On the test of the modified BCS at finite temperature

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Abstract

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 [1, 2, 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 [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 [7]. We concentrate only on the major issues without repeating minor arguments already discussed in [2, 3] or inconsistent comparisons in Fig. 9 and footnote [11] of [7] (See [8]).

1) 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 $T \geq 4$ 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 [9], the neutron energies are $\epsilon_j' = \epsilon_j(1 + \gamma T^2)$ with $\gamma = -1.2 \times 10^{-4}$ if $|j| \leq |1g_{9/2}|$. For $|j| > |1g_{9/2}|$, we took $\gamma$ equal to $0.49 \times 10^{-3}$ and $-0.7 \times 10^{-3}$ for negative and positive $\epsilon_j$, respectively. The obtained MBCS gap has a smooth and positive $T$ dependence similar to the solid line in Fig. 7 of [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.

2) 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 [7]). Therefore, the region of $T > 1.2$ MeV,
FIG. 1: (a) MBCS quasiparticle-number fluctuations \( \delta N_j \) 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).

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 \[3\]), which in fact requires that the line shapes of the quasiparticle-number fluctuations \( \delta N_j \equiv \sqrt{n_j(1-n_j)} \) should be included symmetrically related to the Fermi level [Fig. 1 (f) of \[3\] 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, \( \delta N_j \) 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 \( \delta N_j \) 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 \( 0 \leq T \leq 4 \) 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. We also carried out the calculations for larger particle numbers \( N \). This eventually increases \( T_M \), and also makes the line shapes of \( \delta N_j \) very symmetric at much higher \( T \). For \( \Omega = 50 \) and 100, e.g., we found \( T_M > 5 \) 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
FIG. 2: Total energies (a) and heat capacities (b) within the PFM for \((N = 10, \Omega = 11, G = 0.4 \text{ MeV})\) versus \(T\). Dotted, thin-, and thick-solid lines denote the BCS, MBCS and exact results, respectively. A quantity equivalent to the self-energy term \(-G \sum v_j^4\), 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 5 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.

\(Z\) becomes practically impossible.

3) 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 [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 [7] no longer holds at \(T \neq 0\) since the BCS gap is now defined by Eq. (7) of [7], instead of Eq. (3). Fig. 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 [7].
In conclusion, the test of [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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