# Modified Hartree-Fock-Bogoliubov theory at finite temperature

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The modified Hartree-Fock-Bogoliubov (MHFB) theory at finite temperature is derived, which conserves the unitarity relation of the particle-density matrix. This is achieved by constructing a modified-quasiparticle-density matrix, where the fluctuation of the quasiparticle number is microscopically built in. This matrix can be directly obtained from the usual quasiparticle-density matrix by applying the secondary Bogoliubov transformation, which includes the quasiparticle-occupation number. It is shown that, in the limit of constant pairing parameter, the MHFB theory yields the previously obtained modified BCS (MBCS) equations. It is also proved that the modified quasiparticle-random-phase approximation, which is based on the MBCS quasiparticle excitations, conserves the Ikeda sum rule. The numerical calculations of the pairing gap, heat capacity, level density, and level-density parameter within the MBCS theory are carried out for $^{120}$Sn. The results show that the superfluid-normal phase transition is completely washed out. The applicability of the MBCS up to a temperature as high as $T\sim 5$ MeV is analyzed in detail.

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## I. INTRODUCTION

The finite-temperature Hartree-Fock-Bogoliubov (FT-HFB) theory has been successfully applied to highly excited nuclei [1,2]. It offers a fully self-consistent treatment of the interplay between single-particle, pairing as well as rotational degrees of freedom for nuclei in thermal equilibrium.

A major drawback of this theory is the omission of fluctuation effects, which can be classified as quantal and statistical fluctuations. Quantal fluctuations arise from the mean-field approximation to the exact density operator $\mathcal{D}$. As a result, the HFB density operator $\mathcal{D}_{\rm HFB}$ violates the symmetries of the single-particle Hamiltonian $H$ such as the conservation of particle number and spin. However, quantal fluctuations decrease as the temperature increases. Various methods, such as the Lipkin-Nogami [3] method, particle-number projection [4], angular-momentum projection [5], particle-number conserving pairing correlations [6], etc., have been proposed to eliminate quantal fluctuations.

On the contrary, statistical fluctuations, which appear at finite temperature $(T\neq 0)$, increase with increasing $T$ [7–9]. Even the knowledge of the exact density operator $\mathcal{D}$ cannot eliminate statistical fluctuations from the FT-HFB theory. The omission of statistical fluctuation effect leads to the violation of another symmetry, namely, the unitarity relation of the particle-density matrix [1,9]. An immediate consequence of this symmetry violation is the collapse of the pairing gap $\Delta(T)$ at a critical temperature $T_{\rm c}\approx\frac{1}{2}\Delta(T=0)$ in all calculations for realistic nuclei within the FT-HFB theory and its limit, FT-BCS theory [1,2,9,10]. Such a collapse of the pairing gap has been usually speculated as the signature of the superfuid-normal phase transition in finite nuclei. However, by using the Landau macroscopic theory of phase transition [11], Moretto had shown a long time ago that statistical fluctuations wash out such phase transition in finite systems such as nuclei, where these fluctuations are indeed quite large [12]. This conclusion has been confirmed recently by the calculations within the modified BCS (MBCS) theory [13,14]. The latter employs the modified quasiparticles obtained by a secondary Bogoliubov transformation of usual quasiparticles explicitly involving the quasiparticle-occupation numbers. Other approaches such as the static-path approximation [15,16], shell-model Monte Carlo approach [17], modern nuclear shell model calculations [18], as well as the exact solution of the pairing problem [19] also show that pairing correlations do not abruptly disappear at $T\neq 0$.

Another example of symmetry violation caused by the HFB and/or BCS theories is the violation of the Ikeda sum rule within the renormalized quasiparticle random-phase approximation (renormalized QRPA). The Ikeda sum rule states that the difference $\mathcal{S}^{-}-\mathcal{S}^{+}=(2J+1)(N-Z)$ between the total strength $\mathcal{S}^{-}$ of $\beta^{-}$ transitions and of $\beta^{+}$ ones, $\mathcal{S}^{+}$, is independent of models, where $N$ and $Z$ are the neutron and proton numbers, respectively, and $J$ is the angular momentum of the transitions [20]. The renormalized RPA (or the renormalized QRPA, which includes pairing correlations) is an approach taking into account the Pauli principle between the particle (quasiparticle) pairs, which the RPA (QRPA) ignores [21–23]. This renormalizes the RPA forward-going $X$ and backward-going $Y$ amplitudes as well as the two-body interaction matrix elements by a factor, which involves the particle (quasiparticle) occupation numbers in the correlated ground state. As a result, the collapse of the RPA (QRPA) at a critical value of the interaction parameter is avoided. However, it was soon realized that the renormalized QRPA violates the Ikeda sum rule [24]. Several approaches were proposed recently to resolve this problem [25,26].

 

The goal of this paper is to derive a modified HFB (MHFB) theory at finite temperature, which conserves the unitarity relation of the particle-density matrix. It will be shown that this can be achieved by using a modified quasiparticle-density matrix, which takes into account statistical fluctuation of the quasiparticle number microscopically. This modified quasiparticle-density matrix can be alternatively obtained by applying the secondary Bogoliubov transformation in Refs. [13,14] on the particle-density matrix at zero temperature. It will be demonstrated that the BCS limit of the MHFB equations yields the MBCS equations, which have been obtained previously in Refs. [13,14]. It will also be proved that the modified QRPA [13], obtained by using the MBCS quasiparticles, conserves the Ikeda sum rule.

The paper is organized as follows. Section II summarizes the main features of the FT-HFB theory and its violation of the unitarity relation. The MHFB theory, which restores the unitarity relation, is derived in Sec. III. The MBCS equations are derived as the limit of the MHFB ones in the same section. The restoration of the Ikeda sum rule within the modified QRPA is shown in the Appendix. The theory is illustrated in Sec. IV by numerical calculations of the pairing gap and thermodynamic quantities such as the heat capacity, level-density parameter, and level-density as functions of temperature for $^{120}$Sn. The same section also discusses in detail the applicability of the MBCS equations in numerical calculations using realistic single-particle energies at high temperature. The paper is summarized in Sec. V, where conclusions are drawn.

## II. REVIEW OF THE FT-HFB THEORY

This section summarizes the main features of the FT-HFB theory, which has been derived by Goodman in Ref. [1]. They are essential for deriving the MHFB theory at finite temperature in the present paper.

### A. HFB Hamiltonian

The HFB theory is based on the self-consistent Hartree-Fock (HF) Hamiltonian with two-body interaction,

$$H=\sum_{ij}\mathcal{T}_{ij}a_i^\dagger a_j+\frac{1}{4}\sum_{ijkl}v_{ijkl}a_i^\dagger a_j^\dagger a_l a_k, \tag{1}$$

where $i,j,\ldots$ denote the quantum numbers characterizing the single-particle orbitals, $\mathcal{T}_{ij}$ are the kinetic energies, and $v_{ijkl}$ are antisymmetrized matrix elements of the two-body interaction. The HFB theory approximates Hamiltonian (1) by an independent-quasiparticle Hamiltonian $H_{\rm HFB}$,

$$H-\mu\hat{N}\approx H_{\rm HFB}=E_0+\sum_i E_i\alpha_i^\dagger\alpha_i, \tag{2}$$

where $\hat{N}$ is the particle-number operator, $\mu$ is the chemical potential, $E_0$ is the energy of the ground state $|0\rangle$, which is defined as the vacuum of quasiparticles,

$$\alpha_i|0\rangle=0, \tag{3}$$

and $E_i$ are quasiparticle energies. The quasiparticle creation $\alpha_i^\dagger$ and destruction $\alpha_i$ operators are obtained from the single-particle operators $a_i^\dagger$ and $a_i$ by the Bogoliubov transformation, whose matrix form is

$$\begin{pmatrix}\alpha^\dagger\\ \alpha\end{pmatrix}=\begin{pmatrix}U & V\\ V^* & U^*\end{pmatrix}\begin{pmatrix}a^\dagger\\ a\end{pmatrix} \tag{4}$$

with properties

$$UU^\dagger+VV^\dagger=\mathbf{1},\quad UV^{\rm T}+VU^{\rm T}=0, \tag{5}$$

where $\mathbf{1}$ is the unit matrix, and the superscript $^{\rm T}$ denotes the transposing operation. The two-body interaction term of Hamiltonian (1), expressed in terms of quasiparticle operators using transformation (4), also contains the terms $\sim\alpha_i^\dagger\alpha_j^\dagger\alpha_k^\dagger\alpha_l^\dagger, \alpha_i^\dagger\alpha_j^\dagger\alpha_k^\dagger\alpha_l, \alpha_i^\dagger\alpha_j^\dagger\alpha_l\alpha_k$, and their Hermitian conjugated parts. These terms are neglected in the HFB approximation. They play the role of residual interaction beyond the quasiparticle mean field. The quasiparticle energies $E_i$ and matrices $U$ and $V$ are determined as the solutions of the HFB equations, which are usually derived by applying either the variational principle of Ritz or Wick's theorem [5].

### B. Thermodynamic and statistical quantities within the FT-HFB theory

At finite temperature $T$, the condition for a system to be in thermal equilibrium requires the minimum of its grand potential $\Omega$,

$$\Omega=\mathcal{E}-TS-\mu N, \tag{6}$$

with the total energy $\mathcal{E}$, the entropy $S$, and particle number $N$, namely,

$$\delta\Omega=0. \tag{7}$$

This variation defines the density operator $\mathcal{D}$ with trace equal to 1:

$${\rm Tr}\mathcal{D}=1,\quad \delta\Omega/\delta\mathcal{D}=0 \tag{8}$$

in the form

$$\mathcal{D}=Z^{-1}e^{-\beta(H-\mu\hat{N})},\quad Z={\rm Tr}[e^{-\beta(H-\mu\hat{N})}],\quad \beta=T^{-1}, \tag{9}$$

where $Z$ is the grand partition function. The expectation value $<\hat{\mathcal{O}}>$ of any operator $\hat{\mathcal{O}}$ is then given as the average in the grand canonical ensemble,

$$<\hat{\mathcal{O}}>={\rm Tr}(\mathcal{D}\hat{\mathcal{O}}). \tag{10}$$

This defines the total energy $\mathcal{E}$, entropy $S$, and particle number $N$ as

$$\mathcal{E}=<H>={\rm Tr}(\mathcal{D}H),\quad S=-<\mathcal{D}\ln\mathcal{D}>=-{\rm Tr}(\mathcal{D}\ln\mathcal{D}),$$

$$N=<\hat{N}>={\rm Tr}(\mathcal{D}\hat{N}). \tag{11}$$

The FT-HFB theory replaces the unknown exact density operator $\mathcal{D}$ in Eq. (9) with the approximated one, $\mathcal{D}_{\rm HFB}$, which is found in Ref. [1] by substituting Eq. (2) into Eq. (9) as

$$\mathcal{D}_{\rm HFB}=\prod_i [n_i\hat{\mathcal{N}}_i+(1-n_i)(1-\hat{\mathcal{N}}_i)], \tag{12}$$

where $\hat{\mathcal{N}}_i$ is the operator of the quasiparticle number on the $i$th orbital,

$$\hat{\mathcal{N}}_i=\alpha_i^\dagger\alpha_i, \tag{13}$$

and $n_i$ is the quasiparticle-occupation number. Within the FT-HFB theory, $n_i$ is defined according to Eq. (10) as

$$n_i=\langle\hat{\mathcal{N}}_i\rangle=\frac{1}{e^{\beta E_i}+1}, \tag{14}$$

where the symbol $\langle\cdots\rangle$ denotes the average similar to Eq. (10), but in which the approximated density operator $\mathcal{D}_{\rm HFB}$ (12) replaces the exact one, i.e.,

$$\langle\hat{\mathcal{O}}\rangle={\rm Tr}(\mathcal{D}_{\rm HFB}\hat{\mathcal{O}}). \tag{15}$$

That the quasiparticle-occupation number $n_i$ at finite temperature is given by the Fermi-Dirac ditsribution as in Eq. (14), within the framework of the independent-quasiparticle approximation (2) has been also proved a long time ago by Zubarev using the double-time Green function method [27] (see also Appendix A of Ref. [14]). The quasiparticle energy $E_i$ in Eq. (14) is found by solving the FT-HFB equations summarized in the following section.

