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Thermal pairing in Richardson model

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Abstract

The modified BCS theory (MBCS) is applied to the Richardson model for pairing with a level distance of 1 MeV at various values for the number of levels Ω and particles N. It is shown that the limitation of the configuration space sets a limiting temperature T_{M} up to which the MBCS can be applied. Enlarging the space in the half-filled case ($\Omega = N$) by one valence level ($\Omega = N + 1$) extends T_{M} to a much higher temperature so that the predictions by the MBCS can be compared directly with the exact results up to $T \sim 4$–5 MeV even for small N. The MBCS gap does not collapse, but decreases monotonously with increasing T. The total energy and heat capacity predicted by the MBCS are closer to the exact results than those predicted by the BCS, especially in the region of the BCS superfluid-normal phase transition. The discontinuity in the BCS heat capacity at the BCS phase-transition temperature T_c is smoothed out within the MBCS, especially for small N, showing the disappearance of superfluid-normal phase transition in very light systems. With increasing N the peak at T_c in the heat capacity becomes more pronounced, showing a phase-transition-like behavior in heavy systems.

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1. Introduction

Infinite systems undergo a sharp phase transition from the superfluid phase to the normal-fluid one at finite temperature. This phase transition is a second-order one as it is marked by a collapse of the pairing correlations (pairing gap), and a near divergence of the heat capacity at a critical temperature T_c called the phase-transition point. For metal superconductors and nuclear matter,

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by solving the BCS equation at finite temperature (FTBCS) for a constant level density around the Fermi surface, the critical temperature is found to be $T_c \simeq 0.567\Delta(0)$, where $\Delta(0)$ is the pairing gap at zero temperature $T = 0$ [1].

The application of the BCS theory and its generalization, the Hartree–Fock–Bogoliubov (HFB) theory, to finite Fermi systems paved the way to study the superfluid-normal (SN) phase transition in nuclei at finite temperature T [2–4]. Soon it has been realized, however, that the BCS and HFB theories ignore a number of quantal and thermodynamic fluctuations, which become large in small systems due to their finiteness. Several papers have studied the effect of thermal fluctuations in the pairing field and showed that the pairing gap does not collapse as has been predicted by the BCS theory, but decreases monotonously as the temperature increases, and remains finite even at rather high T [5–7]. The conclusion is that thermal fluctuations in the pairing field wash out the second-order SN phase transition. It was unclear, however, about the origin of these fluctuations. Indeed the approach based on the macroscopic Landau theory of phase transitions refers to them as the fluctuations of the most probable values of the paring gap [5,6]. This concept is close to that of the static-path approximation, which treats thermal fluctuations on all possible static paths around the mean field [7].

In the recently proposed modified-BCS (MBCS) theory [8,9], and its generalization, the modified-HFB (MHFB) theory [10], it has been shown for the first time that it is the fluctuations of quasiparticle number that smooth out the sharp SN phase transition and lead to the non-vanishing thermal pairing in finite systems. These quasiparticle-number fluctuations are ignored in the standard BCS and HFB theories at finite temperature, as has been pointed out by Goodman [4]. As a consequence, these theories violate the unitarity relation for the generalized particle-density matrix R, which requires $R^2 = R$. Goodman has shown that $R^2(T) \neq R(T)$ within the HFB theory at $T \neq 0$, and the difference is proportional to the square $\delta\mathcal{N}^2$ of the quasiparticle-number fluctuation, namely

$$\mathrm{Tr}\big[R^2(T) - R(T)\big] = 2\delta\mathcal{N}^2 \equiv 2\sum_i \delta\mathcal{N}_i^2 = 2\sum_i n_i(1-n_i), \tag{1}$$

where

$$n_i = \big[e^{\beta E_i} + 1\big]^{-1} \tag{2}$$

is the occupation number of non-interacting quasiparticles with energy E_i at temperature $T = 1/\beta$ on the ith orbital [4]. The MHFB theory restores the unitarity relation by explicitly including the quasiparticle-number fluctuations, making use of a secondary Bogoliubov transformation from quasiparticle operators to modified quasiparticle ones. The modified single-particle density matrix $\bar{\rho}$ and particle-pairing tensor $\bar{\tau}$ in the MHFB equation have additional terms, which contain the quasiparticle-number fluctuation $\delta\mathcal{N}$. In the limiting case of a constant pairing interaction G the MHFB equation is reduced to the MBCS one. The numerical calculations carried out for realistic nuclei within the MBCS theory have confirmed that the pairing gap does not vanish but decrease with increasing T, and the sharp discontinuity in the heat capacity is smoothed out. Among the merits of the MBCS and MHFB theories are their microscopic nature and simplicity. As a matter of fact, solving the MBCS (MHFB) equation turns out to be as simple as the BCS (HFB) one.

Since the experimental evidences of the thermal non-vanishing pairing gap and smoothing out the sharp bump of the heat capacity are currently scarce [11], a convincing test of the effectiveness of the MBCS (MHFB) theory is to use a model, which allows exact solutions to be compared with. The Richardson model [12] can serve very well this aim as it is a model for pure pairing, which can be solved exactly. An attempt of testing the MBCS theory by using the Richardson model was undertaken in Ref. [13]. Unfortunately, as has been point out in Ref. [14], the consideration of only a single half-filled case with a small number of levels $\Omega = 10$ (equal to the particle number N) has biased the conclusion by the authors of Ref. [13] on the predictive power of the MBCS theory.

The aim of the present paper is to conduct a systematic test of the MBCS theory at finite temperature within the Richardson model for pairing. By comparing the predictions of the MBCS theory with the exact results obtained at various values of level and particle numbers as well as temperature, it will be possible to give an exhausting answer to the applicability and validity of this theory.

The paper is organized as follows. The outline of the Richardson model and its BCS, MBCS and exact solutions at finite temperature are given in Section 2. The results of numerical calculations are analyzed in Section 3. The last section summarizes the paper, where conclusions are drawn.

