Mean field calculation of thermal properties of simple nucleon matter on a lattice

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Thermal properties of single species nucleon matter are investigated assuming a simple form of the nucleon-nucleon interaction. The nucleons are placed on a cubic lattice, hopping from site to site and interacting through a spin-dependent force, as in the extended, attractive Hubbard model. A mean field calculation in the Hartree-Fock-Bogoliubov approximation suggests that the superfluid ground state generated by strong nucleon pairing undergoes a second-order phase transition to a normal state as the temperature increases. The calculation is shown to lead to a promising description of the thermal properties of low-density neutron matter. A possibility of a density wave phase is also examined.

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I. INTRODUCTION

Nuclear excitations are complicated dynamical phenomena, depending on the detailed structure of the individual nucleus, and must be examined based on the specific structure of the nucleus, such as whether it is closed or open shell. As the excitation energy gets higher, however, the excitations depend less on specific nuclear structure and start to exhibit more common features among (heavy) nuclei. These features are expected to be reasonably well represented by excitations of nuclear matter. Furthermore, dynamics of supernovae and neutron stars, which have been of much astronomical interest, are expected to be better understood through the study of excitations of neutron matter [1,2]. The gross features of the thermal properties of nucleon matter have been examined by means of statistical models [3] and lattice gas models [4]. More realistic descriptions of the thermal properties have been provided through applications of various approaches in the nuclear many-body theories [5–10]. Applications of the traditional nuclear many-body theories regarding nucleon matter at zero temperature have been extensive [2,11–13], and provide the most reliable information on the properties of nucleon matter at low temperatures.

Previously, one of us (R.S.) collaborated on a Monte Carlo calculation of nuclear matter on a lattice [14], which provides a new framework for studying the thermal properties of nucleon matter. Though the computational space was small and the nucleon-nucleon interaction was simple, the calculation has proven to be of much promise, demonstrating the occurrence of a phase transition around 15 MeV using the parameters adjusted to reproduce the saturation properties. A similar calculation of nucleon matter of a single species has also been initiated in the same work, using the same form of the Hamiltonian. Though a phase transition appeared to take place at a few MeV, the evidence for it was not quite solid owing to statistical fluctuations, which are enhanced at low temperature (a sign problem). The phase transitions may correspond to those expected through paired nucleons (Cooper pairs) in nucleon matter [1,2].

In order to gain a better understanding of the possible, latter phase transition, we apply in this work the analytic means of a mean field approach to the problem in the same lattice formulation. From this work, we do not expect to be able to draw precise quantitative conclusions, but rather we will try to learn the nature of the phase transition at a semi-quantitative level. For this purpose, we take the thermodynamical (infinite volume) limit for numerical results, so as to obtain a clear signal of the phase transition. The mean field results in this work will also serve as a reference for the more extensive Monte Carlo calculation that we are currently carrying out.

Our Hamiltonian for single-species nucleon matter turns out to be an extended, attractive Hubbard model, which has been studied as a simple model of high-temperature superconductivity [15]. The mean field calculation shows that the low-temperature, low-density state is a superfluid state and undergoes a continuous (second-order) phase transition to the normal state as the temperature and/or density increases. As the Hamiltonian is not yet fully realistic and the values of the interaction parameters are uncertain, our results are not quite comparable to those for neutron matter, except perhaps at a very low density. But we demonstrate that the approach is promising for the study of low-density neutron matter.

Furthermore, we find that a density-wave state coexists with the superfluid state, suggesting that the state of neutron matter may be more complicated than the simple description of a superfluid state as it is often characterized.

The outline of this work is as follows. After the introduction in Sec. I, the Hamiltonian and its discretized form in the coordinate space are presented and are identified as an extended Hubbard model in Sec. II. The Hartree-Fock-Bogoliubov approximation is applied and the Hamiltonian is diagonalized in Sec. III. Thermodynamical properties numerically calculated are shown in Sec. IV, an attempt to apply our calculation to the problem of low-density neutron matter is discussed in Sec. V, and the possibility of a density-wave phase is examined in Sec. VI. Discussions and conclusion are presented in Sec. VII.

II. SIMPLIFIED HAMILTONIAN AND EXTENDED HUBBARD MODEL

The Hamiltonian consists of the kinetic and potential terms $\hat{K}$ and $\hat{V}$, respectively:

$$\hat{H} = \hat{K} + \hat{V} = -\frac{\hbar^2}{2m_N}\sum_{\sigma\tau}\int d\mathbf{r}\hat{\psi}^\dagger_{\sigma\tau}(\mathbf{r})\nabla^2\hat{\psi}_{\sigma\tau}(\mathbf{r}) + \frac{1}{2}\sum_{\substack{\sigma\sigma'\\ \tau\tau'}}\int d\mathbf{r}\int d\mathbf{r}'\,\hat{\psi}^\dagger_{\sigma\tau}(\mathbf{r})\hat{\psi}^\dagger_{\sigma'\tau'}(\mathbf{r}') \times V(\mathbf{r}-\mathbf{r}')\hat{\psi}_{\sigma'\tau'}(\mathbf{r}')\hat{\psi}_{\sigma\tau}(\mathbf{r}), \quad (1)$$

where m_N is the nucleon mass, and $\sigma = \pm 1/2$ and $\tau = \pm 1/2$ are the spin ($\uparrow$ or $\downarrow$) and the isospin (p or n), respectively. $\hat{\psi}^\dagger_{\sigma\tau}(\mathbf{r})$ and $\hat{\psi}_{\sigma\tau}(\mathbf{r})$ are the creation and annihilation operators of the nucleon, with the spin σ and isospin τ at the position $\mathbf{r}$. As in the previous Monte Carlo lattice calculation [14], we include only the central and spin-exchange interactions, V_c and V_σ, respectively:

$$V(\mathbf{r}-\mathbf{r}') = V_c(\mathbf{r}-\mathbf{r}') + V_\sigma(\mathbf{r}-\mathbf{r}')\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'. \quad (2)$$

V_c and V_σ are taken to consist of on-site and next-neighbor interactions,

$$V_c(\mathbf{r}-\mathbf{r}') = V_c^{(0)}\delta(\mathbf{r}-\mathbf{r}') + V_c^{(2)}[\nabla^2_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}')]$$
$$V_\sigma(\mathbf{r}-\mathbf{r}') = V_\sigma^{(0)}\delta(\mathbf{r}-\mathbf{r}') + V_\sigma^{(2)}[\nabla^2_{\mathbf{r}}\delta(\mathbf{r}-\mathbf{r}')], \quad (3)$$

where $V^{(2)}$ terms can be written explicitly exhibiting their hermiticity.

As physics of the lattice description is more apparent in the coordinate space, we consider the discretized coordinate with an internucleon spacing a in the cubic lattice with the torus boundary conditions. We thus focus our interest on the physics of the spatial separation greater than a in each direction, or of the momentum component roughly between π/a and $-\pi/a$, by eliminating (or integrating out) the physics of the shorter distance. The discretization corresponds to

$$\mathbf{r} \to a\mathbf{n}_i,$$

$$\int \mathrm{d}\mathbf{r} \to a^3\sum_i,$$

$$\sum_{\sigma\tau}\int d\mathbf{r}\hat{\psi}^\dagger_{\sigma\tau}(\mathbf{r})\hat{\psi}_{\sigma\tau}(\mathbf{r}) \to \sum_{i\sigma\tau}\hat{c}^\dagger_{i\sigma\tau}\hat{c}_{i\sigma\tau},$$

where i denotes a lattice site specified by $\mathbf{n}_i$ with its component ranging $[-aN/2, aN/2]$. Here, N is the number of sites in each spatial direction. Note that the creation and annihilation operators, $\hat{c}^\dagger_{i\sigma\tau}$ and $\hat{c}_{i\sigma\tau}$, have no dimension as defined. We also apply the identity

$$\sum_i \sigma^{(i)}_{\alpha\beta}\sigma^{(i)}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta},$$

where i denotes the spatial components (x,y,z), and the Greek indices denote the components of the Pauli spin matrix, 1 or 2.