### C. FT-HFB equations

The generalized particle-density matrix $R$ is related to the generalized quasiparticle-density matrix $Q$ through the Bogoliubov transformation (4) as

$$R=\mathcal{U}^\dagger Q\mathcal{U}, \tag{16}$$

where

$$R=\begin{pmatrix}\rho & \tau\\ -\tau^* & 1-\rho^*\end{pmatrix},\quad Q=\begin{pmatrix}q & t\\ -t^* & 1-q^*\end{pmatrix}=\begin{pmatrix}n & 0\\ 0 & 1-n\end{pmatrix}, \tag{17}$$

with

$$\mathcal{U}=\begin{pmatrix}U^* & V^*\\ V & U\end{pmatrix},\quad \mathcal{U}\mathcal{U}^\dagger=\mathbf{1}. \tag{18}$$

The matrix elements of the single-particle matrix $\rho$ and the particle pairing tensor $\tau$ within the FT-HFB approximation are evaluated as

$$\rho_{ij}=\langle a_j^\dagger a_i\rangle,\quad \tau_{ij}=\langle a_j a_i\rangle, \tag{19}$$

while those of the quasiparticle matrix $q$ are given in terms of the quasiparticle-occupation number since

$$q_{ij}=\langle\alpha_j^\dagger\alpha_i\rangle=\delta_{ij}n_i,\quad t_{ij}=\langle\alpha_j\alpha_i\rangle=0, \tag{20}$$

which follow from the HFB approximation (2). Using the inverse transformation of Eq. (4), the particle densities are obtained as [1]

$$\rho=U^{\rm T}nU^*+V^\dagger(1-n)V,\quad \tau=U^{\rm T}nV^*+V^\dagger(1-n)U. \tag{21}$$

By minimizing the grand potential $\Omega$ according to Eq. (7), Goodman had derived in Ref. [1] the FT-HFB equations in the following form:

$$\begin{pmatrix}\mathcal{H} & \Delta\\ -\Delta^* & -\mathcal{H}^*\end{pmatrix}\begin{pmatrix}U_i\\ V_i\end{pmatrix}=E_i\begin{pmatrix}U_i\\ V_i\end{pmatrix}, \tag{22}$$

where

$$\mathcal{H}=\mathcal{T}-\mu+\Gamma,\quad \Gamma_{ij}=\sum_{kl} v_{ikjl}\rho_{lk},\quad \Delta_{ij}=\frac{1}{2}\sum_{kl} v_{ijkl}\tau_{kl}. \tag{23}$$

(for details of the derivation, see Sec. 4 of Ref. [1]). The total energy $\mathcal{E}$, entropy $S$, and particle number $N$ from Eq. (11) are now given within the FT-HFB theory as

$$\mathcal{E}={\rm Tr}[(\mathcal{T}+\tfrac{1}{2}\Gamma)\rho+\tfrac{1}{2}\Delta\tau^\dagger], \tag{24}$$

$$S=-\sum_i [n_i\ln n_i+(1-n_i)\ln(1-n_i)], \tag{25}$$

$$N={\rm Tr}\rho, \tag{26}$$

from which one can easily calculate the grand potential $\Omega$ (6).

In the limit

$$v_{i\tilde{i}j\tilde{j}}=-G_{ij}, \tag{27}$$

where $|\tilde{i}\rangle$ denotes the time-reversal state of $|i\rangle$, Eqs. (22), (23), and (26) yield the well-known FT-BCS equations. For spherical nuclei and with all the pairing matrix elements equal to $G_{ij}=G$, the FT-BCS equations have the form

$$\Delta=G\sum_j \Omega_j u_j v_j(1-2n_j), \tag{28}$$

$$N=2\sum_j \Omega_j[(1-2n_j)v_j^2+n_j], \tag{29}$$

where $2\Omega_j=2j+1$ is the shell degeneracy. The quasiparticle energies $E_j$ and coefficients $u_j$ and $v_j$ are given as

$$E_j=\sqrt{(\epsilon_j-\mu)^2+\Delta^2}, \quad u_j^2=\frac{1}{2}\left(1+\frac{\epsilon_j-\mu}{E_j}\right),$$

$$v_j^2=\frac{1}{2}\left(1-\frac{\epsilon_j-\mu}{E_j}\right). \tag{30}$$

### D. Violation of unitarity relation within the FT-HFB theory

At zero temperature ($T=0$), the quasiparticle-occupation number vanishes: $n_i=0$, and average (15) reduces to the average in the quasiparticle vacuum (3). The quasiparticle-density matrix $Q$ (17) becomes

$$Q(T=0)\equiv Q_0=\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{for which} \quad Q_0^2=Q_0. \tag{31}$$

Therefore, for the generalized particle-density matrix $R_0=R(T=0)$ the following unitarity relation holds:

$$R_0^2=R_0, \tag{32}$$

where

$$R_0=\mathcal{U}^\dagger Q_0 \mathcal{U}. \tag{33}$$

However, idempotent (32) no longer holds at $T\neq 0$. Indeed, from Eqs. (16) and (17) it follows that

$$R-R^2=\mathcal{U}^\dagger(Q-Q^2)\mathcal{U}, \tag{34}$$

which leads to

$$\begin{aligned}\mathrm{Tr}(R-R^2)&=\mathrm{Tr}(Q-Q^2)\\ &=2\sum_i n_i(1-n_i)\\ &\equiv 2(\delta\mathcal{N})^2\neq 0 \quad (T\neq 0).\end{aligned} \tag{35}$$

The quantity $\delta\mathcal{N}^2=\Sigma_i n_i(1-n_i)$ in Eq. (35) is nothing but the quasiparticle-number fluctuation. This can be easily checked by calculating

$$\begin{aligned}\delta\mathcal{N}^2&=\langle\hat{\mathcal{N}}^2\rangle-\langle\hat{\mathcal{N}}\rangle^2\\ &=\left\langle\sum_i \hat{\mathcal{N}}_i+\sum_{i\neq j}\hat{\mathcal{N}}_i\hat{\mathcal{N}}_j\right\rangle-\sum_i n_i^2-\sum_{i\neq j} n_i n_j\\ &=\sum_i n_i(1-n_i)=\sum_i \delta\mathcal{N}_i^2,\end{aligned} \tag{36}$$

where

$$\delta\mathcal{N}_i^2=n_i(1-n_i) \tag{37}$$

is the fluctuation of quasiparticle number on the $i$th orbital. We have just seen that the violation of the unitarity relation (32) for the generalized single-particle density matrix $R$ occurs at $T\neq 0$ due to the fact that the HFB approximation (2) and the density operator $\mathcal{D}_{\rm HFB}$ (12) exclude the quasiparticle-number fluctuation (36) from the quasiparticle-density matrix (17) [9]. Therefore, in order to restore the idempotent of type (32) at $T\neq 0$ a new approximation should be found such that it includes the quasiparticle-number fluctuation [Eqs. (36) and (37)] in the quasiparticle-density matrix.

## III. THE MHFB THEORY AT FINITE TEMPERATURE

By including the quasiparticle-number fluctuation (36), a part of the higher-order terms $\sim\alpha_i^\dagger\alpha_j^\dagger\alpha_l\alpha_k$, neglected as the residual interaction beyond the FT-HFB quasiparticle mean field, will be taken into account. As a result, the mean field of usual quasiparticles itself will be modified. This leads to the new quasiparticle energy $\overline{E_i}$ and chemical potential $\overline{\mu}$, which will be found as the solution of the MHFB equations to be derived in this section.

### A. Restoration of the unitarity relation

Let us consider, instead of the FT-HFB density operator $\mathcal{D}_{\rm HFB}$ (12), an improved approximation, $\overline{\mathcal{D}}$, to the density operator $\mathcal{D}$. This approximated density operator $\overline{\mathcal{D}}$ should satisfy the two following requirements.

(a) The average

$$\langle\langle\hat{\mathcal{O}}\rangle\rangle\equiv\mathrm{Tr}(\overline{\mathcal{D}}\hat{\mathcal{O}}), \tag{38}$$

in which $\overline{\mathcal{D}}$ is used in place of $\mathcal{D}$ (or $\mathcal{D}_{\rm HFB}$), yields

$$\overline{R}=\mathcal{U}^\dagger\overline{Q}\mathcal{U} \tag{39}$$

for the Bogoliubov transformation $\mathcal{U}$ (18), where one has the modified matrices

$$\overline{R}=\begin{pmatrix} \overline{\rho} & \overline{\tau} \\ -\overline{\tau^*} & 1-\overline{\rho^*} \end{pmatrix}, \quad \overline{Q}=\begin{pmatrix} \overline{q} & t \\ -\overline{t^*} & 1-\overline{q^*} \end{pmatrix}, \tag{40}$$

with

$$\overline{\rho_{ij}}=\langle\langle a_j^\dagger a_i\rangle\rangle, \quad \overline{\tau_{ij}}=\langle\langle a_j a_i\rangle\rangle, \tag{41}$$

$$\overline{q_{ij}}=\langle\langle\alpha_j^\dagger\alpha_i\rangle\rangle=\delta_{ij}\overline{n_i}, \quad \overline{t_{ij}}=\langle\langle\alpha_j\alpha_i\rangle\rangle=\mathbf{\Lambda}_{ij} \tag{42}$$

instead of matrices $R$ and $Q$ in Eqs. (17), (19), and (20). The nonzero values of $\overline{t_{ij}}$ in Eq. (42) are caused by the quasiparticle correlations in thermal equilibrium, which are now included in the average $\langle\langle\cdots\rangle\rangle$ using the density operator $\overline{\mathcal{D}}$.

(b) The modified-quasiparticle-density matrix $\overline{Q}$ satisfies the unitarity relation

$$(\overline{Q})^2=\overline{Q}. \tag{43}$$

The solution of Eq. (43) immediately yields the matrix $\mathbf{\Lambda}$ in the canonical form

$$\mathbf{\Lambda}=\sqrt{\overline{n}(1-\overline{n})}\equiv\begin{pmatrix} & & & & 0 & -\Lambda_1\\ & & & & \Lambda_1 & 0\\ & & 0 & -\Lambda_2 & & \\ & & \Lambda_2 & 0 & & \\ & \iddots & & & & \\ \iddots & & & & & \end{pmatrix},\quad \Lambda_i=\sqrt{\overline{n_i}(1-\overline{n_i})}. \tag{44}$$

Comparing this result with Eqs. (36) and (37), it is clear that tensor $\mathbf{\Lambda}$ consists of the quasiparticle-number fluctuation $\delta\overline{\mathcal{N}}_i=\sqrt{\overline{n_i}(1-\overline{n_i})}$. From Eq. (39) it is easy to see that the unitarity relation holds for the modified generalized single-particle density matrix $\overline{R}$ since

$$\overline{R}-\overline{R}^2=\mathcal{U}^\dagger(\overline{Q}-\overline{Q}^2)\mathcal{U}=0 \tag{45}$$

due to Eq. (43) and the unitary matrix $\mathcal{U}$.

Let us define the modified-quasiparticle operators $\overline{\alpha_i^\dagger}$ and $\overline{\alpha_i}$, which behave in average (38) exactly as the usual-quasiparticle operators $\alpha_i^\dagger$ and $\alpha_i$ do in the quasiparticle ground state, namely,

$$\langle\langle\overline{\alpha_i^\dagger}\overline{\alpha_k}\rangle\rangle=\langle\langle\overline{\alpha_i^\dagger}\overline{\alpha_k^\dagger}\rangle\rangle=\langle\langle\overline{\alpha_k}\overline{\alpha_i}\rangle\rangle=0. \tag{46}$$

In the same way as for the usual Bogoliubov transformation (4), we search for a transformation between these modified-quasiparticle operators $(\overline{\alpha_i^\dagger},\overline{\alpha_i})$ and the usual-quasiparticle ones $(\alpha_i^\dagger,\alpha_i)$ in the following form:

$$\begin{pmatrix}\overline{\alpha^\dagger}\\ \overline{\alpha}\end{pmatrix}=\begin{pmatrix} w & z\\ z^* & w^*\end{pmatrix}\begin{pmatrix}\alpha^\dagger\\ \alpha\end{pmatrix}, \tag{47}$$

with the unitary property similar to Eq. (5) for $U$ and $V$ matrices

$$ww^\dagger+zz^\dagger=\mathbf{1}. \tag{48}$$

Using the inverse transformation of Eq. (47) and requirement (46), we obtain

$$\overline{n}_i=\langle\langle\alpha_i^\dagger\alpha_i\rangle\rangle=\sum_k z_{ik}z_{ik}^*. \tag{49}$$

From this equation and the unitary condition (48), it follows that $zz^\dagger=\overline{n}$ and $ww^\dagger=\mathbf{1}-\overline{n}$. Since $\mathbf{1}-\overline{n}$ and $\overline{n}$ are real diagonal matrices, the canonical form of matrices $w$ and $z$ is found as

$$w=\sqrt{1-\overline{n}}\equiv\begin{pmatrix} w_1 & 0 & & & & \\ 0 & w_1 & & & & \\ & & w_2 & 0 & & \\ & & 0 & w_2 & & \\ & & & & \ddots & \\ & & & & & \ddots\end{pmatrix},$$

$$z=\sqrt{\overline{n}}\equiv\begin{pmatrix} & & & & 0 & -z_1\\ & & & & z_1 & 0\\ & & 0 & -z_2 & & \\ & & z_2 & 0 & & \\ & \iddots & & & & \\ \iddots & & & & & \end{pmatrix}, \tag{50a}$$

where

$$w_i=\sqrt{1-\overline{n}_i},\quad z_i=\sqrt{\overline{n}_i}. \tag{50b}$$

We now see that, just like Eq. (4), which is the generalized form of the Bogoliubov transformation for the BCS case, Eq. (47) with matrices $w$ and $z$ uniquely defined in Eq. (50) is the genearlized form of the secondary Bogoliubov transformation used in Refs. [13,14]. It expresses a simple relationship between the modified-quasiparticle operators $(\overline{\alpha_i^\dagger},\overline{\alpha_i})$ and the usual-quasiparticle operators $(\alpha_i^\dagger,\alpha_i)$ in the same manner as that between the latter and the single-particle operators in the Bogoliubov transformation (4).