2. Exact and approximate solutions for Richardson model at finite temperature

2.1. The model

The Richardson model, considered in the present paper, consists of Ω doubly-folded equidistant levels, which interact via a pairing force with a constant parameter G.[1] The Hamiltonian of this model is written as

$$H = \sum_{i=1}^{\Omega} \epsilon_i N_i - G \sum_{i,j=1}^{\Omega} P_i^\dagger P_j, \tag{3}$$

where ϵ_i are the single-particle energies, λ denotes the chemical potential. The particle-number operator N_i and pairing operators $P_i^\dagger$, P_i are given in terms of the creation and destruction particle operators $a_i^\dagger$ and a_i as

$$N_i = a_i^\dagger a_i + a_{-i}^\dagger a_{-i}, \qquad P_i^\dagger = a_i^\dagger a_{-i}^\dagger, \qquad P_i = \left(P_i^\dagger\right)^\dagger. \tag{4}$$

They satisfy the following commutation relations

$$\left[P_i, P_j^\dagger\right] = \delta_{ij}(1 - N_i), \qquad \left[N_i, P_j^\dagger\right] = 2\delta_{ij} P_j^\dagger, \qquad [N_i, P_j] = -2\delta_{ij} P_j. \tag{5}$$

The single-particle energies take the values $\epsilon_i = i\epsilon$ with index i running over all Ω levels. The model is called half-filled when the number Ω of levels is equal to the number N of particles. This particle–hole (ph) symmetric case means that, in the absence of interaction ($G = 0$), the lowest $\Omega_h = \Omega/2$ hole levels are occupied with $N = \Omega$ particles (two particles on each level), while the upper $\Omega_p = \Omega/2$ particle levels are empty. In general, the number Ω_h of hole levels is not necessary to be the same as the number Ω_p of particle levels, i.e. $\Omega_h \neq \Omega_p \neq \Omega/2$. Numerating particle ($p$) and hole ($h$) levels from the levels closest to the Fermi surface, the particle and hole energies are equal to $\epsilon_p = \epsilon(\Omega_h + p)$ and $\epsilon_h = \epsilon(\Omega_h - h + 1)$, respectively, with p indices running from 1 to Ω_p, and h indices running from 1 to $\Omega_h = \Omega - \Omega_h$. The level distance $\epsilon =$ 1 MeV will be used in the present paper.

[1] This model is also called the picket-fence model, ladder model, doubly degenerate equidistant pairing model, or simply pairing model. It was solved exactly for the first time by Richardson in the sixties [12]. This is the reason why it is also known under the name "Richardson model", adopted in the present paper.

2.2. Exact solutions

There exist several methods of solving exactly the pairing problem described by the Hamiltonian (3). They include the Richardson's method [12], the infinite-dimensional algebras in Ref. [15], or the recently proposed exact-pairing (EP) method [16], which amounts to a direct diagonalization in the Fock space. The latter is used in the present paper because of its simplicity. By noticing that the pairing Hamiltonian (3) does not affect unpaired particles, leaving them stationary on given levels, the EP method uses these partially occupied levels, called seniority, as quantum numbers to label the levels. Each level k can contain $s_k = 0$ or 1 unpaired particle. In the case of $s_k = 1$ the unpaired particle can be on either one of two time-conjugated orbitals, which doubles the degeneracy of the resulting many-body state. Hence, in the exact solution, the pairing eigenstate with energy e_k can be labeled with the set of seniorities $\{s_1, s_2, \dots, s_\Omega\}$ and has the degeneracy $d_k = 2^s$, where the total seniority $s = \sum_k s_k$ is the total number of unpaired particles with the values $s = 0, 2, \dots, \Omega$.

Thermodynamics is introduced into the Richardson model by averaging its exact eigenvalues e_k over a statistical ensemble. As the number N of particles in the system is fixed, the preferable choice is the canonical ensemble, which does not allow the particle-number fluctuations, but can share the total energy $\mathcal{E}(T)$ among its possible thermodynamical states following a distribution $Z(\beta)$ called the partition function at temperature β^{-1} [17,18]

$$Z(\beta) = \sum_k d_k \mathrm{e}^{-\beta e_k}. \tag{6}$$

The total energy $\mathcal{E}(T)$ of the system, and its heat capacity C are then defined from the partition function in a standard way as

$$\mathcal{E}(\beta) = -\frac{\partial[\ln Z(\beta)]}{\partial\beta}, \qquad C = -\beta^2 \frac{\partial \mathcal{E}(\beta)}{\partial\beta}. \tag{7}$$

2.3. BCS solutions

By using the canonical Bogoliubov transformation from the particle operators $a_i^\dagger$ and a_i to the quasiparticle ones, $\alpha_i^\dagger$ and α_i

$$a_i^\dagger = u_i\alpha_i^\dagger + v_i\alpha_{-i}, \qquad a_{-i} = u_i\alpha_{-i} - v_i\alpha_i^\dagger, \tag{8}$$

the pairing Hamiltonian (3) is written in the quasiparticle representation as [6,9]

$$H = a + \sum_i b_i\mathcal{N}_i + \sum_i c_i\big(\mathcal{A}_i^\dagger + \mathcal{A}_i\big) + \sum_{ij} d_{ij}\mathcal{A}_i^\dagger\mathcal{A}_j + \sum_{ij} g_i(j)\big(\mathcal{A}_j^\dagger\mathcal{N}_i + \mathcal{N}_i\mathcal{A}_j\big)$$
$$+ \sum_{ij} h_{ij}\big(\mathcal{A}_i^\dagger\mathcal{A}_j^\dagger + \mathcal{A}_j\mathcal{A}_i\big) + \sum_{ij} q_{ij}\mathcal{N}_i\mathcal{N}_j. \tag{9}$$

Here $\mathcal{N}_i$ is the operator of the quasiparticle number, $\mathcal{A}_i^\dagger$ and $\mathcal{A}_i$ are the creation and destruction operators of a time-conjugate quasiparticle pair:

$$\mathcal{N}_i = \alpha_i^\dagger\alpha_i + \alpha_{-i}^\dagger\alpha_{-i}, \qquad \mathcal{A}_i^\dagger = \alpha_i^\dagger\alpha_{-i}^\dagger, \qquad \mathcal{A}_i = \big(\mathcal{A}_i^\dagger\big)^\dagger. \tag{10}$$

