Study of the entanglement in systems with periodic boundary conditions

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(joint work with
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Abstract

In this work we give a new definition for the linking number between two oriented closed or open chains in a system with three periodic boundary conditions (p.b.c.), and of the self-linking number and the writhe of one oriented closed or open chain in a system with three p.b.c.. Furthermore, we show how this definition of the linking number, for two oriented closed chains in a system with p.b.c., coincides with the Gauss linking number of two oriented closed chains in 3-space, and also with the Gauss linking number of two oriented closed chains in a 3-manifold. This definition is suitable for studying entanglement in a collection of closed, or open polymer chains, as they are given by a computer generated atomistic polymer sample. Using this new measure of linking for chains in systems with three p.b.c., we study numerically the effect of CReTA (Contour Reduction Topological Analysis) algorithm on the entanglement of polyethylene chains. Our results show that the new linking measure is consistent for the original and reduced systems. It can be used to characterize entanglement under periodic boundary conditions.

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