We now show that we can obtain the idempotent $\overline{R}^2=\overline{R}$ (45) by applying the secondary Bogoliubov transformation (47), which automatically leads to Eq. (43). Indeed, using the inverse transformation of Eq. (47) with matrices $w$ and $z$ given in Eq. (50), we found that the modified-quasiparticle-density matrix $\overline{Q}$ can be obtained as

$$\mathcal{W}^{\dagger}\bar{Q}_0\mathcal{W}=\begin{pmatrix} \bar{n} & [\sqrt{\bar{n}(1-\bar{n})}]^{\dagger} \\ \sqrt{\bar{n}(1-\bar{n})} & 1-\bar{n}\end{pmatrix}\equiv\bar{Q}, \quad (51)$$

where

$$\mathcal{W}=\begin{pmatrix} (\sqrt{1-\bar{n}})^* & (\sqrt{\bar{n}})^* \\ \sqrt{\bar{n}} & \sqrt{1-\bar{n}}\end{pmatrix}, \quad \mathcal{W}\mathcal{W}^{\dagger}=\mathbf{1}, \quad (52)$$

and

$$\bar{Q}_0=\begin{pmatrix} \langle\langle\bar{\alpha}^{\dagger}\bar{\alpha}\rangle\rangle & \langle\langle\bar{\alpha}\bar{\alpha}\rangle\rangle \\ \langle\langle\bar{\alpha}^{\dagger}\bar{\alpha}^{\dagger}\rangle\rangle & 1-\langle\langle\bar{\alpha}^{\dagger}\bar{\alpha}\rangle\rangle\end{pmatrix}=\begin{pmatrix} 0 & 0 \\ 0 & 1\end{pmatrix}, \quad \bar{Q}_0^2=\bar{Q}_0, \quad (53)$$

due to Eq. (46). This result shows another way of deriving the modified quasiparticle-density matrix $\bar{Q}$ (40) from the density matrix $\bar{Q}_0$ of the modified quasiparticles $(\bar{\alpha}_i^{\dagger},\bar{\alpha}_i)$. This matrix $\bar{Q}_0$ is identical to the zero-temperature quasiparticle-density matrix $Q_0$ (31). Substituting this result into the right-hand side (rhs) of Eq. (39), we obtain

$$\bar{R}=\bar{\mathcal{U}}^{\dagger}\bar{Q}_0\bar{\mathcal{U}}, \quad (54)$$

where

$$\bar{\mathcal{U}}=\mathcal{W}\mathcal{U}=\begin{pmatrix} \bar{U}^* & \bar{V}^* \\ \bar{V} & \bar{U}\end{pmatrix}$$
$$=\begin{pmatrix} (\sqrt{1-\bar{n}})^*U^*+(\sqrt{\bar{n}})^*V & (\sqrt{1-\bar{n}})^*V^*+(\sqrt{\bar{n}})^*U \\ \sqrt{1-\bar{n}}V+\sqrt{\bar{n}}U^* & \sqrt{1-\bar{n}}U+\sqrt{\bar{n}}V^*\end{pmatrix}. \quad (55)$$

This equation is the generalized form of the modified Bogoliubov coefficients $\bar{u}_j$ and $\bar{v}_j$ given in Eq. (6) of Ref. [13] or Eq. (38) of Ref. [14]. From Eqs. (18), (52), and (55), it follows that $\bar{\mathcal{U}}\bar{\mathcal{U}}^{\dagger}=\mathbf{1}$, i.e., transformation (54) is unitary. Therefore, from idempotent (53) it follows that $\bar{R}^2=\bar{R}$. We have just shown that the secondary Bogoliubov transformation (47) allows us to take into account fluctuation of the quasiparticle number and restore the unitarity relation of the generalized particle-density matrix.[1] In this sense, the approximation discussed in the present section is a step beyond the thermal mean field of usual quasiparticles. As a result, the thermal quasiparticle mean field, which was defined within the FT-HFB approximation, is modified due to thermal quasiparticle-number fluctuation.[2]

### B. MHFB equations at finite temperature

With all the thermal degrees of freedom now included in $\bar{\mathcal{U}}$, Eq. (54) formally looks the same as the usual HFB approximation at $T=0$ (33), which connects $R_0$ to $Q_0$. Applying Wick's theorem for the ensemble average [5], one obtains the expressions for the modified total energy $\bar{\mathcal{E}}$,

$$\bar{\mathcal{E}}=\mathrm{Tr}[(\mathcal{T}+\tfrac{1}{2}\bar{\Gamma})\bar{\rho}+\tfrac{1}{2}\bar{\Delta}\bar{\tau}^{\dagger}], \quad (56)$$

where

$$\bar{\Gamma}_{ij}=\sum_{kl} v_{ikjl}\bar{\rho}_{lk}, \quad (57)$$

$$\bar{\Delta}_{ij}=\frac{1}{2}\sum_{kl} v_{ijkl}\bar{\tau}_{kl}. \quad (58)$$

From Eq. (54) we obtain the modified single-particle-density matrix $\bar{\rho}$ and the modified particle-pairing tensor $\bar{\tau}$ in the following form:

$$\bar{\rho}=U^{\mathrm{T}}\bar{n}U^*+V^{\dagger}(1-\bar{n})V+U^{\mathrm{T}}[\sqrt{\bar{n}(1-\bar{n})}]^{\dagger}V$$
$$+V^{\dagger}\sqrt{\bar{n}(1-\bar{n})}U^*, \quad (59)$$

$$\bar{\tau}=U^{\mathrm{T}}\bar{n}V^*+V^{\dagger}(1-\bar{n})U+U^{\mathrm{T}}[\sqrt{\bar{n}(1-\bar{n})}]^{\dagger}U$$
$$+V^{\dagger}\sqrt{\bar{n}(1-\bar{n})}V^*. \quad (60)$$

As compared to Eq. (21) within the FT-HFB approximation, Eqs. (59) and (60) contain the last two terms $\sim[\sqrt{\bar{n}(1-\bar{n})}]^{\dagger}$ and $\sim\sqrt{\bar{n}(1-\bar{n})}$, which arise due to quasiparticle-number fluctuation. Also, the quasiparticle-occupation number is now $\bar{n}$ [see Eq. (42)] instead of $n$ (14).

We derive the MHFB equations following the same variational procedure, which was used to derive the FT-HFB equations in Sec. 4 of Ref. [1]. According to this, we minimize the grand potential $\delta\bar{\Omega}=0$ by varying $U$, $V$, and $\bar{n}$, where

[1]An alternative approach to the unitarity problem was proposed in Ref. [28] making use of the thermofield dynamics [29].

[2]An exact theory on quasiparticle excitations at $T=0$ should define the vacuum and quasiparticles in terms of exact eigenstates of the many-body system [5]. But in this case, a simple mathematical relationship between the exact quasiparticles and the usual particles of the system no longer exists. The advantage of the Bogoliubov-type quasiparticles is the linear relationship between them and the usual particles. However, the corresponding vaccum and single-quasiparticle state are now only approximations of the exact eigen functions of the many-body Hamiltonian. Similarly, at $T\neq0$, when the average over the individual compound systems is replaced by that over the grand canonical ensemble (10), the density operators $\mathcal{D}_{\mathrm{HFB}}$ (12) and $\bar{\mathcal{D}}$ (38) are different approximations of the exact density operator $\mathcal{D}$ (9).

$$\bar{\Omega}=\bar{\mathcal{E}}-T\bar{S}-\bar{\mu}N. \tag{61}$$

Due to Eq. (5), the variations $\delta U$ and $\delta V$ are not independent. They are found by using an infinitesimal unitary tranformation of Eq. (4). The obtained infinitesimal variations $U'=U+\delta U$ and $V'=V+\delta V$ together with $\overline{n'}=\bar{n}+\delta\bar{n}$ are then used in Eqs. (59) and (60) to obtain $\overline{\rho'}=\bar{\rho}+\delta\bar{\rho}$ and $\overline{\tau'}=\bar{\tau}+\delta\bar{\tau}$. Substituting them into Eq. (61) one obtains $\bar{\Omega}'=\bar{\Omega}+\delta\bar{\Omega}$, where $\delta\bar{\Omega}$ is expressed in terms of $\delta\bar{\rho}$, $\delta\bar{\tau}$, and $\delta\bar{n}$ as independent variations. By requiring that the coefficients of $\delta\bar{\rho}$ and $\delta\bar{\tau}$ vanish and following the rest of the derivation as for the zero-temperature case, we finally obtain the MHFB equations, which formally look like the FT-HFB ones (22):

$$\begin{pmatrix} \bar{\mathcal{H}} & \bar{\Delta} \\ -\bar{\Delta}^* & -\bar{\mathcal{H}}^* \end{pmatrix}\begin{pmatrix} U_i \\ V_i \end{pmatrix}=\bar{E}_i\begin{pmatrix} U_i \\ V_i \end{pmatrix}, \tag{62}$$

where, however,

$$\bar{\mathcal{H}}=\mathcal{T}-\bar{\mu}+\bar{\Gamma}, \tag{63}$$

with $\bar{\Gamma}$ and $\bar{\Delta}$ given by Eqs. (57) and (58), respectively. The equation for particle number $N$ within the MHFB theory is

$$N=\mathrm{Tr}\bar{\rho}. \tag{64}$$

By solving Eq. (62), one obtains the modified-quasiparticle energy $\bar{E}_i$, which is different from $E_i$ in Eqs. (22) and/or (30) due to the change of the HF and pairing potentials. Hence, the MHFB quasiparticle Hamiltonian $H_{\mathrm{MHFB}}$ can be written as

$$H-\bar{\mu}\hat{N}\approx H_{\mathrm{MHFB}}=\bar{E}_0+\sum_i \bar{E}_i\hat{\mathcal{N}}_i, \tag{65}$$

instead of Eq. (2). This implies that the approximated density operator $\bar{D}$ (38) within the MHFB theory can be represented in the form similar to Eq. (12), namely,

$$\bar{\mathcal{D}}\equiv\mathcal{D}_{\mathrm{MHFB}}=\prod_i [\bar{n}_i\hat{\mathcal{N}}_i+(1-\bar{n}_i)(1-\hat{\mathcal{N}}_i)]. \tag{66}$$

From here it follows that the formal expression for the modified entropy $\bar{S}$ is the same as that given in Eq. (25), i.e.,

$$\bar{S}=-\sum_i [\bar{n}_i\ln\bar{n}_i+(1-\bar{n}_i)\ln(1-\bar{n}_i)]. \tag{67}$$

Using the thermodynamic definition of temperature in terms of entropy $T=\delta\bar{S}/\delta\bar{\mathcal{E}}$ and carrying out the varition over $\delta\bar{n}_i$, we find

$$\frac{\delta\bar{\mathcal{E}}}{\delta\bar{n}_i}\equiv\bar{E}_i=T\frac{\delta\bar{S}}{\delta\bar{n}_i}=T\ln\left(\frac{1-\bar{n}_i}{\bar{n}_i}\right). \tag{68}$$

Inverting Eq. (68), we obtain

$$\bar{n}_i=\frac{1}{e^{\beta\bar{E}_i+1}}. \tag{69}$$

This result shows that the functional dependence of quasiparticle-occupation number $\bar{n}_i$ on the quasiparticle energy and the temperature within the MHFB theory is also given by the Fermi-Dirac distribution of noninteracting quasiparticles but with the modified energies $\bar{E}_i$ defined by the MHFB equations (62).[3] Therefore, in the rest of the paper we will omit the bar over $\bar{n}_i$ and use the same Eq. (14) with $E_i$ replaced with $\bar{E}_i$ for the MHFB equations.