The commutation relations for operators $\mathcal{N}_i$, $\mathcal{A}_i^\dagger$, and $\mathcal{A}_i$ are similar to those given by Eq. (5) for operators N_i, $P_i^\dagger$, and P_i, namely

$$\big[\mathcal{A}_i, \mathcal{A}_j^\dagger\big] = \delta_{ij}(1-\mathcal{N}_i), \qquad \big[\mathcal{N}_i, \mathcal{A}_j^\dagger\big] = 2\delta_{ij}\mathcal{A}_i^\dagger, \qquad [\mathcal{N}_i, \mathcal{A}_j] = -2\delta_{ij}\mathcal{A}_i. \tag{11}$$

The explicit expressions of the functions a, b_i, c_i, d_{ij}, $g_i(j)$, h_{ij}, and q_{ij} in Eq. (9) in terms of the coefficients u_i and v_i, and pairing-interaction parameter G can be obtained from Eqs. (7)–(13) of Ref. [9] after setting the shell degeneracy $2\Omega_j = 2$ therein. The BCS equation is a special case of the HFB equation at finite temperature. The later was derived by Goodman [3] using the variational principle, which minimizes the grand potential $\boldsymbol{\Omega} = E - TS - \lambda N$ so that

$$\delta\boldsymbol{\Omega} = 0, \tag{12}$$

where $E = \mathrm{Tr}(DH)$ is the average energy, and $S = -\mathrm{Tr}(D\ln D)$ is the entropy. This variational principle defines a density operator $D = \exp[-\beta(H - \lambda N)]/\mathbf{Z}$ with $\mathbf{Z} = \mathrm{Tr}\{\exp[-\beta(H - \lambda N)]\}$ being the grand partition function, which includes the summation over the thermodynamical states with different particle numbers N. In the limit with a constant pairing parameter G the HFB equation is reduced to the BCS equation at finite temperature. The latter is a set of two coupled sub-equations for the pairing gap Δ and particle number N,

$$\Delta = G\sum_i \tau_i, \qquad N = 2\sum_i \rho_i, \tag{13}$$

where ρ_i and τ_i,

$$\rho_i = v_i^2 + \left(1 - 2v_i^2\right)n_i, \qquad \tau_i = u_i v_i(1 - 2n_i), \tag{14}$$

are the single-particle density and particle-pairing tensor, respectively, with the quasiparticle-occupation number n_i given by the Fermi–Dirac distribution (2), and the quasiparticle energy $E_i = \sqrt{(\epsilon_i - \lambda)^2 + \Delta^2}$. The internal energy $\mathcal{E}$ of the system is given by

$$\mathcal{E} = \mathrm{Tr}\left[(\epsilon - G\rho)\rho - \Delta\tau^\dagger\right] = 2\sum_i\left(\epsilon_i - 2G\sum_k \rho_k\right)\rho_i - \frac{\Delta^2}{G}. \tag{15}$$

In the standard BCS theory the contribution of $G\rho$ to the Hartree–Fock (HF) potential, which leads to the self-energy correction $-G\sum_i v_i^4$ in the internal energy, is often neglected.[2] As the result, the BCS internal energy is obtained as

$$\mathcal{E}_{\mathrm{BCS}} = 2\sum_i \epsilon_i\rho_i - \frac{\Delta^2}{G} = 2\sum_i \epsilon_i\left[(1 - 2n_i)v_i^2 + n_i\right] - \frac{\Delta^2}{G}. \tag{16}$$

The heat capacity C_{BCS} and entropy S_{BCS} are given in a standard way as

$$C_{\mathrm{BCS}} = \frac{\partial\mathcal{E}_{\mathrm{BCS}}}{\partial T}, \qquad S_{\mathrm{BCS}} = -2\sum_i\left[n_i\ln n_i + (1 - n_i)\ln(1 - n_i)\right]. \tag{17}$$

The use of the grand-canonical ensemble within the variational principle (12) within the HFB theory yields the generalized particle-density matrix $R(T)$ in the form

$$R(T) = \begin{pmatrix} \rho & \tau \\ -\tau^* & 1 - \rho^* \end{pmatrix}, \tag{18}$$

which leads to the violation of the unitarity relation in Eq. (1) [4].

[2] In such approximated particle-number projections like the Lipkin–Nogami method [19], the introduction of the term $\sim \lambda_2 v_k^2$ nearly suppresses the self-energy correction $\sim Gv_k^2$.

2.4. MBCS solutions

The MBCS theory includes the quasiparticle-number fluctuations by using the following secondary Bogoliubov transformation from quasiparticle operators, $\alpha_i^\dagger$ and α_i, to the modified quasiparticle ones, $\bar{\alpha}_i^\dagger$ and $\bar{\alpha}_i$

$$\bar{\alpha}_i^\dagger = \sqrt{1-n_i}\alpha_i^\dagger + \sqrt{n_i}\alpha_{-i}, \qquad \bar{\alpha}_{-i} = \sqrt{1-n_i}\alpha_{-i} - \sqrt{n_i}\alpha_i^\dagger. \tag{19}$$

The derivations of the MBCS and MHFB equations are presented in detail in Refs. [9,10]. In Ref. [9], the two transformations (8) and (19) were combined into

$$a_i^\dagger = \bar{u}_i\bar{\alpha}_i^\dagger + \bar{v}_i\bar{\alpha}_{-i}, \qquad a_{-i} = \bar{u}_i\bar{\alpha}_{-i} - \bar{v}_i\bar{\alpha}_i^\dagger, \tag{20}$$

which transforms the particle operators directly to the modified quasiparticle ones. The coefficients $\bar{u}_i$ and $\bar{v}_i$ of the combined transformation (20) are given as

$$\bar{u}_i = u_i\sqrt{1-n_i} + v_i\sqrt{n_i}, \qquad \bar{v}_i = v_i\sqrt{1-n_i} - u_i\sqrt{n_i}. \tag{21}$$

