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Comment on "Test of the modified BCS model at finite temperature"

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The results and conclusions by Ponomarev and Vdovin [Phys. Rev. C **72**, 034309 (2005)] are inadequate to judge the applicability of the modified BCS because they were obtained either in the temperature region, where the use of zero-temperature single-particle spectra is no longer justified, or in too limited configuration spaces.

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The modified BCS theory (MBCS) was proposed and developed in Refs. [1–3] as a microscopic approach to take into account fluctuations of quasiparticle numbers, which the BCS theory neglects. The use of the MBCS in nuclei at finite temperature T washes out the sharp superfluid-normal phase transition. This agrees with the predictions by the macroscopic theory [4], the exact solutions [5], and experimental data [6]. The authors of Ref. [7] claimed that the MBCS is thermodynamically inconsistent and its applicability is far below the temperature where the conventional BCS gap collapses. The present Comment points out the shortcomings of Ref. [7]. We concentrate only on the major issues without repeating minor arguments already discussed in Refs. [2,3] or inconsistent comparisons in Fig. 9 and Ref. [11] of Ref. [7] (see Ref. [8]).

(i) The application of the statistical formalism in finite nuclei requires that T should be small compared to the major-shell spacings ($\sim$5 MeV for ^{120}Sn). In this case zero-T single-particle energies can be extended to $T \neq 0$. As a matter of fact, the T-dependent Hartree-Fock (HF) calculations for heavy nuclei in [9] have shown that already at $T \geqslant 4$ MeV the effect of T on single-particle energies cannot be neglected. We carried out a test calculation of the neutron pairing gap for ^{120}Sn, where, to qualitatively mimic the compression of the single-particle spectrum at high T as in Ref. [9], the neutron energies are $\epsilon'_j = \epsilon_j(1+\gamma T^2)$ with $\gamma = -1.2\times 10^{-4}$ if $|j\rangle \leqslant |1g_{9/2}\rangle$. For $|j\rangle$ above $|1g_{9/2}\rangle$, we took γ equal to 0.49×10^{-3} and -0.7×10^{-3} for negative and positive ϵ_j, respectively. The obtained MBCS gap has a smooth and positive T dependence similar to the solid line in Fig. 7 of Ref. [1] with a flat tail of around 0.2 MeV from $T = 5$ MeV up to $T = 7$ MeV. For the limited spectrum used in the calculations of Ni isotopes [2], the major-shell spacing between (28–50) and (50–82) shells is about 3.6 MeV, so the region of valid temperature is $T \ll 3.6$ MeV. Hence, the strange behaviors in the results obtained at large T for ^{120}Sn and Ni isotopes in [7] occurred because the zero-T spectra were extended to too high T. Moreover, the configuration spaces used for Ni isotopes are too small for the MBCS to be applied at large T. The same situation takes place within the picket-fence model (PFM) analyzed below.

(ii) The virtue of the PFM is that it can be solved exactly in principle at $T = 0$. However, at $T \neq 0$ the exact solutions of a system with pure pairing do not represent a fully thermalized system. As a result, temperatures defined in different ways do not agree [10]. The limitation of the configuration space with $\Omega = 10$ causes a decrease of the heat capacity C at $T_M > 1.2$ MeV (Schottky anomaly) [3] (See Fig. 4 (c) of Ref. [7]). Therefore, the region of $T > 1.2$ MeV, generally speaking, is thermodynamically unphysical. The most crucial point here, however, is that such limited space deteriorates the criterion of applicability of the MBCS (See Sec. IV. A. 1 of Ref. [3]), which in fact requires that the line shapes of the quasiparticle-number fluctuations $\delta\mathcal{N}_j \equiv \sqrt{n_j(1-n_j)}$ should be included symmetrically related to the Fermi level [Fig. 1(f) of Ref. [3] is a good example]. The dashed lines in Fig. 1(a) shows that, for $N = 10$ particles and $\Omega = 10$ levels ($G = 0.4$ MeV), at T close to 1.78 MeV, where the MBCS breaks down, $\delta\mathcal{N}_j$ are strongly asymmetric and large even for lowest and highest levels. At the same time, by just adding one more valence level ($\Omega = 11$) and keeping the same $N = 10$ particles, we found that $\delta\mathcal{N}_j$ are rather symmetric related to the Fermi level up to much higher T [solid lines in Fig. 1(a)]. This restores the balance in the summation of partial gaps $\delta\Delta_j$ [3]. As a result the obtained MBCS gap has no singularity at $0 \leqslant T \leqslant 4$ MeV [Fig. 1(b)]. The total energy and heat capacity obtained within the MBCS also agree better with the exact results than those given by the BCS [Fig. 2]. It is worth noticing that, even for such small N, adding one valence level increases the excitation energy E^* by only $\sim$10% at $T = 2$ MeV, while at $T < 2$ MeV the values of E^* for $\Omega = 10$ and 11 are very close to each other.