### C. The MBCS theory at finite temperature

#### 1. MBCS equations

The MBCS equations at finite temperature have been derived previously in Refs. [13,14] using the secondary Bogoliubov transformation (47) for the BCS case. We will show below that these MBCS equations emerge as the limit of the MHFB equations derived in the preceding section.

In the BCS limit (27) with equal pairing matrix elements $G_{ij}=G$, neglecting the contribution of $G$ to the HF potential so that $\bar{\Gamma}=0$, the HF Hamiltonian becomes

$$\bar{\mathcal{H}}_{ij}=(\epsilon_i-\bar{\mu})\delta_{ij}. \tag{70}$$

The pairing potential (58) now takes the simple form

$$\bar{\Delta}=-G\sum_{k>0}\bar{\tau}_{k\tilde{k}}. \tag{71}$$

The Bogoliubov transformation (4) for spherical nuclei reduces to

$$\alpha^{\dagger}_{jm}=u_j a^{\dagger}_{jm}+v_j(-)^{j+m}a_{j-m},$$
$$(-)^{j+m}\alpha_{j-m}=u_j(-)^{j+m}a_{j-m}-v_j a^{\dagger}_{jm}, \tag{72}$$

while the secondary Bogoliubov transformation (47) becomes [13,14]

$$\bar{\alpha}^{\dagger}_{jm}=\sqrt{1-n_j}\alpha^{\dagger}_{jm}-\sqrt{n_j}(-)^{j+m}\alpha_{j-m},$$
$$(-)^{j+m}\bar{\alpha}_{j-m}=\sqrt{1-n_j}(-)^{j+m}\alpha_{j-m}+\sqrt{n_j}\alpha^{\dagger}_{jm}. \tag{73}$$

[3] Note that there remains the residual interaction, even due to pairing alone, beyond the MHFB quasiparticle mean field. At $T=0$ this can be treated as ground-state correlations within the renormalized and/or modified QRPA [13,22]. As a result, $\bar{n}_i$ deviates from the Fermi-Dirac distribution, especially if different multipolarities of the two-body residual interaction are taken into account. However, for the monopole pairing interaction alone, as considered in this paper, such deviation is negligible (see Appendix B of Ref. [14]). At $T\neq 0$ the quasiparticle-number fluctuation beyond the quasiparticle mean field leads to the entropy effect within the renormalized RPA, which was studied in Ref. [30].

The $U$, $V$, $1-n$, $n$, and $\sqrt{n(1-n)}$ matrices are now block diagonal in each two-dimensional subspace spanned by the quasiparticle state $|j\rangle$ and its time-reversal partner $|\tilde{j}\rangle = (-)^{j+m}|j-m\rangle$:

$$U=\begin{pmatrix} u_j & 0 \\ 0 & u_j \end{pmatrix}, \quad V=\begin{pmatrix} 0 & v_j \\ -v_j & 0 \end{pmatrix}, \tag{74}$$

$$1-n=\begin{pmatrix} 1-n_j & 0 \\ 0 & 1-n_j \end{pmatrix}, \quad n=\begin{pmatrix} n_j & 0 \\ 0 & n_j \end{pmatrix},$$

$$\sqrt{n(1-n)}=\begin{pmatrix} 0 & -\sqrt{n_j(1-n_j)} \\ \sqrt{n_j(1-n_j)} & 0 \end{pmatrix}. \tag{75}$$

Substituting these matrices into the rhs of Eqs. (59) and (60), we find

$$\overline{\rho_{j\tilde{j}}}=(1-2n_j)v_j^2+n_j-2\sqrt{n_j(1-n_j)}u_jv_j, \tag{76}$$

$$\overline{\tau_{j\tilde{j}}}=-(1-2n_j)u_jv_j+\sqrt{n_j(1-n_j)}(u_j^2-v_j^2). \tag{77}$$

Substituting now Eqs. (77) and (76) into the rhs of Eqs. (71) and (64), respectively, we obtain the MBCS equations for spherical nuclei in the following form:

$$\overline{\Delta}=G\sum_j \Omega_j[(1-2n_j)u_jv_j-\sqrt{n_j(1-n_j)}(u_j^2-v_j^2)], \tag{78}$$

$$N=2\sum_j \Omega_j[(1-2n_j)v_j^2+n_j-2\sqrt{n_j(1-n_j)}u_jv_j]. \tag{79}$$

Equations (78) and (79) are exactly the same as the MBCS equations (23) and (24) in Ref. [13] or Eqs. (39) and (40) in Ref. [14]. We have just shown that the MBCS equations in Refs. [13,14] emerge as the natural limit of the MHFB equations at finite temperature.

For convenience in further discussions we rewrite the MBCS gap in Eq. (78) as a sum of quantal $\Delta_{\rm Q}$ and thermal-fluctuation $\delta\Delta$ parts as

$$\overline{\Delta}=\Delta_{\rm Q}+\delta\Delta, \tag{80}$$

where the quantal gap $\Delta_{\rm Q}$ is

$$\Delta_{\rm Q}=\sum_j (\Delta_{\rm Q})_j, \quad (\Delta_{\rm Q})_j=G\Omega_ju_jv_j(1-2n_j). \tag{81}$$

It is called quantal since it is caused by quantal effects starting from $T=0$, where it is equal to the BCS gap, and decreases as $T$ increases because the Pauli blocking becomes weaker. The thermal-fluctuation gap $\delta\Delta$, referred to, hereafter, as the thermal gap, is given as

$$\delta\Delta=\sum_j \delta\Delta_j, \quad \delta\Delta_j=G\Omega_j(v_j^2-u_j^2)\delta\mathcal{N}_j, \tag{82}$$

and arises due to the thermal quasiparticle-number fluctuation $\delta\mathcal{N}_j$ at $T\neq 0$. Therefore, comparing the FT-BCS equations (28) and (29) with the MBCS ones, Eqs. (78) and (79), we see that the latter explicitly include the effect of quasiparticle-number fluctuation $\sim\delta\mathcal{N}_j$ (37) in the last terms on their rhs, which are the thermal gap (82) in Eq. (78) and the thermal fluctuation of particle number $\delta N=\Sigma_j\delta N_j = -4\Sigma_j\Omega_ju_jv_j(\delta\mathcal{N}_j)$ in Eq. (79). These terms are ignored within the FT-BCS theory. Hence, Eqs. (78) and (79) show for the first time how the effect of statistical fluctuations is included in the MBCS (MHFB) theory at finite temperature on a microscopic ground. So far, this effect was treated only within the framework of the macroscopic Landau theory of phase transition [12].

### *2. Thermodynamics quantities*

The total energy $\overline{\mathcal{E}}$ is found as

$$\overline{\mathcal{E}}=2\sum_j \Omega_j\epsilon_j[(1-2n_j)v_j^2+n_j-2\sqrt{n_j(1-n_j)}u_jv_j]-\frac{\overline{\Delta}^2}{G}. \tag{83}$$

The heat capacity $C$ is calculated as the derivative of energy $\overline{\mathcal{E}}$ (83) with respect to temperature $T$,

$$C=\frac{\partial\overline{\mathcal{E}}}{\partial T}. \tag{84}$$

The level-density parameter $a$ is defined by the Fermi-gas formula as

$$a=\frac{E^*}{T^2}=\frac{\overline{\mathcal{E}}(T)-\overline{\mathcal{E}}(0)}{T^2}, \tag{85}$$

where $E^*\equiv\overline{\mathcal{E}}(T)-\overline{\mathcal{E}}(0)$ is the excitation energy of the system. The quasiparticle entropy (67) is written for spherical nuclei as

$$\overline{S}=-2\sum_j \Omega_j[n_j\ln n_j+(1-n_j)\ln(1-n_j)]$$
$$=2\sum_j \Omega_j\left[\frac{\beta\overline{E_j}}{e^{\beta\overline{E_j}}+1}+\ln(1+e^{-\beta\overline{E_j}})\right]. \tag{86}$$

Using the MBCS equations (78) and (79), Eqs. (83), and (86) together with the expressions for $\overline{E_i}$, $u_i$, and $v_i$, which are the same as in Eq. (30) (with $\overline{E_i}$ replacing $E_i$ and $\overline{\Delta}$ replacing $\Delta$), we found that the formal expression for the grand potential $\Phi$ is also the same as that given within the FT-BCS theory [31,32], namely,

$$\Phi\equiv-\beta\overline{\Omega}$$
$$=-\beta\sum_j \Omega_j[\epsilon_j-\overline{\mu}-\overline{E_j}]+2\sum_j \Omega_j\ln[1+e^{-\beta\overline{E_j}}]-\beta\frac{\overline{\Delta}^2}{G}. \tag{87}$$

The level-density $\rho(N,Z)$ is calculated as the inverse Laplace transform of the grand partition function $e^{\Phi}$. It is approximated as [32,33]

$$\rho(N,Z)=\frac{e^{\mathbf{S}}}{2\pi\sqrt{2\pi\mathbf{D}}},\tag{88}$$

where $\mathbf{S}=\overline{S_N}+\overline{S_Z}$ is the total entropy of the system and $\mathbf{D}$ is the determinant of the second derivatives of the grand partition function taken at the saddle point. It is given as

$$\mathbf{D}=\frac{\partial^2\Phi}{\partial\alpha_N^2}\mathbf{D}_Z+\frac{\partial^2\Phi}{\partial\alpha_Z^2}\mathbf{D}_N,$$

$$\mathbf{D}_i=\begin{vmatrix}\frac{\partial^2\Phi_i}{\partial\alpha_i^2} & \frac{\partial^2\Phi_i}{\partial\alpha_i\partial\beta}\\ \frac{\partial^2\Phi_i}{\partial\alpha_i\partial\beta} & \frac{\partial^2\Phi_i}{\partial\beta^2}\end{vmatrix},\quad i=N,Z,\quad \alpha_i=\beta\overline{\mu_i}.\tag{89}$$

The formal expressions for the derivatives in determinant $\mathbf{D}_i$ are the same as given in Eqs. (B.15)–(B.17) of Ref. [32]. However, the derivatives of the gap $\overline{\Delta}$ entering in these expressions are more complex due to Eq. (78). They are obtained here as

$$\frac{\partial\overline{\Delta}}{\partial\alpha}=\frac{\sum_j\Omega_j\left\{\frac{\sqrt{2a_j}}{\beta}\frac{\overline{\Delta}^2}{E_j^2}-(\epsilon_j-\overline{\mu})[(\epsilon_j-\overline{\mu})c_j+\overline{\Delta}(a_j-b_j)]\right\}}{\frac{2}{G}-\beta\sum_j\Omega_j[E_j^2b_j+\overline{\Delta}^2(a_j-b_j)]-\overline{\Delta}\sum_j\Omega_j(\epsilon_j-\overline{\mu})\left(\beta c_j+\frac{\sqrt{2a_j}}{E_j^2}\right)},\tag{90}$$

$$\frac{\partial\overline{\Delta}}{\partial\beta}=\frac{\sum_j\Omega_j\left\{\overline{\Delta}[(\epsilon_j-\overline{\mu})(\epsilon_ja_j-\overline{\mu}b_j)+\overline{\Delta}^2a_j]-\frac{\overline{\mu}}{\beta}\overline{\Delta}^2\frac{\sqrt{2a_j}}{E_j^2}+(\epsilon_j-\overline{\mu})[(\epsilon_j-\overline{\mu})\epsilon_j+\overline{\Delta}^2]c_j\right\}}{\frac{2}{G}-\beta\sum_j\Omega_j[E_j^2b_j+\overline{\Delta}^2(a_j-b_j)]-\overline{\Delta}\sum_j\Omega_j(\epsilon_j-\overline{\mu})\left(\beta c_j+\frac{\sqrt{2a_j}}{E_j^2}\right)},\tag{91}$$

where

$$a_j=\frac{\mathrm{sech}^2(z)}{2E_j^2},\quad b_j=\frac{\tanh(z)}{\beta E_j^3},\quad c_j=\frac{\mathrm{sech}(z)\tanh(z)}{2E_j^2},$$

$$z=\frac{1}{2}\beta E_j.\tag{92}$$

We have just derived the MHFB theory at finite temperature, which includes the quasiparticle-number fluctuation to preserve the unitarity of the modified generalized particle-density matrix. We have shown that the limit of this MHFB theory reproduces the MBCS equations obtained previously in Refs. [13,14]. For the sake of completeness, we give in the Appendix the proof that, by using the secondary Bogoliubov transformation (73), the modified QRPA indeed conserves the Ikeda sum rule.