The Hamiltonian (3) in the modified-quasiparticle representation has the same form (9) as that of the quasiparticle one, but with the modified-quasiparticle operators $\bar{\alpha}_i^\dagger$ and $\bar{\alpha}_i$ replacing the quasiparticle ones $\alpha_i^\dagger$ and α_i, $\bar{u}_i$ and $\bar{v}_i$ coefficients replacing u_i and v_i in the expressions for the functions a, b_i, c_i, d_{ij}, $g_i(j)$, h_{ij}, and q_{ij}. The rest of the derivation followed the same way as that for the BCS equation. The final result yields the MBCS equation in the form

$$\bar{\Delta} = G\sum_i \bar{\tau}_i, \qquad N = 2\sum_i \bar{\rho}_i, \tag{22}$$

where the modified single-particle density matrix $\bar{\rho}_i$ and modified particle-pairing tensor $\bar{\tau}_i$ are given as

$$\bar{\rho}_i = \rho_i - 2u_iv_i\delta\mathcal{N}_i, \qquad \bar{\tau}_i = \tau_i - \left(u_i^2 - v_i^2\right)\delta\mathcal{N}_i. \tag{23}$$

The MBCS internal energy is given by an expression similar to that of the BCS one (16). Neglecting $G\bar{\rho}$ from

$$\bar{\mathcal{E}} = \mathrm{Tr}\left[(\epsilon - G\bar{\rho})\bar{\rho} - \bar{\Delta}\bar{\tau}^\dagger\right] = 2\sum_i\left(\epsilon_i - 2G\sum_k\bar{\rho}_k\right)\bar{\rho}_i - \frac{\bar{\Delta}^2}{G}, \tag{24}$$

one obtains

$$\mathcal{E}_{\mathrm{MBCS}} = 2\sum_i\epsilon_i\bar{\rho}_i - \frac{\bar{\Delta}^2}{G} = 2\sum_i\epsilon_i\left[(1-2n_i)v_i^2 + n_i - 2u_iv_i\sqrt{n_i(1-n_i)}\right] - \frac{\bar{\Delta}^2}{G}, \tag{25}$$

where the modified quasiparticle energy $\bar{E}_i \equiv \sqrt{(\epsilon_i - \bar{\lambda})^2 + \bar{\Delta}^2}$ replaces the quasiparticle energy E_i in the expression for the quasiparticle-occupation number n_i. The heat capacity and entropy are calculated within the MBCS theory using the same expressions as given in Eq. (17), where $\mathcal{E}_{\mathrm{BCS}}$ and $n_i(E_i)$ are replaced with $\mathcal{E}_{\mathrm{MBCS}}$ and $n_i(\bar{E}_i)$, respectively.

These results clearly show that the MBCS equation indeed takes the quasiparticle-number fluctuations $\delta\mathcal{N}_i$ on all ith orbitals into account. In Ref. [10], by generalizing of the secondary Bogoliubov transformation (19), the MHFB equation was derived using the variational principle in the same way as for the derivation of the HFB equation at finite temperature [3]. In the limit of constant pairing interaction G of the obtained MHFB equation one recovers the MBCS equation

(22) above. In the same Ref. [10] it has been also proved that the MHFB theory restores the unitarity relation $\bar{R}^2(T) = \bar{R}(T)$ for the modified generalized particle-density matrix $\bar{R}(T)$, in which the single-particle density ρ and particle-pairing tensor τ are replaced with their modified partners, $\bar{\rho}$ and $\bar{\tau}$.

An important feature of Eq. (22) is that the MBCS gap $\bar{\Delta}$ is a sum of a quantal part $\Delta = G\sum_i \tau_i$ and a thermal part $\delta\Delta$

$$\delta\Delta = G\sum_i \delta\Delta_i, \quad \delta\Delta_i = -G\big(u_i^2 - v_i^2\big)\delta\mathcal{N}_i. \tag{26}$$

The latter contains the factors $-(u_i^2 - v_i^2)$, and therefore can be positive- or negative-definite depending on the structure of the single-particle space. As a result, in the extreme case when $|\delta\Delta| \gg \Delta$, the MBCS gap $\bar{\Delta}$ can increase with T at high T if $\delta\Delta > 0$, or become negative if $\delta\Delta < 0$. A test-example for such case with the Woods–Saxon spectrum for neutrons in ^{120}Sn was analyzed in Ref. [10]. This sets the criterion of applicability of the MBCS, which requires that the single-particle space used in practical calculations should be sufficiently large so that the line-shape of $\delta\mathcal{N}_i$ as a function of the single-particle energies ϵ_i is symmetric with respect to the Fermi surface. The reason of why this works has been analysed in detail in Section IV.A.1 of Ref. [10], where Fig. 1(f) shows that a symmetric line shape of $\delta\mathcal{N}_i$ ultimately leads to a large cancellation of the positive and negative wings in $\delta\Delta_i$ (see Fig. 2(b) therein). As a result $|\delta\Delta|$ becomes smaller than Δ so that the MBCS gap $\bar{\Delta}$ remains always positive. This criterion of applicability of the MBCS theory is examined in the next section by analyzing the results of numerical calculations carried out within the Richardson model.

3. Numerical analysis

3.1. Half-filled case: $\Omega = N$

The BCS equation (13) and MBCS equation (22) were numerically solved at finite temperature. The solid lines in Fig. 1(a) represent the MBCS gaps as functions of T, which are obtained

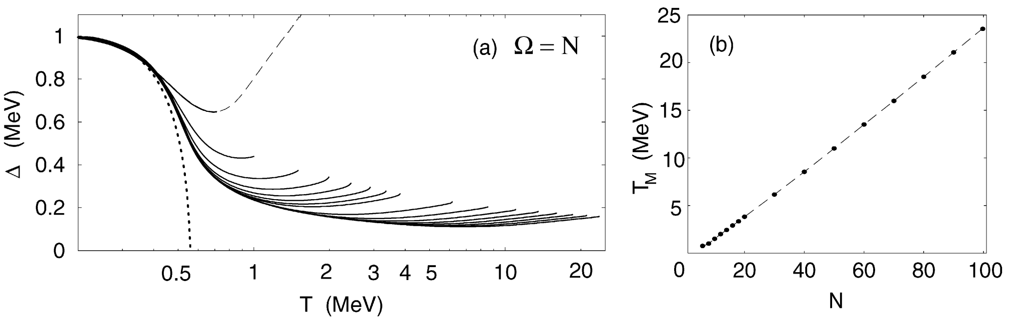

Fig. 1. (a) Pairing gaps for $\Omega = N$ as functions of temperature. The dotted line denotes the BCS gap obtained at $N = 100$. The solid lines represent the MBCS gaps obtained at $N = 6, 8, 10, 12, 14, 16, 18, 20, 30, 40, 50, 60, 70, 80, 90$ and 100, where a solid line, which is extended to a higher T_{M} (see (b)), corresponds to a larger value of N. The dashed line at $N = 6$ shows the part of the MBCS gap, which increases with T due to the limitation of the configuration space as discussed in the text. (b) Values T_{M} (full dots), starting from which the MBCS gap increases with T due to the limitation of the configuration space, plotted against the particle numbers $N = \Omega$. The dashed line connecting these values is drawn as an eye-guide line.

