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

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The applicability, predictive power, and internal consistency of a modified BCS (MBCS) model suggested by Dang and Arima have been analyzed in detail in [1]. That analysis concluded that the T-range of the MBCS applicability can be determined as being far below the critical temperature T_c, i.e., $T \ll T_c$. Unfortunately, the source of our conclusions has been misrepresented in [2], which referred to MBCS predictions at $T \gg T_c$.

Since above T_c, particles and holes contribute to an MBCS gap with opposite signs, the model results are rather sensitive to details of a single particle spectrum (s.p.s.) (e.g., discussion in Sec. IV A 1 of [3]). As so, it is indeed possible to find conditions under which the MBCS simulates reasonable thermal behavior of a pairing gap. This can be achieved, e.g., by introducing some particular T-dependence of the s.p.s. (item (i) in [2]) or by adding an extra level to a picket fence model (PFM) (item (ii) in [2]). But such results are very unstable, and accordingly, the model has no predictive power.

Dang and Arima explain poor MBCS results for the PFM ($N = \Omega = 10$) discussed in [1] by referring to strong asymmetry in the line shape of the quasiparticle-number fluctuations $\delta\mathcal{N}_j$ above $T \sim 1.75$ MeV (symmetry of $\delta\mathcal{N}_j$ is announced as a criterion of the MBCS applicability.) The space limitation is blamed for that in [2]. Remember, particle-hole symmetry is an essential feature of the PFM with $N = \Omega$. Thus, strong asymmetry is reported from the MBCS calculation in an ideally symmetric system.

It has been found that a less symmetrical example $N = 10, \Omega = 11$ satisfies better the MBCS criterion [2]. Indeed, the model mimics the behavior of a macroscopic theory in this case [see Fig. 1(b)]. But this example is the only one in which the MBCS does not breakdown, in a long row of physically very close examples with more limited or less limited s.p.s. In all other examples, we witness either negative heat capacity C_ν [Fig. 1(a)] or negative gap $\bar{\Delta}$ [Fig. 1(c)] at rather moderate T (see also [4]).

Unfortunately, the conclusion in [2] that "within extended configuration spaces … the MBCS is a good approximation up to high T even for a system with $N = 10$ particles," is based on a single example, while in all other $N = 10$ examples the MBCS yields unphysical predictions.

The most serious problem of the MBCS is its thermodynamic inconsistency. It is not sufficient to declare two quantities, $\langle H\rangle = \mathrm{Tr}(HD)$ and $\mathcal{E}$ representing the system energy, as being analytically equal by definition (as is done in footnote [8] of [2]) to prove the model consistency. It is easy to find that the expression for $\mathcal{E}_{\mathrm{MBCS}}$ [in the form of Eq. (83) in [3]] can be obtained in the same way as all

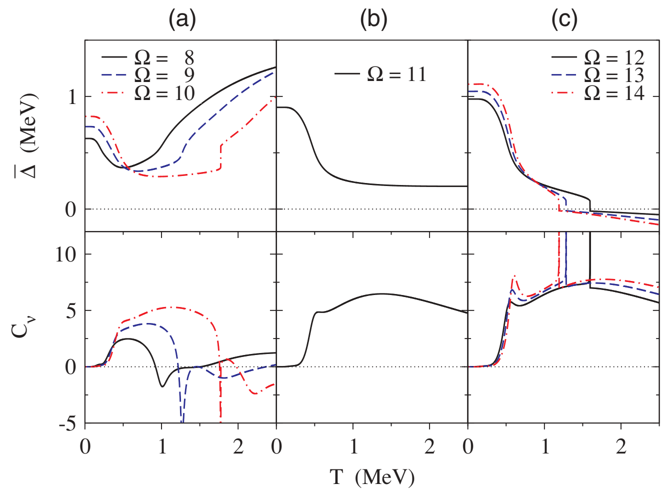

FIG. 1. (Color online) MBCS pairing gap $\bar{\Delta}$ (top panels) and specific heat C_ν (bottom panels) for the PFM with $N = 10$ and (a) $\Omega = 8, 9, 10$, (b) $\Omega = 11$, and (c) $\Omega = 12, 13, 14$. Pairing strength $G = 0.4$ MeV in all cases.