## IV. ANALYSIS OF NUMERICAL RESULTS

As an illustration for the modified HFB theory at finite temperature, we now discuss in detail the results of numerical calculations within its limit, the MBCS theory, of the pairing gap, heat capacity, level-density parameter, and level-density for $^{120}$Sn. The single-particle energies $\epsilon_j$ used in the calculations are obtained within the Woods-Saxon potential at $T=0$. These discrete neutron and proton spectra include not only bound but also quasibound levels, which span an energy interval from around $-40$ MeV up to around 17 MeV. They include all the major shells up to $N(Z)=126$ as well as several levels in the next major shell $N(Z)=126$–184 up to $1k_{17/2}$ orbital. They are assumed here to be independent of $T$. This assumption is supported by the results of temperature-dependent HF calculations, which show that for $T\lesssim 5$ MeV the variation of the single-particle energies with $T$ is negligible [34]. The value $G_\nu=0.13$ MeV is adopted for the neutron pairing parameter so that the gap $\Delta_\nu$ for neutrons is about 1.4 MeV at $T=0$.

### A. Temperature dependence of pairing gap

#### *1. Open-shell case: Neutron pairing in $^{120}$Sn*

Since the modified gap $\overline{\Delta}$ is a function of $T$, the last term $\delta\Delta$ (82) on the rhs of Eq. (78) raises a question about the validity of the MBCS equation at high temperature. In fact, at first glance, it seems that, if the single-particle spectrum is such that $\delta\Delta$ is negative and its absolute value is greater than that of the first term on the rhs of Eq. (78) at a certain value of $T$, the gap $\overline{\Delta}$ turns negative and the MBCS approximation

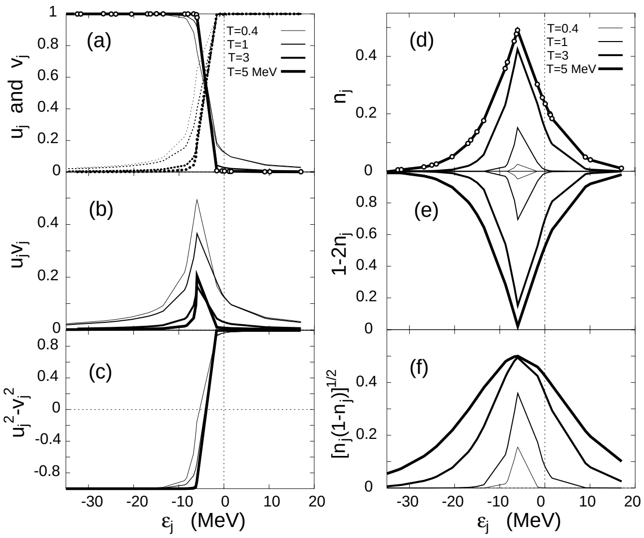


FIG. 1. Occupation probabilities within the MBCS theory as functions of single-particle energies $\epsilon_j$ for neutrons at $T=0.4$, 1, 3, and 5 MeV [thicker line corresponds to a higher $T$, as indicated in panels (a) and (d)]. Panel (a) shows the Bogoliubov coefficients $u_j$ (dotted lines) and $v_j$ (solid lines). Panels (b) and (c) show the product $u_jv_j$ and the difference $u_j^2-v_j^2$, respectively. Panel (d) shows the quasiparticle-occupation number $n_j$. Panels (e) and (f) show the factor $(1-2n_j)$ and $\delta\mathcal{N}_j\equiv\sqrt{n_j(1-n_j)}$, respectively. The open circles marked on the lines at $T=5$ MeV in (a) and (d) correspond to the positions of single-particle levels.

breaks down. In this section, we will show that this does not happen in numerical calculations using the entire single-particle energy spectrum.

Shown in Fig. 1 are the Bogoliubov coefficients $u_j, v_j$, quasiparticle-occupation number $n_j$, together with the combinations $u_jv_j$, $u_j^2-v_j^2$, $1-2n_j$, and $\delta\mathcal{N}_j$ as functions of single-particle energies $\epsilon_j$ for neutrons at several temperatures. These quantities determine the behavior of gap (78) as a function of $T$. They are rather symmetric functions from both sides of the chemical potential $\bar{\mu}$. The latter varies weakly around $-6$ MeV as $T$ increases. The product $u_jv_j$ decreases quickly with increasing $T$. At $T=5$ MeV, it remains effective only in the region of $\pm 5$ MeV around $\bar{\mu}$. The difference $u_j^2-v_j^2$, which enters in the thermal part $\delta\Delta$, remains rather insensitive to the variation of $T$. In general, the effect of pairing on the Bogoliubov coefficients $u_j$ and $v_j$ and their combinations $u_jv_j$ and $u_j^2-v_j^2$ is significant only in the region of at most $\pm 10$ MeV around $\bar{\mu}$. This situation is rather similar to that obtained within the BCS theory. However, for the quasiparticle-occupation number $n_j$ and its combinations $1-2n_j$ and $\delta\mathcal{N}_j$, the situation is different. Here, with increasing $T$, these quantities, although having a peak near $\bar{\mu}$, spread over the whole single-particle spectrum as shown in Figs. 1(d)–1(f). For the quantal component $(\Delta_{\rm Q})_j$, the maximum of $u_jv_j$ comes always with the minimum of $(1-2n_j)$ near $\bar{\mu}$. Beyond this region the product $u_jv_j(1-2n_j)$ is small. However, for the thermal-fluctuation part of the gap, both regions far above and below $\bar{\mu}$ are important. This means that, in difference with the BCS theory, where one can restrict the calculations with valence nucleons on some closed-shell core by renormalizing the pairing parameter $G_\nu$, the calculations for open-shell nuclei within the MBCS theory are necessary to be carried out using the entire single-particle spectrum.

This observation is demonstrated in Fig. 2, where the partial quantal $(\Delta_{\rm Q})_j$ and thermal $\delta\Delta_j$ gaps are shown as functions of single-particle energies $\epsilon_j$ at several temperatures. The quantal part $(\Delta_{\rm Q})_j$ is always larger around $\bar{\mu}$, but its magnitude quickly decreases as $T$ increases. On the contrary, the thermal part $\delta\Delta_j$ is positive at $\epsilon_j<\bar{\mu}$ and negative at $\epsilon_j>\bar{\mu}$. Its absolute value sharply increases with increasing $T$. In a realistic spectrum the number of single-particle levels below $\bar{\mu}$ is usually larger than that of those above it. In the present example of $^{120}$Sn, within the same energy interval of $\sim$20 MeV from $\bar{\mu}$, the one below $\bar{\mu}$ has twelve, while the one above $\bar{\mu}$ has only eight single-particle levels. Therefore, the sum of partial thermal gaps $\delta\Delta_j$ has more components in the region below $\bar{\mu}$, where the difference $v_j^2-u_j^2$ is positive. As a result, by summing over all single-particle levels weighted over the shell degeneracy $\Omega_j$, the ensuing thermal gap $\delta\Delta$ (82) is always positive.

Shown in Fig. 3 are the quantal $\Delta_{\rm Q}$ (dashed line) and thermal $\delta\Delta$ (dash-dotted line) gaps together with the total MBCS gap $\bar{\Delta}$ (thick solid line) as functions of $T$. The BCS gap is also shown as the dotted line for comparison. It collapses at a critical temperature $T_{\rm c}\approx 0.79$ MeV. This value almost coincides with the temperature of superfluid-normal

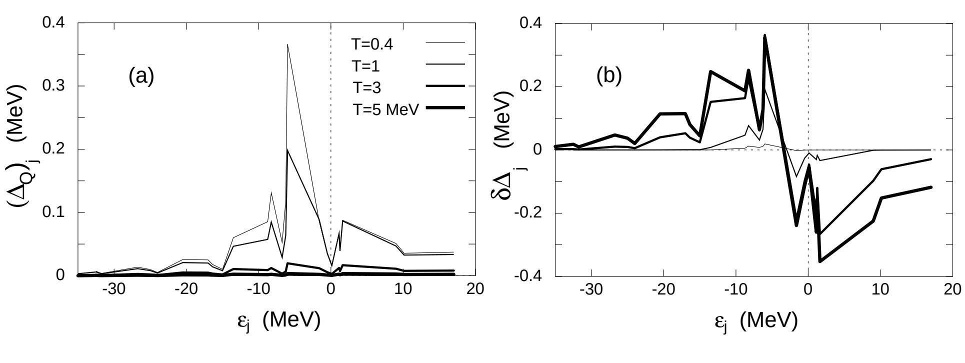


FIG. 2. Partial quantal $(\Delta_{\rm Q})_j$ and thermal $\delta\Delta_j$ gaps as functions of single-particle energies $\epsilon_j$ for neutrons at $T=0.4$, 1, 3, and 5 MeV. A thicker line corresponds to a higher temperature as indicated in panel (a).

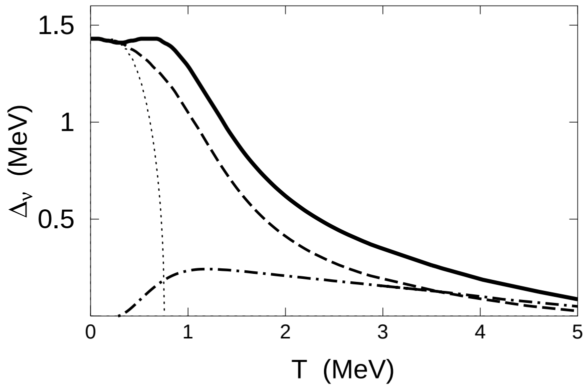


FIG. 3. Neutron pairing gap as a function of temperature $T$. The thick solid line represents the MBCS gap $\bar{\Delta}$. Its two components, the quantal gap $\Delta_{\rm Q}$ and thermal gap $\delta\Delta$, are shown by dashed and dash-dotted lines, respectively. The BCS gap is shown by the dotted line.

phase transition estimated for infinite systems, which is about $0.567\Delta(T=0)$ [11]. On the contrary, within the MBCS theory, the quantal gap $\Delta_{\rm Q}$ never collapses, but decreases monotonously with increasing $T$. The thermal component $\delta\Delta$ increases first with $T$ at $T\lesssim 1$ MeV, then starts to decrease with increasing $T$ further, but still does not vanish even at $T\sim 5-6$ MeV. As a result, the total MBCS gap $\bar{\Delta}$ has a temperature dependence similar to that of the quantal gap $\Delta_{\rm Q}$, except for a low-temperature region 0.5 MeV $\lesssim T \lesssim T_{\rm c}$, where it increases slightly with $T$ because of the thermal gap $\delta\Delta$. As high $T$, the total gap $\bar{\Delta}$ decreases monotonously with increasing $T$. This yields a long tail extending up to $T\sim 5-6$ MeV.

In order to see how the change of configuration space affects the calculation of the MBCS gap, we also carried out several tests using cutoff spectra. Examples are shown in Fig. 4. The dashed line is the neutron gap obtained in the MBCS calculation after removing the three lowest major shells (up to $N=28$) from the single-particle energy spectrum. The calculations are then carried out by putting $N=42$ particles on the $N=28$ core. The balance in the sum over the single-particle levels is lost with less levels below $\bar{\mu}$ participating in the summation. The symmetry of the spectrum with respect to $\bar{\mu}$ is destroyed. The gap collapses again, but at a much higher temperature $T\approx 4$ MeV, although up to $T\simeq 2.5$ MeV its temperature dependence is almost the same as that obtained using the entire spectrum. Removing from the other side of $\bar{\mu}$ two highest levels $1k_{17/2}$ and $1i_{11/2}$ makes the reduced spectrum rather symmetric again with respect to $\bar{\mu}$. The balance in summation of $\delta\Delta_j$ is restored. As a result, the temperature dependence of the gap is recovered as shown by the thin solid line. However, if one removes further one more level, namely, the $1j_{15/2}$ one, i.e., the reduced space consists of only three major shells, 28–50, 50–82, and 82–126, the balance is destroyed again with more weight toward the positive values of $\delta\Delta_j$. The reduced spectrum now spreads from around $-17$ MeV up to around 1.6 MeV, which is strongly asymmetric with respect to $\bar{\mu}$. In consequence, the high-temperature tail of the gap becomes much more enhanced as shown by the dash-dotted line in Fig. 4. Other tests using 8-neutron, 20-neutron, and 50-neutron cores also show a similar feature. In these tests the parameter $G_\nu$ is renormalized so as to obtain the same value for $\Delta_\nu(T=0)$. With such renormalization of $G_\nu$ the BCS gap always remains the same.