using the 16 values for pairing-interaction parameter $G = 0.55$, 0.48, 0.435, 0.403, 0.38, 0.361, 0.346, 0.334, 0.295, 0.272, 0.256, 0.2445, 0.236, 0.2285, 0.225, and 0.2175 MeV at $\Omega = N = 6$, 8, 10, 12, 14, 16, 18, 20, 30, 40, 50, 60, 70, 80, 90, and 100, respectively. These values of G were chosen so that the BCS gap Δ and MBCS gap $\bar{\Delta}$ remain equal to 1 MeV at $T = 0$. The BCS gap Δ sharply drops with increasing T and collapses at T_c, which signals the SN phase transition. The value of T_c increases slightly with N from 0.55 at $N = 6$ to 0.58 MeV at $N = 100$, i.e. remains close to the value 0.567 MeV for the infinite systems. Therefore in Fig. 1(a) only the BCS gap obtained for $N = 100$ is shown as the dotted line. In difference with the BCS gap, the MBCS gap $\bar{\Delta}$ remains finite at all T. The solid lines in Fig. 1(a) show that the MBCS gap $\bar{\Delta}$ first decreases monotonously with increasing T up to a certain value $T_{\rm M}$. At $T > T_{\rm M}$ an abrupt increase of the MBCS with T is seen for all N. To avoid the figure getting clumsy, this sharp increase of the MBCS is shown as the dashed line only for the case with $N = 6$. The value of $T_{\rm M}$ increases with N almost linearly as shown in Fig. 1(b) from $T_{\rm M} \simeq 0.7$ MeV at $N = 6$ to around 24 MeV at $N = 100$.

Shown in Fig. 2 are the values of quasiparticle-number fluctuation $\delta\mathcal{N}_i$ obtained at various particle numbers N and temperatures $T \leqslant T_{\rm M}$. For $N \leqslant 14$ the line shape of $\delta\mathcal{N}_i$ quickly becomes asymmetric at rather low $T_{\rm M}$ as shown by the thin solid lines in Fig. 2(a)–(e). With increasing N, the line shape of $\delta\mathcal{N}_i$ becomes asymmetric at a much higher $T_{\rm M}$ as shown in Fig. 2(f)–(j). This explains why, for large N, the MBCS theory works well up to very high T even in the half-filled case, as has been shown in Fig. 1 and discussed above. For $N \leqslant 14$, the internal energies predicted by the MBCS theory at $T \leqslant T_{\rm M}$ are still closer to the exact results than those offered by the BCS theory, as shown in Fig. 3.

3.2. Asymmetric case with $\Omega = N + 1$

The thick-solid lines in Fig. 2(a)–(e) clearly demonstrate how adding one more valence level ($\Omega = N + 1$) restores the symmetry in the line shape of $\delta\mathcal{N}_i$. As a result, the MBCS theory produces a long tail in the pairing gap $\bar{\Delta}$ up to much higher T for all $N \leqslant 14$, as shown in Fig. 4. Consequently, reasonable internal energies are obtained within the MBCS theory up to $T \sim 4$–5 MeV, as shown in Fig. 5, in better agreement with the exact results as compared to those predicted by the BCS theory.

The signature of the SN phase transition can be checked by examining the heat capacities C as functions of T, which are shown in Fig. 6. At the same pairing-interaction strength $G = 0.4$ MeV, the BCS theory predicts a sharp peak of divergence of C at T_c as the manifestation of a second-order phase transition (dotted lines). Meanwhile, the exact results for C (thin-solid lines) do not have any singularity at all T. The predictions by the MBCS theory go in between these two limits. At a small particle number, $N = 8$, the quasiparticle-number fluctuations are so strong that they completely wash out the phase-transition peak. As N increases, the peak starts to show up, which becomes comparable with that predicted by the BCS theory at $N = 14$. At high T, both the BCS and MBCS theories predict almost the same values for C, which are slightly smaller than the exact ones. At $T > T_c$, one also notices a large bump in C around $T \simeq 1$–2 MeV, beyond which C decreases with increasing T. This bump is the so-called Schottky anomaly, which is caused by the small configuration space. As shown in Fig. 7, with enlarging the configuration space by increasing Ω ($= N$) this bump in C is pushed up to higher T until its complete disappearance at large N within the entire interval $0 \leqslant T \leqslant 5$ MeV.

It is worth mentioning that, since the results in Fig. 7 are obtained by using reduced values of G to maintain the value for the gap $\Delta(0) = 1$ MeV, i.e. within a reasonable range for the