other MBCS equations have been derived: straightforwardly replacing the Bogoliubov $\{u_j, v_j\}$ coefficients in $\mathcal{E}_{\mathrm{BCS}}(T = 0)$ expression by $\{\bar{u}_j, \bar{v}_j\}$ coefficients. Numeric results in Fig. 9 of [1] show that $\langle H\rangle_{\mathrm{MBCS}}$ and $\mathcal{E}_{\mathrm{MBCS}}$ have nothing in common, while $\langle H\rangle_{\mathrm{BCS}} \approx \mathcal{E}_{\mathrm{BCS}}$, as it should be for thermodynamically consistent theory.

Another example of the MBCS thermodynamic inconsistency is shown below. We calculate the system entropy S as

$$S_1 = \int_0^T \frac{1}{t}\frac{\partial\mathcal{E}}{\partial t}\,dt,$$

and

$$S_2 = -\sum_j (2j+1)\big[n_j \ln n_j + (1-n_j)\ln(1-n_j)\big],$$

where n_j are thermal quasiparticle occupation numbers. In Fig. 2, we compare S_1 and S_2 quantities, which refer to thermodynamic and statistical mechanical definitions of entropy, respectively. The calculations have been performed for the neutron system of ^{120}Sn with a realistic s.p.s.

It is not possible to visually distinguish S_1 and S_2 in the FT-BCS calculation (solid curve in Fig. 2 represents both quantities) as it should be for thermodynamically consistent theory. The MBCS S_1 and S_2 quantities are shown by dashed and dot-dashed lines, respectively. They are different by orders of magnitude in the MBCS prediction.

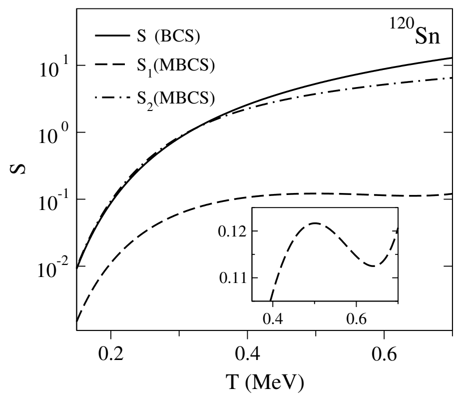

FIG. 2. Entropy of neutron system in ^{120}Sn calculated within the FT-BCS (solid curve) and MBCS (dashed and dot-dashed curves). Notice the logarithmic y scale of the main figure and linear y scale of the insert. See text for details.

We stress that the low T part is presented in Fig. 2. Dramatic disagreement between S_1(MBCS) and S_2(MBCS) representing the system entropy remains at higher T as well, but we do not find it necessary to extend the plot: the model does not describe correctly a heated system even at $T \sim 200$ keV.

We show in the insert of Fig. 2 another MBCS prediction: entropy S_1 decreases as temperature increases. This result is very stable against variation of the pairing strength G within a wide range and contradicts the second law of thermodynamics.

Finally, as we stated before, the conclusion in [1]—that the T-range of the MBCS applicability can be determined as being far below the critical temperature T_c—is based on the analysis of the model predictions from $T \ll T_c$ and not on $T \gg T_c$ results as presented in [2].

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[2] N. D. Dang and A. Arima, Phys. Rev. C **74**, 059801 (2006).
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[4] Dang and Arima put in doubt the validity of the PFM calculations in [1] claiming that "the limitation of the configuration space with $\Omega = 10$ causes a decrease of the heat capacity C at $T_M > 1.2$ MeV.... Therefore, the region of $T > 1.2$ MeV, generally speaking, is thermodynamically unphysical." [2]. It is well-known that such a behavior of the heat capacity is a characteristic feature of finite systems of bound fermions and "does not concern the validity of statistical mechanics. [5]"
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