-+)}(t). \tag{6.6}
$$

We give one more example. Assume we have a nonbilinear coupling $gQ\sum_i q_i^2/2$ in addition to the bilinear coupling $Q\sum_i c_i q_i$. In this case we have only to interpret the lines in Eq. (6.4) slightly differently. In the previous case, the lines always corrspond to $D_{00}^{(lm)}$, while in this case of nonbilinear system-bath coupling, the lines imply various $D_{ij}^{(lm)}$. Namely, the second graph in (6.4) in this case stands for several algebraic expressions. One of them is given by

$$
\left(-\frac{ig}{\hbar}\right)^2 \int_{C_z} \frac{dz}{2\pi i} \sum_{ij} D_{00}^{(-+)}(z) \Sigma_{ij}(z) D_{00}^{(-+)}(z).
$$

The estimation of these formal expressions together with other quantities in the context of quantum optics needs a separate study and is now underway.

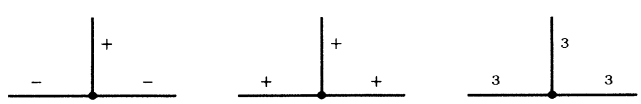


FIG. 5. The three-point vertices appearing in the Feynman rule for the system-bath Hamiltonian.

The coordinate representation of the reduced density matrix has been also derived in a simple way. The result is expressed in Eq. (5.10) with Eq. (5.19). Note that we can immediately derive the Feynman rule from this expression once anharmonicity of the potential V is given.

Though the concept of the unified time path extended a little in this paper is effective in calculation and argument, it may be still considered as in its primitive level. If the Fourier transform counterparts on the unified path were cleverly constructed, our derivation could be more straightforward. This point is now under investigation.

The actual calculation using the Feynman rule derived here has a wide range of applicability. Applications to nonlinear quantum optics and the chemical reaction rate problem are now underway.

In this paper, we demonstrated the calculation of correlation functions based on the perturbative expansion of the anharmonicity of the potential. However if we use a novel method of the Legendre transformation recently developed in the context of quantum field theory [27], we can obtain nonperturbative results for any physical quantities that we are aiming at. In this case the generating functional derived here is a starting quantity to be Legendre-transformed. This line of study is also now under consideration.

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APPENDIX A: THE PATH INTEGRAL ON THE UNIFIED TIME PATH

In this appendix we introduce the concept of the path integration on the unified time path. We assume $m = \hbar = 1$ and consider, as a typical example,

$$\langle q'|K_C|q\rangle \equiv \langle q'|T_C e^{-i\int_C dt[p^2/2+\omega^2 q^2/2-J(t)q]}|q\rangle. \quad \text{(A1)}$$

As mentioned in Sec. II, we divide the unified time path into $N+1$ pieces ($t_0 = 0, t_1, \ldots, t_N, t_{N+1} = -i\beta\hbar$) and introduce ϵ_i's; $\epsilon_i \equiv (\epsilon_0, \epsilon_1, \ldots, \epsilon_N)$ such that

$$t_i = \sum_{k=0}^{i-1} \epsilon_k, \quad t_i - t_j = \sum_{k=j}^{i-1} \epsilon_k \quad (i > j). \quad \text{(A2)}$$

Since we aim at deriving the expression in the limit of large N, we freely deal with ϵ_i as if it were an infinitesimal quantity and N as infinity in the following. Then we obtain the following self-evident generalization of the familiar expression after inserting complete sets of q and p:

$$\langle q'|K_C|q\rangle = \int_{q_0=q}^{q_{N+1}=q'} dq_1 \cdots dq_N \int \frac{dp_0}{2\pi} \cdots \frac{dq_N}{2\pi} e^{iA_{pq}}, \quad \text{(A3)}$$

where

$$A_{pq} = \sum_{i=0}^{N} \epsilon_i \left[p_i(q_{i+1} - q_i) - \frac{1}{2}\epsilon_i p_i^2 - \frac{\omega^2}{2}\epsilon_i \bar{q}_i^2 + \epsilon_i J_i q_i \right]. \quad \text{(A4)}$$