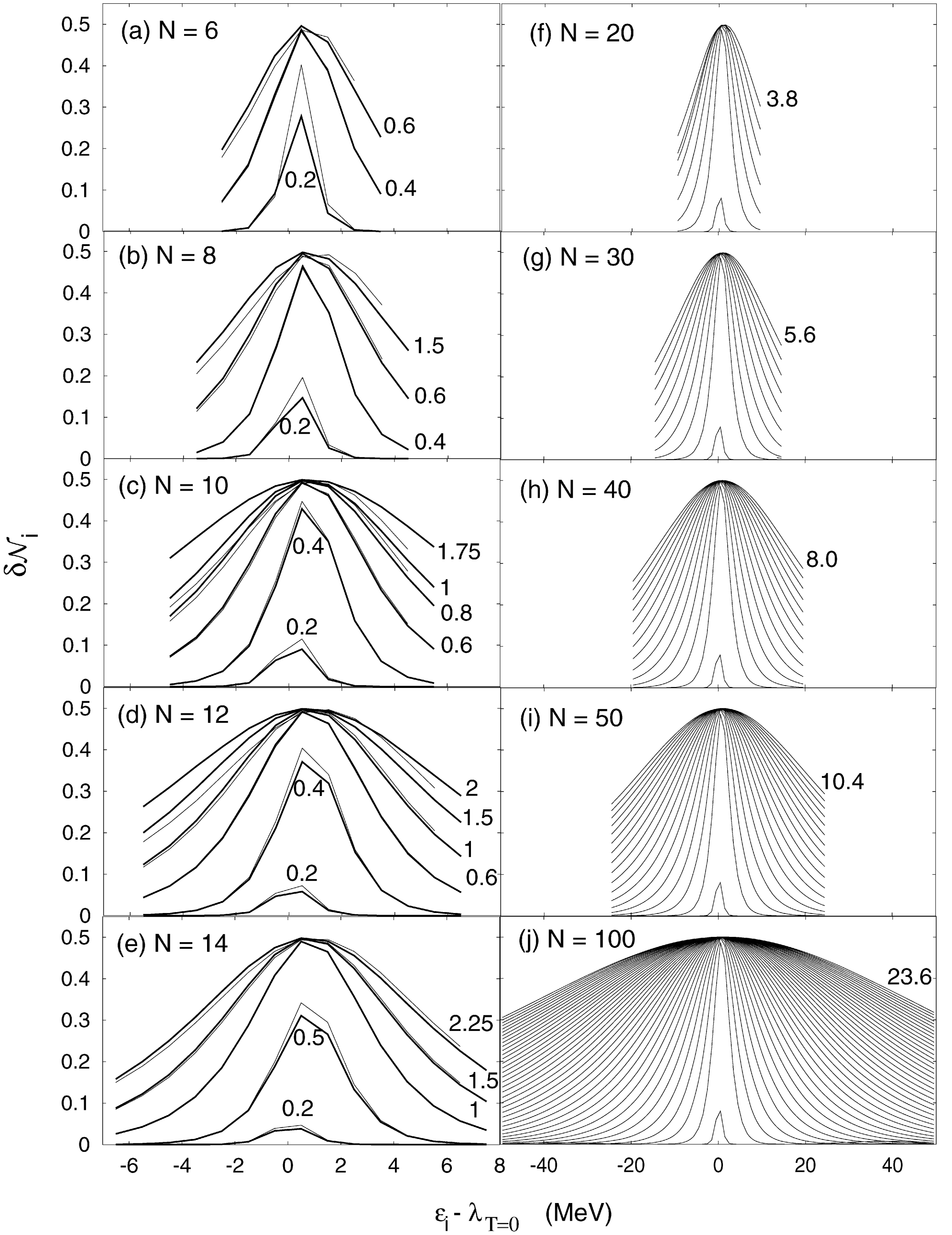

Fig. 2. Quasiparticle-number fluctuation $\delta\mathcal{N}_i$ versus single-particle energies $\epsilon_i - \lambda_{T=0}$ at several particle numbers N and temperatures T. The thin- and thick-solid lines denote the results obtained with $\Omega = N$ and $\Omega = N + 1$, respectively (The lines connecting discrete values at $\epsilon_i - \lambda_{T=0}$ are drawn to guide the eye.) The results for $N \leqslant 14$ are obtained using $G = 0.4$ MeV, while those for larger N are obtained using reduced values of G as described in the text. The results in (a)–(e) are obtained at the values of T (in MeV) shown at the lines, while those in (f)–(i) are obtained with increasing T in step of $\Delta T = 0.4$ MeV from $T = 0.2$ MeV to the value indicated at the top line in each panel.

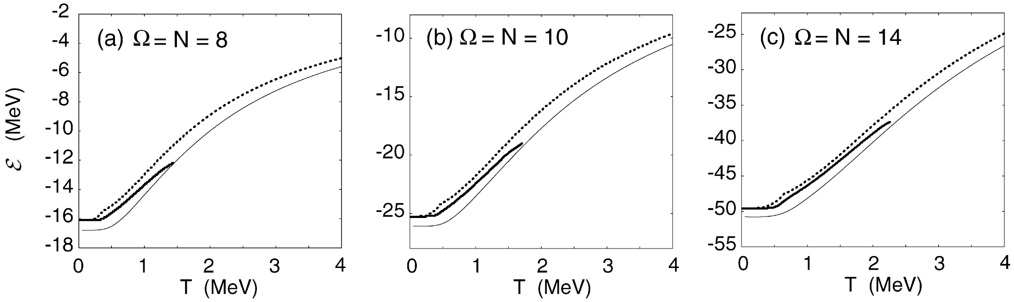

Fig. 3. Internal energies $\mathcal{E}$ within BCS (dotted lines), MBCS (thick solid lines), and exact energies (thin solid lines) for $\Omega = N$ as functions of T at several values of N ($G = 0.4$ MeV). A quantity equivalent to the self-energy term $-G\sum_i v_i^4$, not included in the BCS and MBCS theories, has been subtracted from the exact energies.

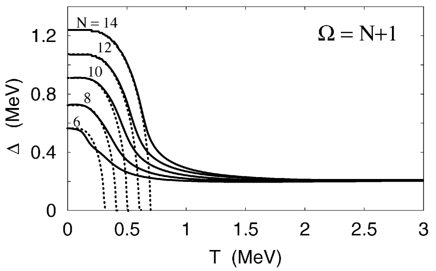

Fig. 4. Pairing gaps within BCS (dotted lines) and MBCS (solid lines) for $\Omega = N + 1$ as functions of temperature at $N \leqslant 14$, as shown atop the lines ($G = 0.4$ MeV).