These results show the difference in practical calculations within the BCS and MBCS theories. In the BCS case, the calculation of the gap using a closed-shell core with a simple renormalizition of the pairing parameter $G_\nu$ yields the same result as that obtained using the entire single-particle energy spectrum. In the MBCS case, the most reliable way is to use the entire or as large as possible single-particle spectrum. If using a limited spectrum is unavoidable, care should be taken to maintain the balance in the summation of partial thermal gap $\delta\Delta_j$. Otherwise, a resulting collapse or an enhanced tail of the gap in the high-$T$ region would be simply an artifact caused by a limited space. As a matter of fact, a criterion for a good reduction is that the cutoff spectrum should be rather symmetric with respect to the region where the quantal pairing correlations are the strongest, namely, from both sides of the chemical potential, so that the effect of quasiparticle-number fluctuation is properly taken into account [see Figs. 1(d)–1(f) and 2(b)]. It is worth noting that the limitation of the configuration space also yields a wrong behavior of the specific heat. This effect is known as the Schottky anomaly, according to which the specific heat reaches a maximum at a certain temperature and decreases as temperature increases further [35].

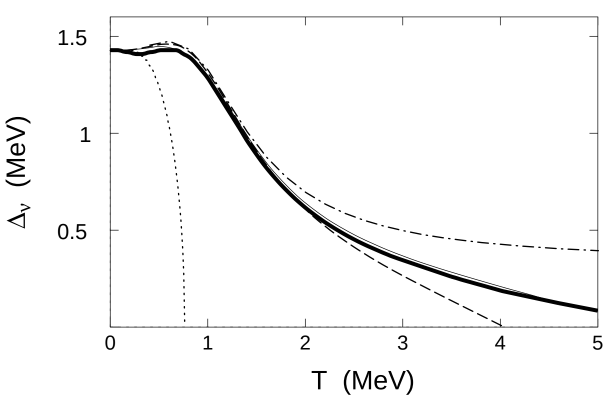


FIG. 4. Neutron pairing gap as a function of temperature $T$. The thick solid line represents the MBCS gap $\bar{\Delta}$ obtained using the entire single-particle spectrum, as in Fig. 3. The dashed line shows the result obtained using an $N=28$ core. The thin solid line represents the result obtained using the same core and removing two highest levels $1k_{17/2}$ and $1j_{11/2}$. The dash-dotted line is the result obtained using the same core and removing three highest levels, $1k_{17/2}$, $1j_{11/2}$, and $1j_{15/2}$. The dotted line shows the BCS gap.

### *2. Closed-shell case: Thermally induced pairing correlations for protons in $^{120}$Sn*

The MBCS gap equation (78) also implies that, in principle, thermal fluctuations can induce pairing correlations even for closed-shell (CS) nuclei. However, the situation here is different from that of the open-shell nuclei because of

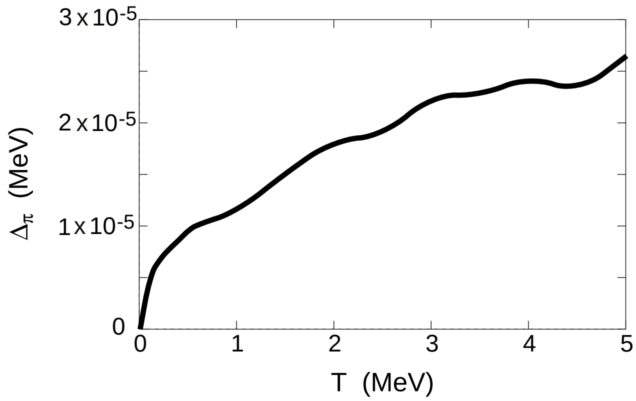


FIG. 5. Thermally induced pairing gap $\overline{\Delta}_\pi$ for protons in $^{120}$Sn as a function of $T$.

a large shell gap between the highest occupied (hole) orbital and the lowest empty (particle) one, which is about 6 MeV for protons in $^{120}$Sn. At $T=0$ all the orbitals below $\overline{\mu}$ are fully occupied ($v_{j_h}=1, u_{j_h}=0, \epsilon_{j_h}-\mu<0$), while those above $\overline{\mu}$ are empty ($v_{j_h}=0, u_{j_h}=1, \epsilon_{j_p}-\mu>0$). Therefore, the quantal gap $\Delta_{\rm Q}$ (81) is always zero. Pairing is so weak that no scattering into the next major shell (particle orbitals) is possible. In such a situation, the approximation of the same pairing matrix elements may not be extended across a too large shell gap separating hole and particle orbitals, especially when $f_{j_h}\equiv 1-n_{j_h}\gg n_{j_p}\equiv f_{j_p}$, where $f_j$ is the single-particle-occupation number. This restricts the summation on the rhs of Eq. (78) to be carried out at most over only the hole states. The MBCS gap $\overline{\Delta}$ in this case is solely determined by the thermal gap $\delta\Delta$ (82) due to the quasiparticle-number fluctuation, namely,

$$\overline{\Delta}_{\rm CS}=\delta\Delta_{\rm CS}\approx G_\pi\sum_{j_h}\Omega_{j_h}\sqrt{n_{j_h}(1-n_{j_h})}. \tag{93}$$

The thermally induced gap $\overline{\Delta}_\pi$ for a closed-shell proton system ($Z=50$) in $^{120}$Sn, obtained using Eq. (93) with the same value of the pairing parameter as that for neutrons, $G_\pi=G_\nu$, is plotted as a function of temperature in Fig. 5. This figure clearly shows that the pairing gap for a closed-shell system is different from zero at $T\neq 0$ and increases as $T$ increases. However, its magnitude, which reaches a value of only around $2.6\times 10^{-5}$ MeV at $T=5$ MeV, is practically negligible as compared to $\overline{\Delta}_\nu$. Therefore, we will put $\overline{\Delta}_\pi$ equal to zero in further discussions.

### 3. Comparison between microscopic and macroscopic descriptions of thermal fluctuation

The effect of thermal fluctuations on the pairing gap was first studied using the Landau macroscopic theory of phase transition [11] by Moretto in Ref. [12]. Within the Landau theory, $\Phi$ (87) is treated as a function of the independent parameter $\Delta$. The probability that the nucleus has any given value of $\Delta$ for the pairing gap is determined by the isothermal distribution

$$P(\Delta)\propto e^{\Phi(\Delta)}. \tag{94}$$

The averaged gap $\langle\Delta\rangle$ is calculated as [12]

$$\langle\Delta\rangle=\frac{\int_0^\infty \Delta P(\Delta)d\Delta}{\int_0^\infty P(\Delta)d\Delta}. \tag{95}$$

This approach does not include quantal fluctuations. Therefore, as has been pointed out in Refs. [9,11,12], at very low temperature or if nonequilibrium states vary too rapidly with time, quantum fluctuations dominate and Eq. (95) is no longer meaningful.

The probability distribution $P(\Delta)$ (94), calculated using the same neutron single-particle spectra for $^{120}$Sn and the same pairing parameter $G_\nu$, is plotted as a function of $\Delta$ at low and high temperatures in Figs. 6(a) and 6(b), respectively. At very low temperature, the most probable value, which is the BCS gap, coincides with the averaged one, resulting in a Gaussian-like shape with a peak at the BCS value of $\Delta(T=0)\simeq 1.4$ MeV. As $T$ increases, the distribution becomes skewed toward the lower values of $\Delta$. Its maximum, which still corresponds to the solution of the BCS equation, moves to lower $\Delta$ and reaches $\Delta=0$ at $T=T_{\rm c}$. This is shown in Fig. 6(a), which is very similar to what was obtained before in Fig. 1 of Ref. [12] for a uniform spectrum. As $T$ increases further, the maximum of the distribution still remains at $\Delta=0$, while its width continues to increase, showing the increase of thermal fluctuations. At hypothetically high temperatures [Fig. 6(b)], the distribution approaches a Gaussian one in the following form:

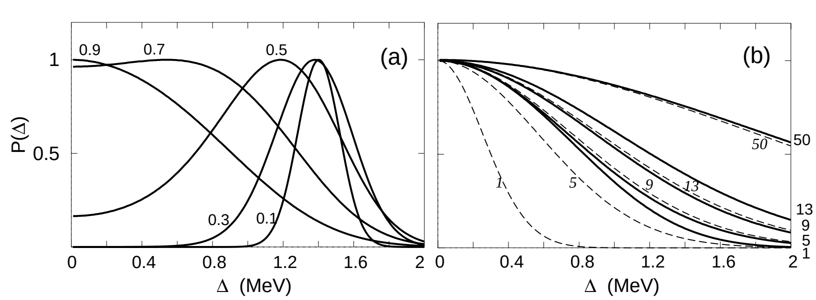


FIG. 6. Probability distribution $P(\Delta)$ for $^{120}$Sn as a function of gap parameter $\Delta$ at different temperatures shown by the numbers (in MeV) next to the thick solid curves. The dashed curves in (b) represent the Gaussian distribution (96) at various temperatures shown by the italic numbers (in MeV) next to these curves.

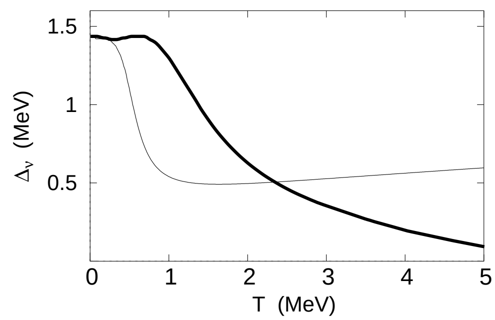


FIG. 7. Neutron pairing gap for $^{120}$Sn as a function of $T$ within the MBCS theory and the macroscopic treatment following the Landau theory of phase transitions. The thick and thin lines show the gap $\bar{\Delta}$ and the averaged gap $\langle\Delta\rangle$, respectively.

$$P(\Delta)|_{T\to\infty} \sim \frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\Delta^2}{2\sigma^2}\right) \quad \text{with} \quad \sigma = \sqrt{\frac{GT}{2}}. \tag{96}$$

This behavior means that Eq. (94) assumes the effect of thermal fluctuations on the pairing gap to be chaotic at both low and high $T$. By substituting Eq. (96) into the rhs of Eq. (95), the integrals can be carried out analytically. The result is

$$\langle\Delta\rangle|_{T\to\infty} = \sqrt{\frac{GT}{\pi}}. \tag{97}$$

This result reveals the increase of the averaged gap $\langle\Delta\rangle$ with increasing $T$ at very high $T$ within the Landau theory using the probability function (94).

The temperature dependence of $\langle\Delta\rangle$ for neutrons in $^{120}$Sn is displayed in Fig. 7 in comparison with the MBCS gap $\bar{\Delta}$. It is seen from this figure that the agreement between the microscopic treatment of thermal fluctuations in the pairing gap within the MBCS theory and the macroscopic one can be called at best qualitative. The gap does not collapse in both treatments, but while the tail of the MBCS gap $\bar{\Delta}$ clearly decreases at high $T$ with increasing $T$, the temperature dependence of the averaged gap $\langle\Delta\rangle$ remains rather flat, and even starts to increase slightly with $T$ already at $T>$ 1 MeV because of Eq. (97). This yields a $\langle\Delta\rangle$ of about 0.6 MeV even at $T\sim4$–5 MeV. In the low-temperature region, $\langle\Delta\rangle$ drops at a lower $T\sim0.5$ MeV as compared to the MBCS gap. The reason is that the MBCS gap incorporates the microscopic interplay between the quantal gap $\Delta_Q$ and thermal one, $\delta\Delta$. At low $T$ the former dominates. The gap $\langle\Delta\rangle$ takes into account only thermal fluctuations around the most probable value following distribution (94). The latter assumes an equally strong coupling between $\Delta$ and all the intrinsic degrees of freedom, disregarding quantal effects.

### B. Temperature dependence of heat capacity, level-density parameter, and level-density

The heat capacity $C$ and inverse level-density parameter $K=A/a$ obtained within the BCS and MBCS theories are shown in Fig. 8 as functions of $T$. The heat capacity usually serves as an indicator for phase transitions. Within the BCS theory, a sharp discontinuity in $C$ is seen at $T=T_c$, where the gap collapses. Together with the collapse at $T_c$ of the BCS gap as an order parameter, this behavior of the heat capacity is a clear signature of the second-order phase transition [11]. However, within the MBCS theory, this phase transition is washed out so that the temperature dependence of the heat capacity is a smooth curve with only a slight effect of the bending of the pairing gap in the region $0.5\lesssim T\lesssim2$ MeV. A similar feature of the heat capacity has been recently reported for iron isotopes within the shell-model Monte Carlo approach [17]. Since both the order parameter $\bar{\Delta}$ and the heat capacity are now continuous functions, we can say that no phase transition actually occurs. At high $T$ both the MBCS and BCS results approach each other.