Here we applied the midpoint difference prescription, that is, $2\bar{q}_i = q_{i+1} + q_i$. The integration over p_i leads to

$$\langle q'|K_C|q\rangle = \left[\prod_{i=0}^{N} \int \frac{dq_i}{(2\pi\epsilon_i i)^{1/2}}\right] e^{iA_q} \equiv \int [q] e^{i\int_C dt\mathcal{L}^J(t)}, \quad \text{(A5)}$$

where

$$A_q = \int_C dt\mathcal{L}^J(t) = \sum_{i=0}^{N} \left[\frac{1}{2\epsilon_i}(q_{i+1} - q_i)^2 - \epsilon_i \frac{\omega^2}{8}(q_{i+1} + q_i)^2 + \epsilon_i J_i q_i \right]. \quad \text{(A6)}$$

If we introduce

$$a_i = \frac{1}{2\epsilon_i} - \frac{\omega^2}{8}\epsilon_i, \quad b_i = \frac{1}{2\epsilon_i} + \frac{\omega^2}{8}\epsilon_i, \quad \text{(A7)}$$

and the vectors

$$\mathbf{q} = (q_1, \ldots, q_N), \quad \mathbf{d} = \left(b_0 q_0, \frac{\epsilon_2}{2}J_2, \frac{\epsilon_3}{2}J_3, \ldots, \frac{\epsilon_{N-1}}{2}J_{N-1}, b_N q_{N+1}\right), \quad \text{(A8)}$$

A_q is expressed as

$$A_q = a_0 q_0^2 + a_N q_{N+1}^2 + \mathbf{q}\cdot M(1,N)\mathbf{q} - 2\mathbf{d}\cdot\mathbf{q}, \quad \text{(A9)}$$

where the $N \times N$ matrix $M(1,N)$ is given through

$$M(j,k) = \begin{pmatrix} a_{j-1}+a_j & -b_j & 0 & 0 & \cdots & 0 \\ -b_j & a_j + a_{j+1} & -b_{j+1} & 0 & \cdots & 0 \\ 0 & -b_{j+1} & a_{j+1}+a_{j+2} & -b_{j+2} & \cdots & 0 \\ & & & \cdots & & \\ 0 & \cdots & 0 & -b_{k-2} & a_{k-2}+a_{k-1} & -b_{k-1} \\ 0 & 0 & \cdots & 0 & -b_{k-1} & a_{k-1}+a_k \end{pmatrix}, \quad \text{(A10)}$$

with $k > j$ and we have assumed $J_1 = J_N = 0$ without loss of generality. Thus, after changing the variable of integration from $\mathbf{q}$ to $\mathbf{x} = \mathbf{q} - [M(1,N)]^{-1}\mathbf{d}$, we can easily perform the integration;

$$\langle q'|K_C|q\rangle = \left[\prod_{i=0}^{N}(2\pi\epsilon_i i)^{-1/2}\right]\left[\frac{(\pi i)^N}{D(1,N)}\right]^{1/2} \times e^{i(a_0 q_0^2 + a_N q_{N+1}^2 - \mathbf{d}\cdot[M(1,N)]^{-1}\mathbf{d})}. \quad \text{(A11)}$$

Here we have denoted the determinant of the $N \times N$ matrix $M(1,N)$ as $D(1,N)$. From now on, we slightly extend the known method of evaluating the inverse of $M(1,N)$ [28]. Let us consider the determinant $D(j,k)$ of the matrix $M(j,k)$. It satisfies the following recurrence relation easily obtained by expansion in terms of the cofactor:

$$D(j,k) = (a_{k-1} + a_k)D(j,k-1) - b_{k-1}^2 D(j,k-2). \quad \text{(A12)}$$

If we introduce

$$\alpha_k = \frac{1}{2\epsilon_k} - \frac{\omega^2}{8}\epsilon_k + i\frac{\omega}{2}, \quad \beta_k = \frac{1}{2\epsilon_k} - \frac{\omega^2}{8}\epsilon_k - i\frac{\omega}{2}, \tag{A13}$$

we can rewrite the above recurrence formula as

$$\begin{aligned} D(j,k) &- \alpha_k D(j,k-1) \\ &= \beta_{k-1}[D(j,k-1) - \alpha_{k-1}D(j,k-2)] \quad (\alpha \leftrightarrow \beta). \end{aligned} \tag{A14}$$