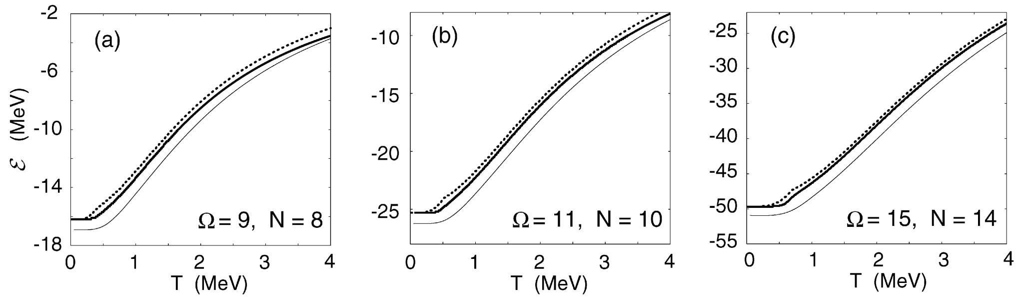

Fig. 5. The same as in Fig. 3 but for $\Omega = N + 1$.

realistic pairing gap at $T = 0$, although thermal fluctuations in the quasiparticle number indeed smooth out the sharp SN phase transition, a remnant of this phase transition can still be seen as shown by the small peak in the temperature-dependence of the heat capacity C at around T_c. Meanwhile, no signature for an SN phase transition is seen in the exact results. Such discrepancy should be interpreted with some caution. The point is that, the exact solutions of a system with pure pairing such as those of the Richardson model do not represent a full thermalization. The seniority conservation prevents a number of particles to interact with each other. As a result, for the exact solutions, the temperature defined in different way do not agree [21,22]. Occupation numbers generally are not described by the Fermi–Dirac distribution, especially at low T, where

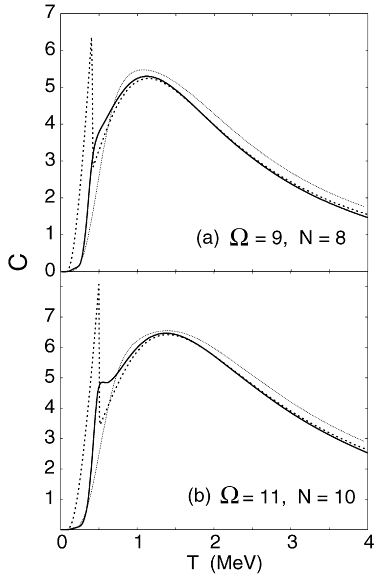

Fig. 6. Heat capacities for $\Omega = N + 1$ as functions of T at several N ($G = 0.4$ MeV). Notation are as in Fig. 3.

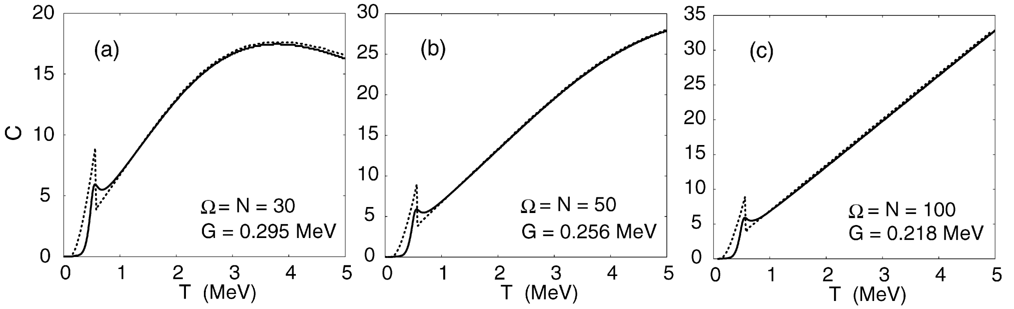

Fig. 7. Heat capacities for $\Omega = N$ as functions of T at $N = 30$, 50, and 100, obtained with reduced values for G so that $\Delta(T = 0) = 1$ MeV. Notation are as in Fig. 3.

the occupation numbers for the levels above the Fermi surface are still quite different from 0, and those for the levels below the Fermi surface are not close to 1. A demonstration of this feature is presented in Fig. 8, where the entropies, predicted by the BCS and MBCS theories, and the exact entropies are shown for both the $\Omega = N$ and $\Omega = N + 1$ cases. For the half-filled case, the MBCS results are slightly closer to the exact ones at $T \geqslant 1$ MeV, while for the asymmetric cases the BCS and MBCS results are nearly the same. In all cases, there is a remarkable agreement between the BCS and MBCS predictions with the exact results at $T > 1$ MeV. One can, however, see that, at $T = 0$, the exact entropy is still positive because the exact occupation numbers are neither 0 nor 1. On the other hand, it is well known that the BCS theory violates the particle number. The inclusion of the quasiparticle-number fluctuation within the MBCS theory removes only a part of this artifact, namely that caused by thermal fluctuations, but does not resolve the problem of particle-number violation in the BCS-based theories.

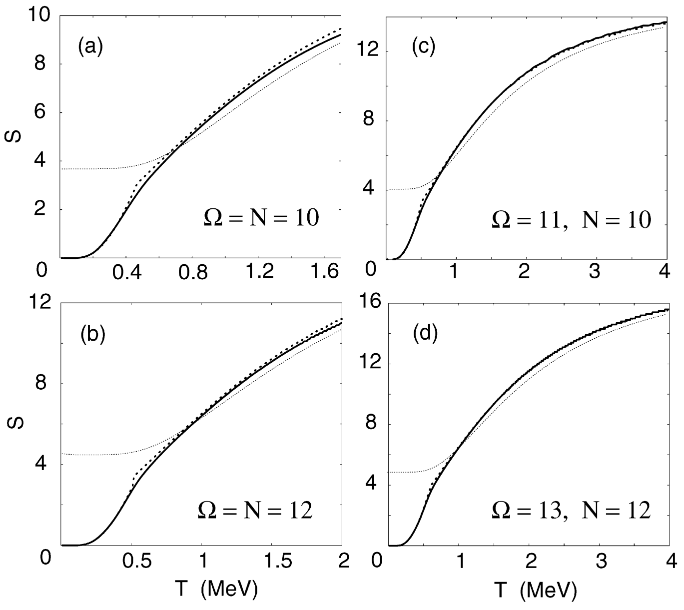

Fig. 8. Entropies S as functions of T ($G = 0.4$ MeV). Notations are as in Fig. 3.