The inverse level-density parameter $K=A/a$ obtained within the MBCS theory is larger than that obtained within the BCS theory at $T\lesssim3$ MeV. At higher temperatures both theories predict almost the same $K$. Except for the low-temperature region (below $T_c$), where the Fermi-gas formula (85) is not valid, $K$ increases with increasing $T$ at $T\gtrsim1$ MeV, and enters the region of the experimentally extracted values between $8\sim12$ MeV at $T\gtrsim2.5$ MeV [36]. At $T\approx1$ MeV, the value of $K$ predicted by the MBCS theory is around 6 MeV, which is about twice as larger than that given by the BCS theory.

Shown in Fig. 9 is the logarithm of level-density $\rho(N,Z)$ (88) as a function of $T$. The BCS result shows a kink at $T=T_c$, while the MBCS result is a smooth curve, which increases monotonously as $T$ increases, exposing no signal of phase transition. At $T\gtrsim2$ MeV, both the BCS and MBCS results practically coincide.

## V. CONCLUSIONS

This work has derived the modified HFB (MHFB) theory at finite temperature, which conserves the unitarity relation

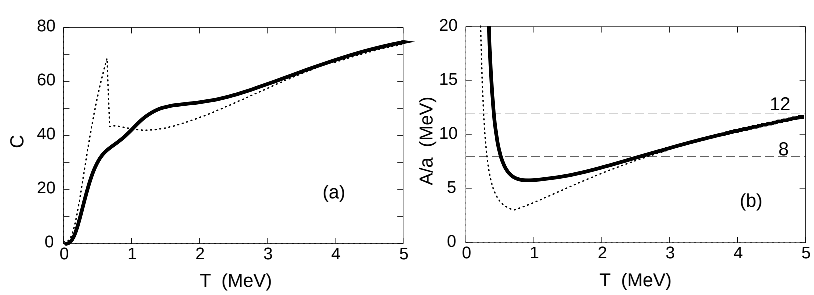


FIG. 8. Heat capacity (a) and the inverse level-density parameter $K=A/a$ (b) as functions of temperature for $^{120}$Sn. The thick solid lines denote results obtained within the MBCS theory. The dotted lines show the BCS results.

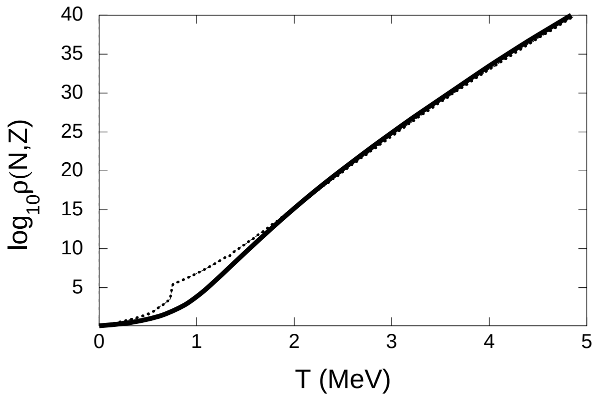


FIG. 9. Logarithm of level-density as a function of $T$ for $^{120}$Sn. The notation is as in Fig. 8.

of the generalized particle-density matrix. This has been done by including the thermal fluctuation of the quasiparticle number microscopically in the quasiparticle-density matrix. It has been shown that the latter can also be obtained by applying the secondary Bogoliubov transformation discussed in Refs. [13,14]. The MHFB equations at finite temperature have been then derived following the standard variational procedure used in Ref. [1]. Its BCS limit yields the modified BCS (MBCS) equations, which have been derived previously in Refs. [13,14] using the above-mentioned secondary Bogoliubov transformation. Apart from being able to restore the unitarity transformation, this secondary transformation helps the modified QRPA to completely restore the Ikeda sum rule for Fermi and Gamow-Teller transitions, which has been violated within the renormalized QRPA.

The illustration of the MHFB theory has been presented within the MBCS theory by calculating the neutron pairing gap and thermodynamic quantities for $^{120}$Sn. Detailed analyses of the results obtained show that the calculations for open-shell nuclei within the MBCS theory need to be carried out using the entire single-particle spectrum, which includes both bound and quasibound levels in a large configuration space of about seven major shells up to 126–184 one. When the use of a reduced spectrum is unavoidable, the reduction should be done symmetrically from both sides of the chemical potential $\overline{\mu}$ so that the distribution of the quasiparticle-occupation number can be properly taken into account as it is symmetric with respect to $\overline{\mu}$. The MBCS gap decreases monotonously with increasing $T$ and does not vanish even at $T\sim5$ MeV. The discontinuity in the BCS heat capacity at the critical temperature $T_c$ is also competely washed out, showing no signature of superfluid-normal phase transition. The temperature dependences of level-density and level-density parameter are also smooth.

The behavior of the MBCS gap as a function of $T$ is found in qualitative agreement with that given by the macroscopic treatment using the Landau theory of phase transitions in the sense that both gaps do not collapse at the critical temperature of the BCS superfluid-normal phase transition. However, quantitative discrepancies between microscopic and macroscopic approaches are evident. In the low-temperature region, due to the microscopic interplay between quantal and thermal components, the MBCS gap starts to decrease at a higher $T$ with increasing $T$ as compared to the macroscopically averaged gap $\langle\Delta\rangle$. At high temperatures $T>2$ MeV the MBCS gap continues to decrease, while $\langle\Delta\rangle$ remains nearly constant and even start to increase with increasing $T$.

The MBCS equations also show that thermal fluctuations can induce a pairing gap even for closed-shell nuclei. Results obtained using a single-particle space restricted to hole orbitals have shown that such a thermally induced gap increases with increasing temperature. However, its magnitude is negligible compared with the gap in open-shell nuclei. Therefore, it can be safely set to be equal to zero at $T \lesssim 5-6$ MeV.

## ACKNOWLEDGMENTS

Numerical calculations were performed using an Alpha AXP workstation and the Visual-Numeric IMSL libraries at the RIKEN Computer Science Laboratory.

## APPENDIX: RESTORATION OF THE IKEDA SUM RULE

At $T=0$, in general, if the quasiparticle correlations are significant so that the correlated ground state $|\tilde{0}\rangle$ deviates appreciably from the quasiparticle vacuum (3) or QRPA vacuum, the secondary Bogoliubov transformation (47) can be used to derive a symmetry-conserving theory, which treats the ground-state correlations within a microscopic and self-consistent framework. In this case the quasiparticle-occupation number $n_j$, which characterizes the magnitude of the ground-state correlations, can be evaluated from the renormalized QRPA backward-going amplitudes $\mathcal{Y}_{jj'}^{(\lambda i)}$, as has been discussed thoroughly in Refs. [13,14,22]. In this section, we will prove that the modified QRPA theory, which has been derived in Ref. [13] using the secondary Bogoliubov transformation in the form of Eq. (73), indeed conserves the Ikeda sum rule.

### 1. The Ikeda sum rule

The Ikeda sum rule for Fermi $(J=0)$ and Gamow-Teller $(J=1)$ transitions is defined with respect to the ground state $|\text{g.s.}\rangle$ of the final nucleus $(N,Z)$ as

$$\mathcal{S}^- - \mathcal{S}^+ = \sum_i |\langle Ji|\beta^-|\text{g.s.}\rangle|^2 - \sum_i |\langle Ji|\beta^+|\text{g.s.}\rangle|^2 = (2J+1)(N-Z), \tag{A1}$$

where the squared $\beta^-$-transition matrix element $|\langle Ji|\beta^-|\text{g.s.}\rangle|^2$ is calculated as

$$|\langle Ji|\beta^-|\mathrm{g.s.}\rangle|^2=|\langle Ji|\sum_{j_\pi j_\nu} q_{j_\pi j_\nu}[u_{j_\pi}v_{j_\nu}A^\dagger_{j_\pi j_\nu}(JM)+u_{j_\nu}v_{j_\pi}A_{j_\pi j_\nu}(J\widetilde{M})]|\mathrm{g.s.}\rangle|^2 \tag{A2}$$

and $\beta^+=(\beta^-)^\dagger$. The notation $\mathcal{O}_{J\tilde{M}}=(-)^{J-M}\mathcal{O}_{J-M}$ is used hereafter, and $q_{j_\pi j_\nu}$ denotes single-particle matrix elements corresponding to the Fermi or the Gamow-Teller transition. The subscripts $\pi$ and $\nu$ denote proton and neutron, respectively. The quasiparticle-pair operators $A^\dagger_{j_\pi j_\nu}(JM)$ and $A_{j_\pi j_\nu}(JM)$ are

$$A^\dagger_{j_\pi j_\nu}(JM)=\sum_{m_\pi m_\nu}\langle j_\pi m_\pi j_\nu m_\nu|JM\rangle \alpha^\dagger_{j_\pi m_\pi}\alpha^\dagger_{j_\nu m_\nu},$$

$$A_{jj'}(JM)=[A_{jj'}(JM)^\dagger]^\dagger. \tag{A3}$$

Their exact commutation relation is

$$[A_{j'_\pi j'_\nu}(J'M'),A^\dagger_{j_\pi j_\nu}(JM)]$$

$$=\delta_{JJ'}\delta_{MM'}\delta_{j_\pi j'_\pi}\delta_{j_\nu j'_\nu}-\delta_{j_\pi j'_\pi}\sum_{m_\pi m_\nu m'_\nu}\langle j_\pi m_\pi j'_\nu m'_\nu|J'M'\rangle$$

$$\times\langle j_\pi m_\pi j_\nu m_\nu|JM\rangle \alpha^\dagger_{j_\nu m_\nu}\alpha_{j'_\nu m'_\nu} \tag{A4}$$

$$-\delta_{j_\nu j'_\nu}\sum_{m_\pi m_\nu m'_\pi}\langle j'_\pi m'_\pi j_\nu m_\nu|J'M'\rangle$$

$$\times\langle j_\pi m_\pi j_\nu m_\nu|JM\rangle \alpha^\dagger_{j_\pi m_\pi}\alpha_{j'_\pi m'_\pi}.$$

#### 2. Fulfillment of the Ikeda sum rule within the QRPA

The QRPA treats the excited state $|Ji\rangle$ as a one-phonon state

$$|Ji\rangle=Q^\dagger_{JMi}|\mathrm{RPA}\rangle, \tag{A5}$$

while the ground state $|\mathrm{RPA}\rangle$ of an even-even nucleus is treated as the phonon vacuum

$$Q_{JMi}|\mathrm{RPA}\rangle=0. \tag{A6}$$

The $\pi\nu$-phonon operator $Q^\dagger_{JMi}$ is defined as

$$Q^\dagger_{JMi}=\sum_{j_\pi j_\nu}[X^{(Ji)}_{j_\pi j_\nu}A^\dagger_{j_\pi j_\nu}(JM)-Y^{(Ji)}_{j_\pi j_\nu}A_{j_\pi j_\nu}(J\widetilde{M})],$$

$$Q_{JMi}=[Q^\dagger_{JMi}]^\dagger. \tag{A7}$$

In order to obtain a set of linear equations with respect to the amplitudes $X^{(Ji)}_{j_\pi j_\nu}$ and $Y^{(Ji)}_{j_\pi j_\nu}$, the QRPA assumes the quasiboson approximation, which neglects the contribution of the last two terms $\sim\alpha^\dagger\alpha$ on the rhs of Eq. (A4) in the average over the ground state $|\mathrm{RPA}\rangle$, i.e.,

$$\langle\mathrm{RPA}|[A_{j'_\pi j'_\nu}(J'M'),A^\dagger_{j_\pi j_\nu}(JM)]|\mathrm{RPA}\rangle$$

$$\approx\delta_{JJ'}\delta_{MM'}\delta_{j_\pi j'_\pi}\delta_{j_\nu j'_\nu}. \tag{A8}$$