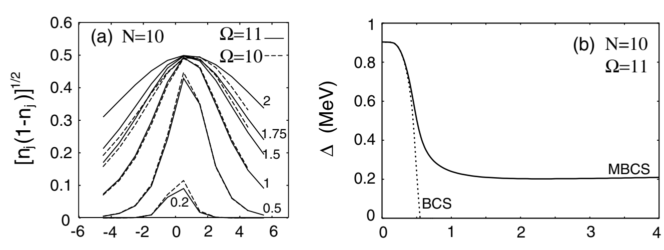

FIG. 1. (a) MBCS quasiparticle-number fluctuations $\delta\mathcal{N}_j$ within the PFM versus single-particle energies at several T. Lines connect discrete values to guide the eyes; numbers at the lines show the values of T in MeV; (b) BCS and MBCS gaps for $N = 10$ and $\Omega = 11$ ($G = 0.4$ MeV).

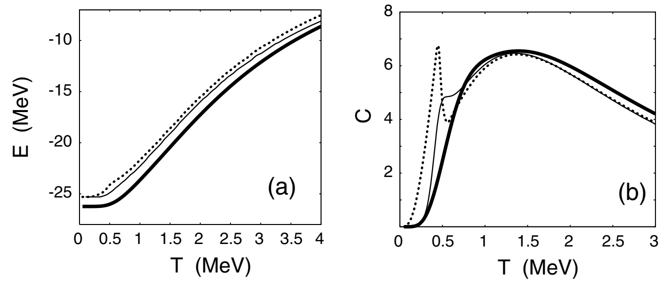

FIG. 2. Total energies (a) and heat capacities (b) within the PFM for ($N = 10$, $\Omega = 11$, $G = 0.4$ MeV) versus T. Dotted, thin-, and thick-solid lines denote the BCS, MBCS, and exact results, respectively. A quantity equivalent to the self-energy term $-G\sum_j v_j^4$, not included within BCS and MBCS, has been subtracted from the exact total energy.

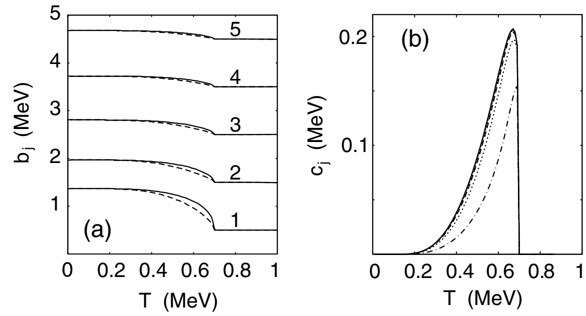

FIG. 3. b_j (a) and c_j (b), obtained within BCS for five lowest levels in the PFM with $\Omega = 10$ versus T. In (a) the solid and dashed lines represent b_j and quasiparticle energies E_j, respectively. In (b) the solid, dashed, dotted, and dash-dotted lines correspond to levels 1–5 in (a), respectively.

We also carried out the calculations for larger particle numbers N. This eventually increases $T_{\rm M}$, and also makes the line shapes of $\delta\mathcal{N}_j$ very symmetric at much higher T. For $\Omega = 50$ and 100, e.g., we found $T_{\rm M} > 5$ MeV, and the MBCS gap has qualitatively the same behavior as that of the solid line in Fig. 1(b) up to $T \sim 5$–6 MeV. However, for large N the exact solutions of PFM turn out to be impractical as a testing tool for $T \neq 0$. Since all the exact eigenstates must be included in the partition function Z, and, since for $N = 50$, e.g., the number of zero-seniority states alone already reaches 10^{14}, the calculation of exact Z becomes practically impossible.

(iii) The principle of compensation of dangerous diagrams was postulated to define the coefficients u_j and v_j of the Bogoliubov canonical transformation. This postulation and the variational calculation of $\partial H'/\partial v_j$ lead to Eq. (19) in Ref. [7] for the BCS at $T = 0$. It is justified so long as divergences can be removed from the perturbation expansion of the ground-state energy. However, at $T \neq 0$ a T-dependent ground state does not exist. Instead, one should use the expectation values over the canonical or grand-canonical ensemble [2,3]. Therefore, Eq. (19) of Ref. [7] no longer holds at $T \neq 0$ since the BCS gap is now defined by Eq. (7) of Ref. [7], instead of Eq. (3). Figure 3 clearly shows how $b_j \neq E_j$ and $c_j \neq 0$ at $T \neq 0$. This invalidates the critics based on Eq. (19) of Ref. [7].

In conclusion, the test of Ref. [7] is inadequate to judge the MBCS applicability because its results were obtained either in the T region, where the use of zero-T spectra is no longer valid (for ^{120}Sn and Ni), or within too limited configuration spaces (the PFM for $N = \Omega = 10$ or 2 major shells for Ni). Our calculations with a T-dependent spectrum for ^{120}Sn, and within extended configuration spaces presented here show that the MBCS is a good approximation up to high T even for a system with $N = 10$ particles.

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