It is easy to check that the general solution to this equation is given by

$$D(j,k) = A\prod_{l=j}^{k}\alpha_l + B\prod_{l=j}^{k}\beta_l \quad (k > j). \tag{A15}$$

Noting the conditions

$$D(j,j) = a_{j-1} + a_j, \quad D(j,j-1) \equiv 1, \tag{A16}$$

we have $A = \alpha_{j-1}/i\omega$, $B = -\beta_{j-1}/i\omega$, which leads to, in the large N limit,

$$D(j,k) = \frac{2}{\omega}\left[\prod_{l=j-1}^{k}\frac{1}{2\epsilon_l}\right]\sin\omega(t_{k+1} - t_{j+1}) \quad (k > j). \tag{A17}$$

Thus we have a formula,

$$2\epsilon_{j-1}\tilde{D}(j,k) = \frac{2\sin\omega(t_k - t_j)}{\omega} \quad (k > j), \tag{A18}$$

where

$$\tilde{D}(j,k) = D(j,k)\prod_{l=j}^{k}2\epsilon_l. \tag{A19}$$

Thereby the prefactor in (A11) is given by

$$\begin{aligned} \left[\prod_{i=0}^{N}(2\pi\epsilon_i i)^{-1/2}\right]\left[\frac{(\pi i)^N}{D(1,N)}\right]^{1/2} &= \frac{1}{2\pi\epsilon_0 i\tilde{D}(1,N)} \\ &= \frac{\omega}{2\pi\sinh\omega\beta}, \end{aligned} \tag{A20}$$

Since the i-j element of the cofactor of the matrix M is given by, for $j > i$,

$$\begin{aligned} \Delta_{ij} &= D(1,i-1)\left(\prod_{l=i}^{j-1}b_l\right)D(j+1,N) \\ &\approx \frac{2\epsilon_j}{\prod_{l=i}^{N}2\epsilon_l}\tilde{D}(1,i-1)\tilde{D}(j+1,N), \end{aligned} \tag{A21}$$

we get, for $j > i$,

$$\begin{aligned} [M(1,N)]^{-1}_{ji} &= \frac{\Delta_{ij}}{D(1,N)} \\ &= \frac{\tilde{D}(1,i-1)}{\tilde{D}(1,N)}2\epsilon_j\tilde{D}(j+1,N). \end{aligned} \tag{A22}$$

Thus we have

$$\begin{aligned} [M(1,N)]^{-1}_{ji} = \theta(j-i)&\frac{2\sin\omega(t_i - t_j)\sin\omega(t_j - t_N)}{\omega\sin(-i\omega\beta)} \\ &+(i \leftrightarrow j). \end{aligned} \tag{A23}$$

By recovering m and $\hbar$ we arrive at the result given in (2.19).

APPENDIX B: DERIVATION OF EQ. (2.26)

Equation (2.26) is simply derived by using the relation

$$\begin{aligned} &\int dx_i \cdots dx_n e^{-\frac{1}{2}x_i(A+B)_{ij}x_j + J_i x_i} \\ &= e^{-\frac{\partial}{\partial J_i}A_{ij}\frac{\partial}{\partial J_j}}\int dx_i \cdots dx_n e^{-\frac{1}{2}x_i B_{ij}x_j + J_i x_i} \end{aligned} \tag{B1}$$

and the well-known identity

$$\begin{aligned} &\int dx_i \cdots dx_n e^{-\frac{1}{2}x_i A_{ij}x_j + J_i x_i} \\ &= (2\pi)^{n/2}(\det A)^{1/2}e^{\frac{1}{2}J_i A^{-1}_{ij}J_j}. \end{aligned} \tag{B2}$$

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