In this work, we study the simplified case of nucleon matter consisting of a single nucleon species, such as neutron matter. The Hamiltonian Eq. (1) is then expressed in a spatially discretized form:

$$\hat{H} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + 6t\sum_{i\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma} + \tilde{U}\sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + V_1\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j\sigma}\hat{c}_{j\sigma}\hat{c}_{i\sigma} + V_2\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j-\sigma}\hat{c}_{j-\sigma}\hat{c}_{i\sigma} + V_3\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}^\dagger_{j-\sigma}\hat{c}_{j\sigma}\hat{c}_{i-\sigma}, \quad (4)$$

where $\langle i,j\rangle$ denotes the pairs of next-neighbor sites, and t is the hopping (kinetic energy) parameter defined as

$$t = \frac{\hbar^2}{2m_N a^2}. \quad (5)$$

Here, the potential parameters $\tilde{U}$ and V's are expressed in terms of linear combinations of $V^{(0)}$'s and $V^{(2)}$'s. The Hamiltonian Eq. (4) is now in the form of an extended Hubbard model, which is the Hubbard model with the on-site spin-pairing interaction of the $\tilde{U}$ term, modified by the next-neighbor interaction of the V terms. As the $\tilde{U}$ value will be taken to be negative, our model is an extended, attractive Hubbard model. The repulsive Hubbard model has been well studied in condensed matter physics as a model of strongly correlated electron systems [16], but the attractive model is generally less studied. In recent years, however, the extended, attractive Hubbard model has drawn much attention as the model describing the essential features of high-temperature superconductivity [15]. Note that the extended, attractive (negative-U) Hubbard model used in condensed matter physics, however, is usually of the simpler form shown below and has no $6t$ term as a part of the kinetic energy [17].

When the spin-dependent next-neighbor interaction is taken to be small and negligible,

$$V_\sigma^{(2)} = 0, \quad (6)$$

the Hamiltonian is simplified:

$$\hat{H} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + 6t\sum_{i\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma} + U\sum_i \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}_{i\uparrow} + V\sum_{\langle i,j\rangle\sigma\sigma'}\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}\hat{c}^\dagger_{j\sigma'}\hat{c}_{j\sigma'}, \quad (7)$$

where

$$U = \frac{1}{a^3}\left(V_c^{(0)} - 6\frac{V_c^{(2)}}{a^2} - 3V_\sigma^{(0)} \right),$$

$$V = \frac{1}{2a^5} V_c^{(2)}. \tag{8}$$

Apart from the lattice spacing a, the Hamiltonian of Eq. (7) now describes dynamics with two parameters. The Hamiltonian Eq. (4) [and thus also Eq. (7)] possesses an underlying particle-hole symmetry, which affects thermodynamical properties as discussed in Sec. VI. The symmetry is not an explicit property in our original Hamiltonian, Eqs. (1)–(3). We elaborate on the symmetry in Appendix A.

III. HARTREE-FOCK-BOGOLIUBOV APPROXIMATION AND GAP EQUATIONS

We now apply the mean field method in the Hartree-Fock-Bogoliubov approximation [18]. Here, we expect effects of the U term to dominate the thermal properties of the single species matter as in the standard BCS description [19–21], but we also wish to treat their single-particle aspects in the Hartree-Fock approximation on the same footing. Since the method is well known, we limit the description of the formalism to the key steps that are specifically relevant to our calculation.

The nature of the mean field approximation is apparent in the spatial representation. Through the application of the Wick theorem, the decoupling scheme for the U term is

$$\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}\hat{c}_{i\uparrow} \simeq -\Delta_i^* \hat{c}_{i\downarrow}\hat{c}_{i\uparrow} - \Delta_i \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger - |\Delta_i|^2 + n_{i\uparrow}\hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} + n_{i\downarrow}\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} - n_{i\uparrow}n_{i\downarrow},$$

where

$$\Delta_i \equiv \langle \hat{c}_{i\uparrow}\hat{c}_{i\downarrow}\rangle = -\langle \hat{c}_{i\downarrow}\hat{c}_{i\uparrow}\rangle,$$

$$n_{i\uparrow} \equiv \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow}\rangle \text{ and } n_{i\downarrow} \equiv \langle \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}\rangle.$$

Here, $\langle\cdots\rangle$ denotes the expectation value in the BCS-like ground state, which is to be determined in a self-consistent way. The order parameters Δ_i's are related to the local density of the condensate of nucleon pairs, while n_i's are the average number of nucleons. Note that the inclusion of n_i as a variational parameter distinguishes the present treatment from the standard BCS [18]. For the V terms, we have

$$\hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}\hat{c}_{j\sigma'}^\dagger \hat{c}_{j\sigma'} \simeq n_{i\sigma}\hat{c}_{j\sigma'}^\dagger \hat{c}_{j\sigma'} + n_{j\sigma'}\hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - n_{i\sigma}n_{j\sigma'}.$$

In the following, Δ_i and n_i's will be assumed to be independent of the site i, or global, and will be formally treated as the variational parameters:

$$\Delta \simeq 2U\Delta_i = 2U\Delta_i^*,$$

$$n \simeq 2n_{i\uparrow} = 2n_{i\downarrow}.$$

Our Δ is defined to be the gap energy itself, with the dimension of energy in the unit of $2U$, and carries an extra factor of 2 in comparison to the often-used Δ. We also note that we ignore the V-term contribution to the hopping term, as they merely change somewhat the strength of the hopping term and of the constant part of the energy, without affecting the physics of the phase transition. The mean field approximation then yields in a cubic lattice with six neighboring sites

$$\hat{H} = -t\sum_{\langle i,j\rangle\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \left(6t + \frac{n}{2}\overline{U}\right)\sum_{i\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} - \frac{\Delta}{2}\sum_i (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger + \hat{c}_{i\downarrow}\hat{c}_{i\uparrow}) - \frac{N^3}{4}\left(\frac{\Delta^2}{U} + n^2\overline{U}\right), \tag{9}$$

where $\overline{U} \equiv U + 24V$.

For convenience, we will carry out the mean field calculations in the momentum space. The momentum representation is introduced by discretizing the momentum as $\mathbf{p} \to 2\pi\mathbf{k}/(Na)$, with each component of $\mathbf{k}$ being an integer, ranging $[-N/2, N/2]$. Note that we now have $\mathbf{r}\cdot\mathbf{p} \to 2\pi\mathbf{n}_i\cdot\mathbf{k}/N$. The coordinate and momentum representations of the operator $\hat{c}$ are related through the Fourier transformations

$$\hat{c}_{j\sigma} = \frac{1}{\sqrt{N^3}}\sum_{\mathbf{k}} e^{-2i\pi\mathbf{k}\cdot\mathbf{n}_j/N}\hat{c}_{\mathbf{k}\sigma},$$

$$\hat{c}_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N^3}}\sum_{j} e^{2i\pi\mathbf{k}\cdot\mathbf{n}_j/N}\hat{c}_{j\sigma},$$

and similarly for the nucleon creation operator, $\hat{c}^\dagger$. Note that the discretized orthonormality relation is

$$\sum_j \exp(2i\pi\mathbf{k}\cdot\mathbf{n}_j/N) = N^3\delta_{\mathbf{k},\mathbf{0}}. \tag{10}$$

With the chemical potential μ, $\hat{H} - \mu N^3\hat{n}$ is in the momentum space

$$\hat{H} - \mu N^3\hat{n} = \sum_{\mathbf{k}} (\hat{c}_{\mathbf{k}\uparrow}^\dagger \hat{c}_{-\mathbf{k}\downarrow}) \begin{pmatrix} \epsilon_{\mathbf{k}} - \overline{\mu} & -\frac{1}{2}\Delta \\ -\frac{1}{2}\Delta & -(\epsilon_{\mathbf{k}} - \overline{\mu}) \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}_{-\mathbf{k}\downarrow}^\dagger \end{pmatrix} - \frac{N^3}{4}\left(\frac{\Delta^2}{U} + n^2\overline{U}\right), \tag{11}$$

where

$$\overline{\mu} = \mu - (6t + n\overline{U}/2), \tag{12}$$

and

$$\epsilon_{\mathbf{k}} = -t\sum_{\mathbf{e}} \exp(2i\pi\mathbf{k}\cdot\mathbf{e}/N) = -2t\sum_{j=x,y,z} \cos(2\pi k_j/N) \tag{13}$$

is a part of the kinetic energy of a quasiparticle expressed in terms of the unit vector $\mathbf{e}$ showing a next-neighbor site. Note that $\epsilon_{-\mathbf{k}} = \epsilon_{\mathbf{k}}$ and $\sum_{\mathbf{k}}\epsilon_{\mathbf{k}} = 0$. We see that in the Hamiltonian, V appears only as $\overline{U} = U + 24V$, and merely shifts the chemical potential and the total energy: It does not actively participate in the generation of the phase transition.