From the discussion above it can be seen that a comparison between the MBCS gap $\bar{\Delta}$ and the exact values at finite T is, generally speaking, not a simple task. First of all, there is no pairing gap per se in the exact solutions. The superfluid pairing field can be well separated from the mean field when the concept of the latter works well, namely in heavy systems where N is large. However, for large N the exact solutions weighed up to high temperature are impracticable. Second, at small N, where exact solutions are feasible, the particle-number violation in the BCS-based theories can be a serious problem. The cure for this problem is to carry out the exact particle-number projection. Unfortunately a rigorous mean-field approximation at finite T, exactly projected before variation, is again impracticable [20]. An approximated particle-number projection at $T \neq 0$ is possible within the context of the Lipkin–Nogami method [6] or static-path approximation (SPA) [7,20], and should be applied on top of the MBCS theory. By carrying out such a study in the future, more conclusive results can be drawn on whether the SN phase transition is completely washed out or there is still a remnant of it in finite systems.[3]

In the meantime, a qualitative comparison can be still carried out by extracting a gap-like quantity from the exact total energy. This is done here by subtracting the first term at the right-hand side of Eq. (25) from the energy $\mathcal{E}(\beta)$ (7) so that the remaining part $\mathcal{E}'(\beta)$, after being corrected by the self-energy term $-G\sum_i v_i^4$ and the effect of residual interaction (see Eq. (24) of Ref. [6]), can be compared with $-\bar{\Delta}^2/G_{\rm eff}$, where $G_{\rm eff} = G(1 + 1/\delta N^2)$ is the renormalized pairing parameter to approximately take into account the effect of approximated particle-number projection following Ref. [23]. The particle-number fluctuations $\delta N^2 = 4\sum_i \bar{u}_i^2\bar{v}_i^2$ are calculated within the MBCS theory [9]. From here a gap-like quantity can be extracted as $\sqrt{-G_{\rm eff}\mathcal{E}'(\beta)}$.

[3] A self-consistent MBCS theory plus approximated particle-number projection within the Lipkin–Nogami method is currently under study.

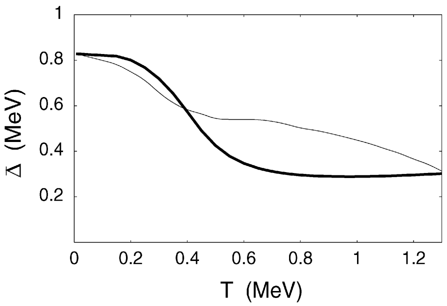

Fig. 9. MBCS pairing gap (thick line) and gap-like quantity extracted from the exact total energy (thin line) as functions of T for $\Omega = N = 10$ with $G = 0.4$ MeV (see the text for details).

This comparison is not intended to be quantitative since the approximate particle-number projection is not carried out self-consistently with solving the MBCS equation.

An illustration for this qualitative comparison is shown in Fig. 9 for $\Omega = N = 10$ with $G = 0.4$ MeV. As the effect of particle-number projection always increases the value of the gap at $T = 0$, to ease the comparison, the gap-like values extracted from the exact total energy (thin line) have been scaled down by a factor of 1.25 to coincide with $\bar{\Delta}$ at $T = 0$. (For comparison, this factor for neutron gaps at $T = 0$ in realistic nuclei is around 1.25 and 1.22 for $N = 30$ [6] and 102 [23], respectively.) Moreover, the method proposed in Ref. [23] is good when $\delta N^2 \gg 1$. At T around T_c this condition is not well satisfied (see Fig. 1 of Ref. [6], e.g.). As a result, the values extracted from the exact results become enhanced at $T \sim 0.4$–0.6 MeV. Albeit being rather crude, this comparison shows that the gap-like quantity extracted from the exact total energy also decreases monotonously with increasing T, showing no signature of a sharp SN phase transition. To reduce the discrepancy at $T > T_c$, apart from using a self-consistent MBCS theory plus particle-number projection mentioned above, the effect of residual interaction beyond the BCS (MBCS) theory should be taken into account within the self-consistent quasiparticle RPA (SQRPA) or SPA plus SQRPA at finite temperature, which is beyond the framework of the present study.

4. Conclusions

This work presents the first systematic test of the MBC theory at finite temperature T by using an exactly solvable model, namely the Richardson model for pairing. The predictions given by the MBCS theory have been compared with those offered by the BCS theory and the exact results, obtained at various level numbers Ω and particle numbers N.

It is shown that the criterion of validity for the MBCS theory is fulfilled up to a temperature $T_{\rm M}$. In the calculations using the reduced values of pairing-interaction parameter G to maintain the same pairing gap at $T = 0$ with increasing the particle number N, the value of $T_{\rm M}$ increases almost linearly with $\Omega = N$ from around 0.6 MeV ($> T_c$) at $\Omega = N = 6$ up to around 24 MeV at $\Omega = N = 100$. For low N, it is demonstrated that enlarging the configuration space by adding one more valence level, i.e. $\Omega = N + 1$, restores the symmetry in the line shape of the quasiparticle-number fluctuation $\delta\mathcal{N}_i$. As a result, the region of applicability of the MBCS theory can be extended up to $T \sim 4$–5 MeV even for $N \leqslant 14$. Hence, the conclusion, previously drawn from the application of the MBCS theory to realistic nuclei, is reconfirmed that the pairing gap does not collapse at T_c within the MBCS theory, but decreases monotonously with increasing T.

As the result, the divergence in the heat capacity C at T_c, which serves as the signature of the second-order SN phase transition, is completely washed out in very small systems ($N \leqslant 8$ for $G = 0.4$ MeV), and smoother in large systems ($N > 20$).

For the small systems with $N \leqslant 14$, where exact solutions are feasible, the predictions by the MBCS theory are found in better agreement with the exact results than those obtained within the BCS theory for all thermodynamic quantities under consideration such as the internal energy, heat capacity, and entropy.

The results of this test adds more confidence in the MBCS theory as an effective and simple microscopic approach to the study of thermal fluctuations in finite systems such as nuclei.

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