Fermi operator expansion method for nuclei and inhomogeneous matter with a nuclear energy density functional†

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It is critically important to calculate nuclear matter in various phases with different temperatures, as it is essential for simulation studies of supernovae and neutron stars. The nuclear energy density functional method at finite temperature is a desirable choice for studying the inhomogeneous neutron-star matter in outer and inner crusts. Moreover, near the boundary between the inner crust and the core, various exotic phases, "nuclear pasta.," are expected to appear.

In order to properly treat thermally dripped nucleons and to study the transition from inhomogeneous to uniform nuclear matter, the coordinate-space representation is preferable. Furthermore, to find novel structure at finite temperature, it is desired to perform the calculation without assuming any spatial symmetry of the configuration using the three-dimensional (3D) coordinate-space representation. As the 3D coordinate-space solution is computationally demanding, most of the finite-temperature mean-field calculations for nuclei either adopt the harmonic-oscillator-basis (shell-model-basis) representation or are restricted to the spherical systems.

A conventional solution of the finite-temperature mean-field theory can be summarized as follows: (1) Construct the mean-field Hamiltonian H, which de pends on one-body densities; (2) diagonalize the Hamiltonian to obtain the eigenvalues and the eigenvectors, $H|i\rangle = \epsilon_i|i\rangle$; and (3) calculate the densities, then, go back to (1) to achieve self-consistency. In step (3), the Fermi-Dirac distribution function $f(x)$ is used to calculate the densities, $\rho = \sum_i f(\epsilon_i)|i\rangle\langle i|$. A truncation with respect to the eigenvector $|i\rangle$ may be possible at low temperature, while, at high temperature, one needs to compute all the eigenvalues and eigenvectors. As this diagonalization is needed every iteration, it requires a large amount of numerical resources.

The objectives of the present study are to investigate an alternative method for the finite-temperature mean-field calculation and to examine its performance for nuclear systems. The methodology is known as the Fermi operator expansion (FOE) method in condensed matter physics.[1,2] It is also known as an order-N ($O(N)$) method;[3] thus, the number of computational operations linearly scales with respect to either the particle number or the dimension of the one-particle space. In $O(N)$ methods, the "nearsightedness" of many elec tron systems plays a crucial role.[4] As the nearsightedness is due to the destructive interference effect in quantum mechanical many-particle systems, I expect that it is applicable to nuclear systems as well. However, as the size of a nucleus is roughly ten femtometers at most, the nearsightedness principle has been assumed to have a minimal effect in practice. The situation may be different for hot nuclei and macroscopic neutron-star matters. It is worthwhile to study $O(N)$ methods used to calculate nuclei at finite temperature and inhomogeneous nuclear matter.

I examine the applicability and the usefulness of the FOE method in nuclear energy density functional approaches at finite temperature. The one-body density matrix, which is identical to the Fermi operator, is expanded in terms of the Chebyshev polynomials up to the finite order. The maximum degree of the polynomials is inversely proportional to the temperature. Thus, the FOE method becomes extremely efficient for calculations at high temperature. Polynomial expansion is applied to calculations of the entropy, which allows for the estimation of the free energy without diagonalization of the Hamiltonian matrix.

I investigate thermal properties of the shape transition and the liquid-gas transition in isolated nuclei. For periodic non-uniform nuclear matter, the self-consistent iteration is initiated with different initial states, such as the simple cubic and bcc configurations. At low temperature, both the simple cubic and bcc states exist as self-consistent solutions. I found that the cubic state is lower in free energy than the bcc state. The transition to the uniform matter takes place at T_c, a value that is smaller than that of a larger cell. This volume effect on the critical temperature T_c is due to the volume dependence of the entropy of the uniform matter.

The advantageous features of the FOE method from a computational perspective can be summarized as follows: (1) The matrix diagonalization is not involved in the calculation, including the calculation of the entropy; (2) the calculation of the density matrix ρ_{ij} is independent of the index j. Thus, it is suitable for distributed-memory parallel computing; and (3) the computational cost could scale linearly with respect to the space dimension N, when N is large enough. Here, N is the dimension of matrix ρ_{ij}.

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