As is well known, the spin density s,

$$s = \langle \hat{s} \rangle \equiv \frac{1}{2N^3} \sum_i \langle \hat{c}^\dagger_{i\uparrow} \hat{c}_{i\uparrow} - \hat{c}^\dagger_{i\downarrow} \hat{c}_{i\downarrow} \rangle = \frac{1}{2N^3} \sum_{\mathbf{k}} \langle \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\uparrow} - \hat{c}^\dagger_{-\mathbf{k}\downarrow} \hat{c}_{-\mathbf{k}\downarrow} \rangle, \tag{14}$$

is conserved in the mean field approach, while n,

$$n = \langle \hat{n} \rangle \equiv \frac{1}{N^3} \sum_{i\sigma} \langle \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma} \rangle = \frac{1}{N^3} \sum_{\mathbf{k}\sigma} \langle \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \rangle \tag{15}$$

(and thus the total nucleon number), is not, as the spin number operator $\hat{s}$ commutes with $\hat{H}$ of Eq. (9), but the number density operator $\hat{n}$ does not. We remedy this problem by the standard method of introducing a Lagrange multiplier corresponding to the chemical potential μ, by subtracting a term $\mu N^3 \hat{n} = \mu \Sigma_{i\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{i\sigma}$ from the $\hat{H}$. μ will be adjusted to achieve the desired value of the conjugate parameter, n. The formalism is thus essentially the canonical ensemble method.

We now diagonalize $\hat{H} - \mu N^3 \hat{n}$ by the use of the Bogoliubov-Valatin transformation,

$$\begin{aligned} \hat{\beta}^\dagger_{\mathbf{k}+} &= u_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} - v_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow}, \\ \hat{\beta}^\dagger_{-\mathbf{k}-} &= u_{\mathbf{k}} \hat{c}^\dagger_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow}, \end{aligned} \tag{16}$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are taken to be real and are given by

$$u^2_{\mathbf{k}} = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}} - \overline{\mu}}{E_{\mathbf{k}}}\right) \quad \text{and} \quad v^2_{\mathbf{k}} = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}} - \overline{\mu}}{E_{\mathbf{k}}}\right),$$

satisfying $u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = 1$. $\hat{H} - \mu N^3 \hat{n}$ is now expressed as that of a system of free quasiparticles:

$$\hat{H} - \mu N^3 \hat{n} = \sum_{\mathbf{k}\lambda=\pm} E_{\mathbf{k}} \hat{\beta}^\dagger_{\mathbf{k}\lambda} \hat{\beta}_{\mathbf{k}\lambda} + N^3 (E_{\mathrm{GS}} - \mu n), \tag{17}$$

with the energy of a quasiparticle

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \overline{\mu})^2 + \Delta^2/4} \tag{18}$$

and the ground-state energy of the system

$$E_{\mathrm{GS}} = -\frac{1}{4}\left(\frac{\Delta^2}{U} + n^2 \overline{U}\right) - \frac{1}{N^3} \sum_{\mathbf{k}} E_{\mathbf{k}} - \overline{\mu} + \mu n. \tag{19}$$

Equation (16) shows that $\hat{\beta}_{\mathbf{k}\lambda}$'s obey anticommutation relations and that the quasiparticles are fermions. Furthermore, Eq. (17) implies that they form a system of free fermions. As a consequence of the thermal average, the internal energy is then given by

$$E \equiv \langle \hat{H} \rangle = \sum_{\mathbf{k}\lambda} E_{\mathbf{k}} n_{\mathbf{k}\lambda} + N^3 E_{\mathrm{GS}}, \tag{20}$$

with the energy per lattice site being E/N^3. Here, $n_{\mathbf{k}\lambda}$ is the momentum distribution of the quasiparticles, $n_{\mathbf{k}\lambda} \equiv \langle \hat{\beta}^\dagger_{\mathbf{k}\lambda} \hat{\beta}_{\mathbf{k}\lambda} \rangle$, and is determined by the requirement that the free energy F introduced below is minimized by a variation of $n_{\mathbf{k}\lambda}$, $\delta F / \delta n_{\mathbf{k}\lambda} = 0$ for $\lambda = \pm$. We obtain

$$n_{\mathbf{k}} \equiv n_{\mathbf{k}+} = n_{\mathbf{k}-} = [\exp(E_{\mathbf{k}}/T) + 1]^{-1}, \tag{21}$$

which have the limiting values, $n_{\mathbf{k}} \to 0$ and $\to 1/2$ as $T \to 0^+$ and $\to \infty$, respectively. Note that throughout this work, we denote the temperature T in the unit of the Boltzmann constant.

By combining with the entropy S, the (Helmholtz) free energy is expressed as

$$\begin{aligned} F(T,a;\Delta,n) &\equiv E - TS \\ &= \sum_{\mathbf{k}\lambda} E_{\mathbf{k}} n_{\mathbf{k}\lambda} + N^3 E_{\mathrm{GS}} \\ &\quad + T \sum_{\mathbf{k}\lambda} [n_{\mathbf{k}\lambda} \ln n_{\mathbf{k}\lambda} + (1 - n_{\mathbf{k}\lambda}) \ln(1 - n_{\mathbf{k}\lambda})], \end{aligned} \tag{22}$$

depending on a through the $\mathbf{k}$ sum because the spatial volume $(aN)^3$ depends on a with N fixed. F is a function of Δ and n. Δ and μ are determined so as to minimize F for variations of Δ and n, while T and a are fixed. The conditions

$$\frac{1}{N^3} \frac{\partial F}{\partial n} = \mu, \quad \frac{\partial F}{\partial \Delta} = 0$$

provide the gap equations

$$\begin{aligned} n - 1 &= \frac{1}{N^3} \sum_{\mathbf{k}} \frac{\epsilon_{\mathbf{k}} - \overline{\mu}}{E_{\mathbf{k}}} (2n_{\mathbf{k}} - 1), \\ \Delta &\left(1 - \frac{U}{2N^3} \sum_{\mathbf{k}} \frac{2n_{\mathbf{k}} - 1}{E_{\mathbf{k}}}\right) = 0 \end{aligned} \tag{23}$$

from which μ and Δ are determined.

IV. THERMODYNAMICAL PROPERTIES

We now apply the formalism so far described, to compute various thermodynamical quantities. For clarifying our presentation, we place some expressions of the thermodynamical variables in Appendix B. All numerical results are calculated in the thermodynamical limit $N \to \infty$. In the limit, the summation over the discretized momentum space of each component of $\mathbf{k}$ ranging in $[-N/2, N/2]$ is replaced by the integral over the first Brillioun zone with each component of the momentum $\mathbf{p}$ ranging $[-\pi/a, \pi/a]$:

$$\frac{1}{N^3} \sum_{\mathbf{k}} \to \left(\frac{a}{2\pi}\right)^3 \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} d^3\mathbf{p}.$$

A. Potential parameters

We apply the parameter values used in the previous Monte Carlo lattice calculation for nuclear matter [14]:

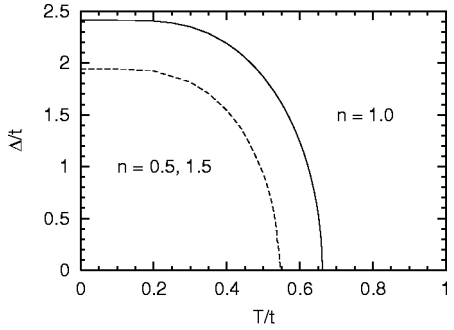

FIG. 1. The order parameter Δ as a function of temperature T in the unit of hopping parameter t for the density $n=0.5$ and 1.5 (long-dashed curve) and $n=1.0$ (solid curve).

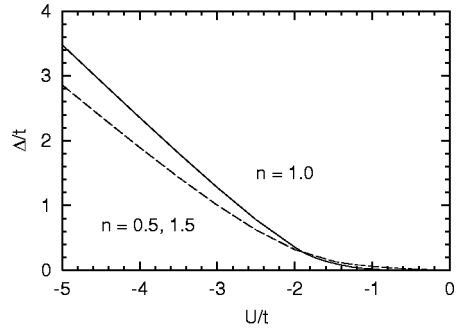

FIG. 2. The order parameter Δ as a function of the on-site potential strength U in the unit of hopping parameter t at zero temperature ($T=0$) for the density $n=0.5, 1.5$ (long-dash curve), $n=1.0$ (solid curve).

$$V_c^{(0)} = -181.5 \text{ MeV fm}^3,$$
$$V_c^{(2)} = 37.8 \text{ MeV fm}^5,$$
$$V_\sigma^{(0)} = -31.25 \text{ MeV fm}^3, \tag{24}$$
$$V_\sigma^{(2)} = 0,$$

with the lattice spacing $a=1.842$ fm. These parameter values give

$$t = 6.11 \text{ MeV},$$
$$U = -24.74 \text{ MeV},$$
$$V = 0.89 \text{ MeV}.$$

The parameter values of Eq. (24) were chosen in Ref. [14] so as to reproduce the saturation density and energy of nuclear matter on a finite $4\times4\times4$ lattice for the same Hamiltonian as ours, Eqs. (1)–(3). Our Hamiltonian has no explicit τ-dependent term, and the parameter values effectively include the strong neutron-proton interactions for nuclear matter. The use of the parameters is thus not quite adequate as a realistic description of the nucleon matter of single species, such as the neutron matter. Furthermore, finite lattice volume effects make the thermodynamical limit ($N\to\infty$) calculation different from the finite volume calculation. For comparison purposes with the previous and future Monte Carlo calculations, however, we use the above parameter values except when the U dependence of Δ is examined. Any conclusion that we could draw from the numerical results in this section is then qualitative.

B. Gap parameter Δ

Equations (23) determine Δ and μ. Figure 1 illustrates Δ as a function of the temperature T for $n=0.5$ (one-quarter filling), 1.0 (one-half filling), and 1.5 (three-quarter filling). In the figure, we see that Δ vanishes at $T=T_c$,

$$T_c = \begin{cases} 0.66t \text{ or } 4.0 \text{ MeV} & \text{for } n=1.0, \\ 0.55t \text{ or } 3.3 \text{ MeV} & \text{for } n=0.5 \text{ and } 1.5. \end{cases}$$

The temperature dependence of Δ is the same for $n=0.5$ and 1.5. This is a consequence of the symmetry with respect to $n=1$ and is discussed further in Sec. IV D and Appendix A. Figure 1 also shows

$$\Delta(T=0) \simeq (2-2.5)t \simeq 12-15 \text{ MeV}.$$

The explicit values of T_c and $\Delta(T=0)$ depend sensitively on the parameter values as discussed below, but T_c and $\Delta(T=0)$ satisfy

$$\Delta(T=0) \simeq 3.6T_c,$$

which is the well-known relation at the weak-coupling limit except for the latter to have a slightly smaller coefficient 3.54 [21]. In comparison to the weak limit, our calculation thus somewhat underestimates T_c in relation to $\Delta(T=0)$. Note that different mean field calculations have been reported to yield the coefficient smaller than the weak-limit value [10] and also even much larger [9] than ours.

Near T_c, the gap equations Eqs. (23) yield

$$\Delta \propto \begin{cases} (T-T_c)^\beta & \text{for } T<T_c, \\ 0 & \text{for } T>T_c, \end{cases}$$

with $\beta\simeq0.45$. Note that the well-known mean field value of the critical exponent β in the simple BCS theory is $1/2$ [22].

The physics of the phase transition depends on the strength of the potential parameter U. Figure 2 illustrates how sensitively the value of Δ depends on U. We see that $\Delta\to0$ as $U\to0$. As is well known, Δ does not vanish for a finite U. In fact, Eq. (23) yields the well-known dependence of Δ on $|U|$ for $U\to0$:

$$\Delta \to Ae^{-B/|U|},$$

where A and B are constant and independent of U.

C. Second-order (continuous) phase transition

The temperature dependence of Δ in Fig. 1 is a well-known dependence of the order parameter for a second-order phase transition. The variation of Δ as shown in Fig. 1 implies that the phase transition takes place from a superfluid state generated by spin pairing to the normal state, as the temperature increases. The features of the second-order phase transition are clearly seen in the temperature dependence of the thermodynamic quantities expressed in terms of

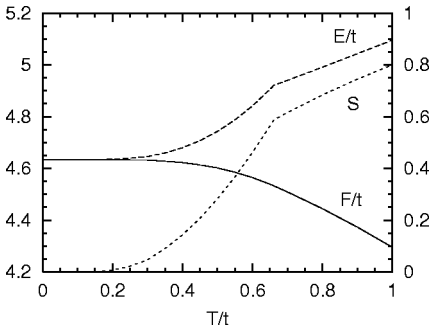

FIG. 3. The Helmholtz free energy F (solid curve), the internal energy E (long-dashed curve), and the entropy of the system S (short-dashed curve) as a function of temperature T in the unit of hopping parameter t for the density $n=1.0$. The left axis refers to F and E, and the right one is for S.

the temperature derivatives of the free energy F in a successive order. We consider the internal energy E, the entropy S, and the heat capacity C_v,

$$E = -T^2\left[\frac{\partial (F/T)}{\partial T}\right]_{a,n},$$

$$S = -\left[\frac{\partial F}{\partial T}\right]_{a,n}, \tag{25}$$

$$C_v = -T\left[\frac{\partial S}{\partial T}\right]_{a,n} = -T\left[\frac{\partial^2 F}{\partial T^2}\right]_{a,n}.$$

The temperature dependence of the quantities is calculated using Eqs. (20), (22), (B1), and (B2), and is illustrated in Figs. 3 and 4. E and S are continuous at the critical temperature T_c as seen in Fig. 3, while C_v has a jump at T_c as in Fig. 4. These behaviors demonstrate the generic features of the second-order phase transition. The amount of the discontinuity in C_v at T_c, ΔC_v, is relative to C_v of the normal phase,

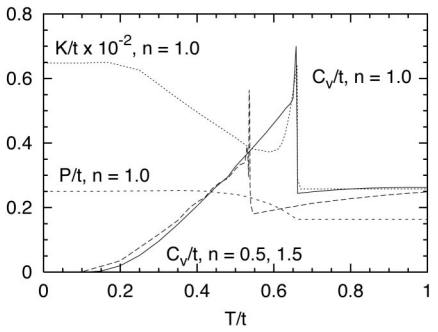

FIG. 4. The heat capacity C_v for the density $n=0.5$ and 1.5 (long-dashed curve) and $n=1.0$ (solid curve), the pressure P for the density $n=1.0$ (short-dashed curve), and the incompressibility K for the density $n=1.0$ (dotted curve) as a function of temperature T in the unit of hopping parameter t.

$$\Delta C_v/C_v(\text{normal}) \simeq \begin{cases} 1.74 & \text{for } n = 1.0, \\ 1.43 & \text{for } n = 0.5 \text{ and } 1.5, \end{cases}$$

while the BCS mean field value is $12/7\zeta(3) \simeq 1.43$, independent of n [21]. (ζ is the zeta function.)

The thermal quantities involving volume derivatives form a set of quantities similar to the temperature derivatives. We consider the pressure P and the isothermal compressibility κ_T. Here, following the common practice in nuclear physics, we examine the incompressibility $K \equiv 9/(\kappa_T \rho)$, defined in terms of the density $\rho = \mathcal{V}/(aN)^3 = n/a^3$ with the spatial volume $\mathcal{V} = (aN)^3$. A volume derivative is then a derivative with respect to the lattice spacing a. A derivative with respect to a requires, however, the knowledge of a dependence of U and V, that is, their renormalization flow when a is varied. In this work, for simplicity, we assume that their a dependence is small, at least around the value of a we use. P and K are written as

$$P = -\left[\frac{\partial F}{\partial \mathcal{V}}\right]_{T,a}, \tag{26}$$

$$K = -9\frac{\mathcal{V}}{\rho}\left[\frac{\partial P}{\partial \mathcal{V}}\right]_{T,a} = -9\frac{\mathcal{V}}{\rho}\left[\frac{\partial^2 F}{\partial \mathcal{V}^2}\right]_{T,a}. \tag{27}$$

P is calculated using Eq. (B4) and K is obtained numerically from the temperature dependence of P. The temperature dependence of P and K confirms the second-order phase transition, as seen in Fig. 4.

There are many other quantities that describe thermodynamic properties of the system described by our Hamiltonian, but they are either related to the quantities already shown, or their features depend strongly on the explicit form of the Hamiltonian. We thus do not show them in this exploratory work. For example, the temperature dependence of double occupancy per site,

$$D \equiv \frac{1}{N^3}\sum_i \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \rangle, \tag{28}$$

provides the amount of the spin pairing that participates in the phase transition. But D, as well as the kinetic energy per site, is related to Δ and n in the mean field approximation [23] and provides no new information, as shown in Appendices A and B.

D. Particle-hole symmetry and phase diagram

For illustrative purposes, however, we show the density dependence of μ, D, E, and KE at $T=0$, in Fig. 5. As noted above, Fig. 1 suggests a symmetric dependence of Δ on the density n, which is more clearly illustrated in Fig. 6. The symmetry is generated as a consequence of the particle-hole symmetry, as seen from the fact that Eq. (23) is invariant under the particle-hole conjugation though the symmetry is implicit in our Hamiltonian, Eqs. (4) and (7). There is a group of Hamiltonians, in which the particle-hole symmetry is implicit, yet yielding (in the mean field results) the energy spectrum of the system with the explicit symmetry. The

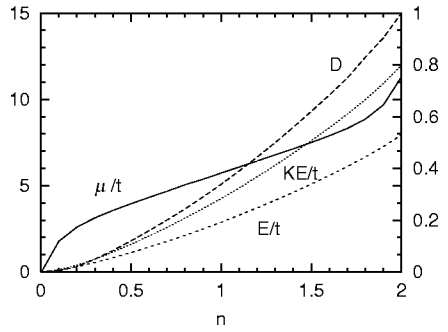

FIG. 5. The chemical potential μ (solid curve), the double occupancy D (long-dashed curve), the internal energy E (short-dashed curve), and the kinetic energy KE (dotted curve) in the unit of hopping parameter t as a function of the density n at zero temperature ($T=0$). The left axis refers to μ, E, and KE, and the right one is for D.

Hamiltonians do yield different behaviors of thermodynamic variables. Figure 5 is an example. We elaborate on the issue of this symmetry in Appendix A.

Some thermodynamic variables are made to exhibit this symmetry explicitly by modifying the Hamiltonian to possess the explicit symmetry. Whether it is explicit or not, however, the thermodynamic properties obtained from the Hamiltonian are affected by the symmetry. The symmetry is a consequence of our computational method using the lattice configuration, and it is an artifact. In order to extract physically realistic results, we should therefore stay away from the region of the symmetry and should confine ourselves to a small value of n by appropriately adjusting the value of the lattice spacing a, so as to simulate the desired density of the nucleon matter. We discuss this point again in the following section, where we attempt to apply our calculation to a case of low-density neutron matter.

Combining the variations of the thermodynamic quantities, some of which have been presented so far, we obtain the phase diagrams of the present system described in the mean field theory. Figure 7 shows the phase diagram in the region of small densities where we expect the above-mentioned symmetry to be generating less distortion.

V. LOW-DENSITY NEUTRON MATTER

In the previous section, we have used the parameter values most appropriate as a description of nuclear matter and

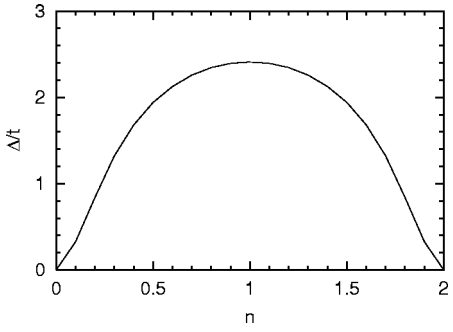

FIG. 6. Δ in the unit of hopping parameter t as a function of the density n at zero temperature ($T=0$).

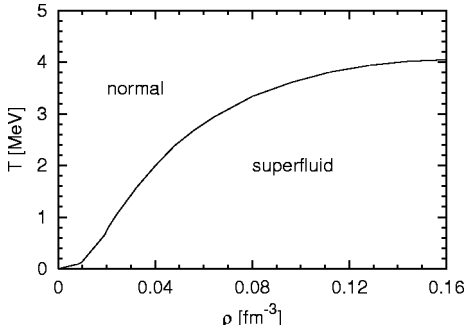

FIG. 7. T-ρ phase diagram.

have examined the nature of the single species nucleon matter described by our model. In this section, we discuss whether our model could be made a realistic description of neutron matter.

First, we have the question of whether our lattice would meet the basic momentum requirement imposed by the lattice spacing. A lattice description can be made realistic when the lattice spacing is less than the momentum scale of the system. By taking the Fermi momentum of the neutron matter as an estimate of the momentum scale, we have

$$\pi/a > p_F. \tag{29}$$

Our lattice spacing, $a=1.842$ fm, yields the density of $\rho = 1/a^3 \simeq 0.160$ fm^{-3} for $n=1.0$ (the lattice space being half full). The Fermi momentum corresponding to this density is

$$p_F \simeq 1.68 \text{ fm}^{-1}$$

using $\rho = p_F^3/3\pi^2$. The value of p_F is practically the same as

$$\pi/a \simeq 1.71 \text{ fm}^{-1},$$

and thus the lattice with the above lattice spacing is applicable to a density much smaller than $\rho \simeq 0.160$ fm^{-3}. Note that the preceding discussion yields that the condition

$$\pi/3 > n$$

meets Eq. (29) independently of a.

Second, there is the question of whether our Hamiltonian is appropriate for a realistic description of low-density neutron matter. The nucleon-nucleon $^1S_0$ phase shift is much greater than the nucleon-nucleon phase shifts of other states below the laboratory energy $E_{lab} \simeq 100$ MeV. The nucleon momentum in the center-of-mass coordinate system $p_{\text{c.m.}}$ corresponding to this E_{lab} is about 1.2 fm^{-1} through $E_{lab} = 4(p_{\text{c.m.}}^2/2m_N)$, and is smaller than the above $\pi/a \equiv p_{cutoff} \simeq 1.7$ fm^{-1}. We thus infer that our Hamiltonian form of the S wave should be reasonable for neutron matter of a density less than 0.17 fm^{-3}, which corresponds to the Fermi momentum of 1.7 fm^{-1}.

As to the parameter values in the Hamiltonian, it would be best to determine them for our lattice size from experimental $^1S_0$ phase shifts by applying the method of effective field theory [24,25]. Instead, as an exploratory study, we simply adjust the U-parameter value so as to see whether our approach could come close to other mean field calculations of low-density neutron matter in the literature. Figure 8 il-

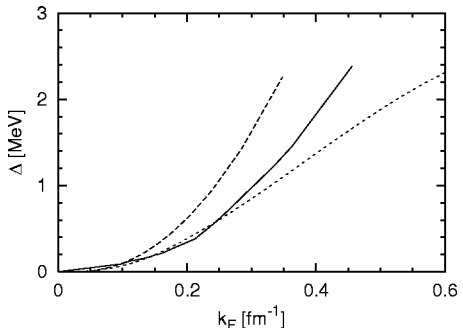

FIG. 8. The gap energy Δ as a function of the Fermi momentum k_F for $U=-45.8$ MeV (solid curve) in comparison to a simple BCS calculation (long-dashed curve) and a more elaborate one [10] (short-dashed curve). The simple calculation is taken from Ref. [26] [using Eq. (8) with the neutron mass of 940 MeV and the neutron-neutron scattering length of −18.8 fm]. Δ in this figure is half the Δ defined in the text, so that its definition agrees with the one used in Refs. [10,26].

lustrates that we could obtain a somewhat reasonable density dependence of Δ by increasing the magnitude of U. We leave a more serious determination of the parameters for our future work.

VI. DENSITY WAVE PHASE

Our analysis has so far been strictly based on the mean field approximation applied to a spin-pairing phase at the same site. In the approximation, the V term merely shifts the effective chemical potential and is inactive in generating the phase transition. As the V term represents the pairing of the spin densities at the adjacent sites, such a role may be a reasonable one in this phase transistion. Would the V term ever play an active role in generating a different phase transition? In this section we briefly examine this possibility.

The most likely phase in which the V term would play the major role would be a density-wave phase generated by a coupling of the densities of the opposite spins at the adjacent sites. We examine how the V term could generate such a phase transition, again in the mean field approximation, and see whether the phase transition would occur with our parameter values.

We follow the Hartree-Fock-Bogoliubov approximation with the same decoupling scheme as before. For simplicity, however, we ignore the superfluid phase. The density wave phase is introduced by making a replacement,

$$\begin{aligned}\langle \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}\rangle &\rightarrow n_{i\sigma} + (\delta/2)\cos(2\pi \mathbf{n}_i\cdot\mathbf{q}/N)\\ &\simeq n/2 + (\delta/2)\cos(2\pi \mathbf{n}_i\cdot\mathbf{q}/N).\end{aligned} \tag{30}$$

Here, the inhomogeneous order parameter for the density-wave depends on the amplitude δ and the wave number vector $\mathbf{q}$. In the following, we examine the wave modes in which the adjacent sites are the maximum and minimum of the amplitude in a cubic lattice. That is, at least one component of $2\pi\hat{q}/N$ is $\pm\pi$. The number of the nonzero components, or the dimension of the density wave d, provides a convenient parameter η,

$$\eta = 3 - 2d. \tag{31}$$

As in the previous spin-pairing case, n and δ are treated as independent parameters, and μ, the parameter conjugate to n, is adjusted to the desired value of n.

The steps to the gap equations are similar to the case of the superfluid phase discussed in Sec. III, and are shown in Appendix C. By minimizing $F-\mu N^3 n$, we obtain

$$\begin{aligned} n &= \frac{1}{N^3}\sum_{\mathbf{k}\lambda} n_{\mathbf{k}\lambda},\\ \delta &\left(1 - \frac{U+8\eta V}{N^3}\sum_{\mathbf{k}}\frac{n_{\mathbf{k}+}-n_{\mathbf{k}-}}{\xi_{\mathbf{k}}}\right) = 0\end{aligned} \tag{32}$$

by varying n and δ, respectively. Equation (32) determines δ and μ. Furthermore, as $n_{\mathbf{k}+} < n_{\mathbf{k}-}$ and

$$U + 8\eta V < 0 \tag{33}$$

for our parameter values, Eq. (32) shows that the density waves of all dimensions are expected to occur owing to the strong, attractive U.

VII. DISCUSSION AND CONCLUSION

The form of the nucleon-nucleon interaction, Eqs. (1)–(3), shows that the nucleon-nucleon interaction used in this work is of the S states. As is well known, the realistic nucleon-nucleon interaction is highly state dependent. The relevant nucleon energy of interest to us here is a few hundred MeV, corresponding to the Fermi energy region of the nuclear matter density. In this energy region, the attractive neutron-neutron interaction is known to be dominated by the $^3P_2$ interaction driven by the spin-orbit force, coupled with the $^3F_2$ interaction associated with the tensor force [27,28]. Our Hamiltonian accommodates none of these features of the interaction. Our objective as noted in Sec. I is to understand the essential physics associated with the thermal properties of nucleon matter, but our finding in this work is limited in this sense and is perhaps most applicable to low-density neutron matter.

There is a serious question of how good the mean field calculation is in our case. A mean field approximation ignores most features of particle correlations. As the particle correlations are the vital ingredient of critical phenomena, the mean field approximation is generally believed to be only of qualitative use, and some times not even qualitative, as fluctuations could alter the nature of the phase transition. The situation, however, depends on the nature of the problem [22], as the prominent success of the Ginzburg-Landau/BCS theory shows [29], especially at temperatures not too close to the critical one. Our problem is in three dimensions, close to the usual upper critical dimension of four under the Ginsburg criterion [22]. We are hoping that our calculation, being similar to the BCS theory, is not far off, but this remains to be seen. This issue is under further investigation by incorporating a renormalization approach, as has recently been done at zero temperature [30].

Our Hamiltonian has a form similar to that of the Skyrme interaction [31] (though ours is a truncated form). The

Skyrme interaction is one of the effective interactions that are phenomenologically introduced to achieve quantitative agreement with experiments, usually by the use of a mean field approximation such as the Hartree-Fock calculations. Though it is still not quite realistic, our Hamiltonian has a justification in this sense. A lattice calculation such as the previous Monte Carlo lattice calculation [14], however, accounts for all the complexity of the many-body interaction with no approximation other than the numerical, in the lattice framework. The nucleon-nucleon interaction used in it should not be then an effective interaction like the Skyrme interaction, but an interaction in free space. The parameters U and V are expected to be determined from scattering data through the use of effective field theory by extending Lüscher's formula [32,33] for the large ${}^1S_0$ scattering length. This issue is presently under investigation [25]. Note that the values of U and V will depend on the lattice spacing a.

In conclusion, our mean field calculation on a lattice with a simple nucleon-nucleon interaction suggests a second-order phase transition taking place at a low temperature in single species nucleon matter described by a simple Hamiltonian. Thermodynamic variables show their dependence on the temperature and density variations as expected under the phase transition in the mean field approach. The transition changes the phase of the matter from a superfluid state due to nucleon pairing, to a normal state as the temperature increases and the density decrease. This dependence is in qualitative agreement with the findings that have been reported in the literature [1].

ACKNOWLEDGMENTS

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APPENDIX A: THE PARTICLE-HOLE SYMMETRY

The Hamiltonian of Eq. (7) does not explicitly exhibit particle-hole symmetry, but it can be modified to do so by adding a single-particle Hamiltonian,

$$\Delta\hat{H} = N^3\overline{U}/4 - (6t + \overline{U}/2)\sum_{i\sigma}\hat{n}_{i\sigma}, \tag{A1}$$

where $\hat{n}_{i\sigma}\equiv\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}$. The new Hamiltonian,

$$\hat{H}' \equiv \hat{H} + \Delta\hat{H} = -t\sum_{\langle i,j\rangle\sigma}\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + U\sum_i\left(\frac{1}{2}-\hat{n}_{i\uparrow}\right)\left(\frac{1}{2}-\hat{n}_{i\downarrow}\right) + V\sum_{\langle i,j\rangle\sigma\sigma'}\left(\frac{1}{2}-\hat{n}_{i\sigma}\right)\left(\frac{1}{2}-\hat{n}_{j\sigma'}\right), \tag{A2}$$

is symmetric under the particle-hole conjugation (or with respect to half filling, $n=1$):

$$\hat{c}^\dagger_{i\sigma}\leftrightarrow\hat{c}_{i\sigma}$$

$$\hat{c}_{i\sigma}\leftrightarrow\hat{c}^\dagger_{i\sigma},$$

or $n_{i\sigma}\leftrightarrow 1-n_{i\sigma}$, which is $n\leftrightarrow 2-n$ with $n\equiv\Sigma_{i\sigma}n_{i\sigma}$. Under the conjugation, the Hamiltonian becomes that of holes, with $t\rightarrow -t$.

When we repeat the BCS formulation in Sec. III, after the Bogoliubov transformation, we obtain the diagonalized form of the new Hamiltonian, Eq. (A2), as

$$\hat{H}' = \sum_{\mathbf{k}\lambda}E'_{\mathbf{k}}\hat{n}'_{\mathbf{k}\lambda} + N^3E'_{\mathrm{GS}} \tag{A3}$$

with the quasiparticle energy

$$E'_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}}-\overline{\mu}')^2 + \Delta^2/4} \tag{A4}$$

and

$$n'_{\mathbf{k}} \equiv n'_{\mathbf{k}+} = n'_{\mathbf{k}-} = [\exp(E'_{\mathbf{k}}/T)+1]^{-1}. \tag{A5}$$

Here, the ground-state energy is

$$E'_{\mathrm{GS}} = -\frac{1}{4}\left(\frac{\Delta^2}{U} + \frac{n^2-1}{4}\overline{U}\right) - \frac{1}{N^3}\sum_{\mathbf{k}}E'_{\mathbf{k}} - \overline{\mu}' + \mu n, \tag{A6}$$

with

$$\overline{\mu}' = \mu - (n-1)\overline{U}/2. \tag{A7}$$

Equations (12) and (A7) show that the μ value is shifted, and Eqs. (19) and (A6) tell us that the expression of the ground-state energy is altered. The kinetic energy is also changed:

$$\mathrm{KE}' \equiv -\frac{t}{N^3}\sum_{\langle i,j\rangle,\sigma}\langle\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma}\rangle = -\frac{1}{N^3}\sum_{\mathbf{k}}\frac{(\epsilon_{\mathbf{k}}-\overline{\mu}')\epsilon_{\mathbf{k}}}{E'_{\mathbf{k}}}, \tag{A8}$$

in comparison to Eq. (B7). We also see that E'_{GS} and KE$'$ for the new Hamiltonian explicitly exhibit the particle-hole symmetry about half filling ($n=1$).

The double occupancy per site for the new Hamiltonian D',

$$D' \equiv \frac{1}{N^3}\sum_i\langle\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\rangle = \frac{\Delta^2}{4U^2} + \frac{n^2}{4}, \tag{A9}$$

differs from that for the original Hamiltonian, Eq. (B6). Note that neither D nor D' is symmetric about $n=1$.

The gap equations for the new Hamiltonian become

$$n-1=\frac{1}{N^3}\sum_{\mathbf{k}}\frac{\epsilon_{\mathbf{k}}-\bar{\mu}'}{E'_{\mathbf{k}}}(2n'_{\mathbf{k}}-1),$$
$$\Delta\left(1-\frac{U}{2N^3}\sum_{\mathbf{k}}\frac{2n'_{\mathbf{k}}-1}{E'_{\mathbf{k}}}\right)=0. \tag{A10}$$

These gap equations are the same as Eqs. (23) except $\bar{\mu}$ is replaced by $\bar{\mu}'$. As we solve the gap equations for Δ and μ (or $\bar{\mu}$) for a fixed n, the gap equations for the two Hamiltonians yield the same set of Δ and $\bar{\mu}$, thus the same T_c. Both Hamiltonians thus provide the same excitation energy spectrum.

APPENDIX B: THERMODYNAMIC VARIABLES

We list here the expressions of the thermodynamic variables, which are used in Sec. IV. The entropy is given in terms of $n_{\mathbf{k}\lambda}$ in Eq. (21) by

$$S=\sum_{\mathbf{k}\lambda}[n_{\mathbf{k}\lambda}\ln n_{\mathbf{k}\lambda}+(1-n_{\mathbf{k}\lambda})\ln(1-n_{\mathbf{k}\lambda})]. \tag{B1}$$

By the use of Eqs. (18), (19), and (22), the heat capacity C_v is expressed as

$$\begin{aligned}C_v&=-T\left[\frac{\partial^2 F}{\partial T^2}\right]_{a,n}\\&=\frac{1}{N^3}\sum_{\mathbf{k}}\frac{\Delta\Delta_T}{4E_{\mathbf{k}}}(2n_{\mathbf{k}}-1)-\frac{2}{N^3}\sum_{\mathbf{k}}n_{\mathbf{k}}^2\left(\frac{\Delta\Delta_T}{4}-\frac{E_{\mathbf{k}}^2}{T^2}\right)e^{E_{\mathbf{k}}/T}\\&\quad-\frac{\Delta\Delta_T}{2U}.\end{aligned} \tag{B2}$$

Here, Δ_T is

$$\Delta_T\equiv\frac{\partial\Delta}{\partial T}, \tag{B3}$$

and is numerically calculated from the solution of the gap equations, Eq. (23).

The pressure P is written in terms of the space volume $\mathcal{V}=(aN)^3$ as

$$\begin{aligned}P&=-\left[\frac{\partial F}{\partial\mathcal{V}}\right]_{T,n}\\&=-\frac{1}{N^3}\sum_{\mathbf{k}}\frac{\partial E_{\mathbf{k}}}{\partial a^3}(2n_{\mathbf{k}}-1)+\frac{n}{2}\left(\frac{n}{2}-1\right)\left(\frac{\partial U}{\partial a^3}+24\frac{\partial V}{\partial a^3}\right),\end{aligned} \tag{B4}$$

where

$$\frac{\partial E_{\mathbf{k}}}{\partial a^3}=\frac{\epsilon_{\mathbf{k}}-\bar{\mu}}{E_{\mathbf{k}}}\left[\frac{\partial\epsilon_{\mathbf{k}}}{\partial a^3}+\frac{n}{2}\left(\frac{\partial U}{\partial a^3}+24\frac{\partial V}{\partial a^3}\right)\right],$$

$$\frac{\partial\epsilon_{\mathbf{k}}}{\partial a^3}=\frac{2t}{3a^2}\sum_{i=x,y,z}k_i\cos\left(\frac{2\pi}{N}k_i\right),$$

$$\frac{\partial U}{\partial a^3}=-\frac{1}{a^6}\left[\left(V_c^{(0)}-5\frac{V_c^{(2)}}{a^2}\right)-3\left(V_\sigma^{(0)}-5\frac{V_\sigma^{(2)}}{a^2}\right)\right],$$

$$\frac{\partial V}{\partial a^3}=-\frac{5}{6a^8}V_c^{(2)}. \tag{B5}$$

The double occupancy per site D is expressed as

$$\begin{aligned}D&\equiv\frac{1}{N^3}\sum_i\langle\hat{c}_{i\uparrow}^\dagger\hat{c}_{i\uparrow}\hat{c}_{i\downarrow}^\dagger\hat{c}_{i\downarrow}\rangle\\&=\frac{1}{N^3}\frac{\partial E}{\partial U}\\&=\frac{\Delta^2}{4U^2}+\frac{n^2}{4}-\frac{n}{N^3}\sum_{\mathbf{k}}(\epsilon_{\mathbf{k}}-\bar{\mu})\frac{n_{\mathbf{k}}^2}{T}e^{E_{\mathbf{k}}/T}.\end{aligned} \tag{B6}$$

The kinetic energy per site KE is written as

$$\begin{aligned}\mathrm{KE}&\equiv-\frac{t}{N^3}\sum_{\langle i,j\rangle,\sigma}\langle\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}\rangle+6\frac{t}{N^3}\sum_{i\sigma}\langle\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\rangle\\&=\frac{t}{N^3}\frac{\partial E}{\partial t}\\&=\frac{1}{N^3}\sum_{\mathbf{k}}\frac{(\epsilon_{\mathbf{k}}-\bar{\mu})(\epsilon_{\mathbf{k}}+6t)}{E_{\mathbf{k}}}\left[2n_{\mathbf{k}}\left(1-\frac{n_{\mathbf{k}}}{T}E_{\mathbf{k}}e^{E_{\mathbf{k}}/T}\right)-1\right]+6t.\end{aligned} \tag{B7}$$

APPENDIX C: DENSITY WAVE PHASE

The Hamiltonian in the coordinate space is reduced to

$$\begin{aligned}\hat{H}&=-t\sum_{\langle i,j\rangle\sigma}\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}+(6t+n\bar{U}/2)\sum_{i\sigma}\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\\&\quad+(U/2+4\eta V)\delta\sum_{i\sigma}\cos(2\pi\mathbf{n}_i\cdot\mathbf{q}/N)\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\\&\quad-[(U/4)(n^2+\delta^2/2)+V(6n^2+\eta\delta^2)]N^3,\end{aligned} \tag{C1}$$

where the parameter η depends on the dimension of the density wave d, $\eta=3-2d$. Here, we have used

$$\begin{aligned}\sum_{\langle i,j\rangle\sigma}(n_{j\uparrow}+n_{j\downarrow})\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}&\to\sum_{\langle i,j\rangle\sigma}(n_{i\uparrow}+n_{i\downarrow})\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\\&\quad+\delta\sum_{i\mathbf{e}\sigma}\cos[2\pi(\mathbf{n}_i+\mathbf{e})\cdot\mathbf{q}/N]\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\\&\simeq 6n\sum_{i\sigma}\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\\&\quad+2\eta\delta\sum_{i\sigma}\cos(2\pi\mathbf{n}_i\cdot\mathbf{q}/N)\hat{c}_{i\sigma}^\dagger\hat{c}_{i\sigma}\end{aligned} \tag{C2}$$

and

$$\sum_{\langle i,j\rangle}(n_{i\uparrow}+n_{i\downarrow})(n_{j\uparrow}+n_{j\downarrow}) \to \sum_{\langle i,j\rangle}(n_{i\uparrow}+n_{i\downarrow})(n_{j\uparrow}+n_{j\downarrow}) + 2\delta\sum_{\langle ij\rangle\sigma}\cos(2\pi\mathbf{n}_i\cdot\mathbf{q}/N)(n_{j\uparrow}+n_{j\downarrow}) + \delta^2\sum_{i\mathbf{e}}\cos(2\pi\mathbf{n}_i\cdot\mathbf{q}/N) \times\cos[2\pi(\mathbf{n}_i+\mathbf{e})\cdot\mathbf{q}/N] \simeq (6n^2+\eta\delta^2)N^3, \quad \text{(C3)}$$

where the nucleon densities n's are defined in the same way as in Sec. III. In the last step of Eq. (C3), we have used the identities

$$\sum_i \cos(2\pi\mathbf{n}_i\cdot\mathbf{q}/N)=0, \qquad \sum_i \cos^2(2\pi\mathbf{n}_i\cdot\mathbf{q}/N)=\frac{N^3}{2} \quad \text{(C4)}$$

by applying the discretized orthonormality relation, Eq. (10).

Using

$$\sum_{i\sigma}\cos\left(\frac{2\pi}{N}\mathbf{n}_i\cdot\mathbf{q}\right)\hat{c}^\dagger_{i\sigma}\hat{c}_{i\sigma}=\frac{1}{2}\sum_{\mathbf{k}\sigma}[\hat{c}^\dagger_{\mathbf{k}-\mathbf{q}/2\sigma}\hat{c}_{\mathbf{k}+\mathbf{q}/2\sigma} + \hat{c}^\dagger_{\mathbf{k}+\mathbf{q}/2\sigma}\hat{c}_{\mathbf{k}-\mathbf{q}/2\sigma}], \quad \text{(C5)}$$

we obtain the momentum space representation

$$\hat{H}-\mu N^3\hat{n}=\frac{1}{2}\sum_{\mathbf{k}\sigma}(\epsilon_+-\overline{\mu})\hat{c}^\dagger_{+\sigma}\hat{c}_{+\sigma}+\frac{1}{2}\sum_{\mathbf{k}\sigma}(\epsilon_--\overline{\mu})\hat{c}^\dagger_{-\sigma}\hat{c}_{-\sigma} + \frac{1}{8}\overline{\delta}\sum_{\mathbf{k}\sigma}(\hat{c}^\dagger_{-\sigma}\hat{c}_{+\sigma}+\hat{c}^\dagger_{+\sigma}\hat{c}_{-\sigma})-\frac{1}{2}\delta\overline{\delta}N^3+E_0N^3 = \frac{1}{2}\sum_{\mathbf{k}\sigma}(\hat{c}^\dagger_{+\sigma}\hat{c}^\dagger_{-\sigma})\begin{pmatrix}\epsilon_+-\overline{\mu} & \frac{1}{4}\overline{\delta}\\ \frac{1}{4}\overline{\delta} & \epsilon_--\overline{\mu}\end{pmatrix}\begin{pmatrix}\hat{c}_{+\sigma}\\ \hat{c}_{-\sigma}\end{pmatrix} - \frac{1}{16}\delta\overline{\delta}N^3+E_0N^3, \quad \text{(C6)}$$

where the subscripts + and − denote $\mathbf{k}+\mathbf{q}/2$ and $\mathbf{k}-\mathbf{q}/2$, respectively; that is, $\hat{c}_{\pm\sigma}=\hat{c}_{\mathbf{k}\pm\mathbf{q}/2\sigma}$. $\epsilon_\pm$ is defined as

$$\epsilon_\pm=-t\sum_{\mathbf{e}}\exp[i2\pi(\mathbf{k}\pm\mathbf{q}/2)\cdot\mathbf{e}/N] = -2t\sum_{j=x,y,z}\cos[2\pi(k_j\pm q_j/2)/N].$$

We have also defined

$$\overline{\delta}=\delta(2U+16\eta V). \quad \text{(C7)}$$

$\hat{H}-\mu N^3\hat{n}$ is diagonalized through the transformation

$$\hat{\alpha}_{\mathbf{k}+}=u_{\mathbf{k}}\hat{c}_{+\sigma}+v_{\mathbf{k}}\hat{c}_{-\sigma}, \qquad \hat{\alpha}_{\mathbf{k}-}=u_{\mathbf{k}}\hat{c}_{-\sigma}-v_{\mathbf{k}}\hat{c}_{+\sigma}, \quad \text{(C8)}$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are taken to be real and are given by

$$u^2_{\mathbf{k}}=\frac{1}{2}\left(1+\frac{\epsilon_+-\epsilon_-}{\xi_{\mathbf{k}}}\right) \quad \text{and} \quad v^2_{\mathbf{k}}=\frac{1}{2}\left(1-\frac{\epsilon_+-\epsilon_-}{\xi_{\mathbf{k}}}\right),$$

satisfying $u^2_{\mathbf{k}}+v^2_{\mathbf{k}}=1$. Here,

$$\xi_{\mathbf{k}}=\sqrt{(\epsilon_+-\epsilon_-)^2+\overline{\delta}^2/4}. \quad \text{(C9)}$$

$\hat{H}-\mu N^3\hat{n}$ is now expressed as that of a system of free quasiparticles:

$$\hat{H}-\mu N^3\hat{n}=\frac{1}{2}\sum_{\mathbf{k}\lambda}E_{\mathbf{k}\lambda}\hat{\alpha}^\dagger_{\mathbf{k}\lambda}\hat{\alpha}_{\mathbf{k}\lambda}+N^3(E_{\mathrm{GS}}-\mu n), \quad \text{(C10)}$$

where $\lambda=\pm$ and

$$E_{\mathbf{k}\pm}=\frac{1}{2}[(\epsilon_++\epsilon_--2\overline{\mu})\pm\xi_{\mathbf{k}}] \quad \text{(C11)}$$

is the energy of the quasiparticles, and

$$E_{\mathrm{GS}}=-\delta\overline{\delta}/16-n^2\overline{U}/4+\mu n \quad \text{(C12)}$$

is the ground-state energy of the system.

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