Within this approximation (A8), the condition for the $\pi\nu$-phonon operators (A7) to be bosons, i.e., satisfying the commutation relation

$$\langle\mathrm{RPA}|[Q_{JMi},Q^\dagger_{J'M'i'}]|\mathrm{RPA}\rangle=\delta_{JJ'}\delta_{MM'}\delta_{ii'}, \tag{A9}$$

leads to the following normalization relation for the amplitudes $X^{(Ji)}_{j_\pi j_\nu}$ and $Y^{(Ji)}_{j_\pi j_\nu}$:

$$\sum_{j_\pi j_\nu}[X^{(Ji)}_{j_\pi j_\nu}X^{(J'i')}_{j_\pi j_\nu}-Y^{(Ji)}_{j_\pi j_\nu}Y^{(J'i')}_{j_\pi j_\nu}]=\delta_{JJ'}\delta_{ii'}. \tag{A10}$$

Using the inverse transformation of Eq. (A7), one expresses $A^\dagger_{j_\pi j_\nu}(JM)$ and $A_{j_\pi j_\nu}(JM)$ in terms of the $\pi\nu$-phonon operators $Q^\dagger_{JMi}$ and $Q_{JMi}$. Substituting the result into Eq. (A2) and using it to evaluate the left-hand side of Eq. (A1) we obtain

$$(\mathcal{S}^--\mathcal{S}^+)_{\mathrm{RPA}}=\sum_i|\langle\mathrm{RPA}|Q_{JMi}\beta^-|\mathrm{RPA}\rangle|^2$$

$$-\sum_i|\langle\mathrm{RPA}|Q_{JMi}\beta^+|\mathrm{RPA}\rangle|^2$$

$$=\left|\sum_{j_\pi j_\nu}q_{j_\pi j_\nu}(u_{j_\pi}v_{j_\nu}X_{j_\pi j_\nu}+v_{j_\pi}u_{j_\nu}Y_{j_\pi j_\nu})\right|^2$$

$$-\left|\sum_{j_\pi j_\nu}q_{j_\nu j_\pi}(v_{j_\pi}u_{j_\nu}X_{j_\pi j_\nu}+u_{j_\pi}v_{j_\nu}Y_{j_\pi j_\nu})\right|^2 \tag{A11}$$

$$=\sum_{j_\pi j_\nu}|q_{j_\pi j_\nu}|^2(v^2_{j_\nu}-v^2_{j_\pi})$$

$$=2(2J+1)\left[\sum_{j_\nu}\Omega_{j_\nu}v^2_{j_\nu}-\sum_{j_\pi}\Omega_{j_\pi}v^2_{j_\pi}\right]$$

$$=(2J+1)(N-Z).$$

In the above derivation, the normalization condition (A10) and the usual BCS equation for the particle number are used together with the property $\Sigma_{j_i}|q_{j_i j_k}|^2=2(2J+1)\Omega_{j_k}$ $[i=(\pi,\nu),k=(\nu,\pi)]$ for the single-particle matrix elements of the Fermi and Gamow-Teller transitions. This derivation shows that the QRPA fulfills the Ikeda sum rule.

**3. Violation of the Ikeda sum rule within the renormalized QRPA**

By neglecting the contribution of the two last terms on the rhs of Eq. (A4) in the ground state (A6), the quasiboson approximation (A8) ignores the Pauli principle between the quasiparticle-pair operators (A3). This causes the collapse of the QRPA at a certain critical value of the interaction parameter, where the solution of the QRPA equations becomes imaginary. The renormalized QRPA has been proposed as a method to remove this inconsistency [21–23].

This approach assumes that, instead of the quasiboson approximation (A8), the following commutation relation holds in the average over the correlated ground state $|\widetilde{\mathrm{RPA}}\rangle$:

$$\langle\widetilde{\mathrm{RPA}}|[A_{j'_\pi j'_\nu}(J'M'),A^\dagger_{j_\pi j_\nu}(JM)]|\widetilde{\mathrm{RPA}}\rangle = \delta_{JJ'}\delta_{MM'}\delta_{j_\pi j'_\pi}\delta_{j_\nu j'_\nu}D_{j_\pi j_\nu}, \tag{A12}$$

where

$$D_{j_\pi j_\nu}=1-n_{j_\pi}-n_{j_\nu}, \quad n_j=\frac{1}{2\Omega_j}\langle\widetilde{\mathrm{RPA}}|\alpha^\dagger_{jm}\alpha_{jm}|\widetilde{\mathrm{RPA}}\rangle\neq 0. \tag{A13}$$

This means that the renormalized QRPA takes into account the contribution of the diagonal elements of the last two terms on the rhs of Eq. (A4) in the correlated ground state $|\widetilde{\mathrm{RPA}}\rangle$.

The renormalized $\pi\nu$-phonon operators $\mathcal{Q}^\dagger_{JMi}$ and $\mathcal{Q}_{JMi}$ are introduced as

$$\mathcal{Q}^\dagger_{JMi}=\sum_{j_\pi j_\nu}\frac{1}{\sqrt{D_{j_\pi j_\nu}}}[\mathcal{X}^{(Ji)}_{j_\pi j_\nu}A^\dagger_{j_\pi j_\nu}(JM)-\mathcal{Y}^{(Ji)}_{j_\pi j_\nu}A_{j_\pi j_\nu}(J\tilde{M})],$$

$$\mathcal{Q}_{JMi}=[\mathcal{Q}^\dagger_{JMi}]^\dagger. \tag{A14}$$

The correlated ground state $|\widetilde{\mathrm{RPA}}\rangle$ is defined as the vacuum with respect to the renormalized phonon operators, i.e.,

$$\mathcal{Q}_{JMi}|\widetilde{\mathrm{RPA}}\rangle=0. \tag{A15}$$

Because of Eq. (A12), these renormalized $\pi\nu$-phonon operators satisfy the boson commutation relation

$$\langle\widetilde{\mathrm{RPA}}|[\mathcal{Q}_{JMi},\mathcal{Q}^\dagger_{J'M'i'}]|\widetilde{\mathrm{RPA}}\rangle=\delta_{JJ'}\delta_{MM'}\delta_{ii'} \tag{A16}$$

in the correlated ground state $|\widetilde{\mathrm{RPA}}\rangle$, provided their $\mathcal{X}$ and $\mathcal{Y}$ amplitudes satisfy the same normalization condition as in the QRPA, i.e.,

$$\sum_{j_\pi j_\nu}[\mathcal{X}^{(Ji)}_{j_\pi j_\nu}\mathcal{X}^{(J'i')}_{j_\pi j_\nu}-\mathcal{Y}^{(Ji)}_{j_\pi j_\nu}\mathcal{Y}^{(J'i')}_{j_\pi j_\nu}]=\delta_{JJ'}\delta_{ii'}. \tag{A17}$$

The phonon energies and $\mathcal{X}^{(Ji)}_{j_\pi j_\nu}$ and $\mathcal{Y}^{(Ji)}_{j_\pi j_\nu}$ amplitudes are found by solving the nonlinear QRPA-like equations, whose submatrices contain the factor $D_{j_\pi j_\nu}$. The latter is found from the equation [13]

$$D_{jj'}=1-\sum_{Ji}(J+1/2)\sum_{j''}\left\{D_{jj''}\frac{[\mathcal{Y}^{(Ji)}_{jj''}]^2}{\Omega_j}+D_{j''j'}\frac{[\mathcal{Y}^{(Ji)}_{j''j'}]^2}{\Omega_{j'}}\right\}. \tag{A18}$$

The presence of the factor $D_{j_\pi j_\nu}$ makes the solution of the renormalized QRPA always real as the interaction strength is reduced by this factor so that the collapse is avoided. However, the inverse transformation of Eq. (A14) now becomes

$$A^\dagger_{j_\pi j_\nu}(JM)=\sqrt{D_{j_\pi j_\nu}}\sum_{JMi}[\mathcal{X}^{(Ji)}_{j_\pi j_\nu}\mathcal{Q}^\dagger_{JMi}+\mathcal{Y}^{(Ji)}_{j_\pi j_\nu}\mathcal{Q}_{J\tilde{M}i}],$$

$$A_{j_\pi j_\nu}(JM)=[A^\dagger_{j_\pi j_\nu}(JM)]^\dagger. \tag{A19}$$

Using Eq. (A19) to evaluate the quantity $S^- - S^+$ in the same way as in derivation (A11), one finds

$$(\mathcal{S}^- - \mathcal{S}^+)_{\mathrm{RRPA}}=\sum_i|\langle\widetilde{\mathrm{RPA}}|\mathcal{Q}_{JMi}\beta^-|\widetilde{\mathrm{RPA}}\rangle|^2 - \sum_i|\langle\widetilde{\mathrm{RPA}}|\mathcal{Q}_{JMi}\beta^+|\widetilde{\mathrm{RPA}}\rangle|^2 = \sum_{j_\nu j_\pi}D_{j_\pi j_\nu}|q_{j_\pi j_\nu}|^2(v^2_{j_\nu}-v^2_{j_\pi}). \tag{A20}$$

This quantity is smaller than $(2J+1)(N-Z)$ since $D_{j_\pi j_\nu}<1$. Hence, Eq. (A20) shows that the renormalized QRPA violates the Ikeda sum rule.

We notice that, although the renormalized QRPA takes into account Eq. (A12), it neglects the following commutation relation between the scattering-quasiparticle pairs:

$$\langle\widetilde{\mathrm{RPA}}|[B^\dagger_{j'_\pi j'_\nu}(J'M'),B_{j_\pi j_\nu}(JM)]|\widetilde{\mathrm{RPA}}\rangle = \delta_{JJ'}\delta_{MM'}\delta_{j_\pi j'_\pi}\delta_{j_\nu j'_\nu}(n_{j_\nu}-n_{j_\pi}), \tag{A21}$$

where

$$B_{j_\pi j_\nu}(JM)=-\sum_{m_\pi m_\nu}\langle j_\pi m_\pi j_\nu m_\nu|JM\rangle\alpha^\dagger_{j_\pi m_\pi}\alpha_{j_\nu\tilde{m}_\nu}, \tag{A22}$$

The omission of the contribution of scattering-quasiparticle operators $B^\dagger_{j'_\pi j'_\nu}(J'M')$ and $B_{j_\pi j_\nu}(JM)$ is the source that leads to the underestimation of the quantity $\mathcal{S}^- - \mathcal{S}^+$ within the renormalized QRPA.

**4. Restoration of the Ikeda sum rule within the modified QRPA**

The modified QRPA takes a step further by taking into account the effects of ground-state correlations on the quasiparticle and collective excitations. This has been realized in Ref. [13] using the secondary Bogoliubov transformation (73), where $n_j$ is the quasiparticle-occupation number in the new correlated ground state $|\widetilde{\mathrm{RPA}}\rangle$:

$$n_j = \langle \overline{\mathrm{RPA}} | \alpha^\dagger_{jm} \alpha_{jm} | \overline{\mathrm{RPA}} \rangle \neq 0. \tag{A23}$$

The modified QRPA phonon operators are introduced as

$$\overline{Q}^\dagger_{JMi} = \sum_{j_\pi j_\nu} [\overline{X}^{(Ji)}_{j_\pi j_\nu} \overline{A}^\dagger_{j_\pi j_\nu}(JM) - \overline{Y}^{(Ji)}_{j_\pi j_\nu} \overline{A}_{j_\pi j_\nu}(J\widetilde{M})],$$

$$\overline{Q}_{JMi} = [\overline{Q}^\dagger_{JMi}]^\dagger, \tag{A24}$$

where $\overline{A}^\dagger_{j_\pi j_\nu}(JM)$ and $\overline{A}_{j_\pi j_\nu}(JM)$ are the creation and destruction operators of a modified-quasiparticle pair

$$\overline{A}^\dagger_{j_\pi j_\nu}(JM) = \sum_{m_\pi m_\nu} \langle j_\pi m_\pi j_\nu m_\nu | JM \rangle \overline{\alpha}^\dagger_{j_\pi m_\pi} \overline{\alpha}^\dagger_{j_\nu m_\nu},$$

$$\overline{A}_{jj'}(JM) = [\overline{A}_{jj'}(JM)^\dagger]^\dagger. \tag{A25}$$

The new ground state $|\overline{\mathrm{RPA}}\rangle$ is defined as the vacuum for the modified phonon operator, i.e.,

$$\overline{Q} | \overline{\mathrm{RPA}} \rangle = 0. \tag{A26}$$

The transformation from the single-particle operators $a^\dagger_{jm}$ and $a_{jm}$ to the modified-quasiparticle opertors $\overline{\alpha}^\dagger_{jm}$ and $\overline{\alpha}_{jm}$ is obtained after successively applying the usual, Eq. (72), and secondary, Eq. (73), Bogoliubov transformations, and has the form similar to the inverse transformation of Eq. (72):

$$a^\dagger_{jm} = \overline{u}_j \overline{\alpha}^\dagger_{jm} + (-)^{j-m} \overline{v}_j \overline{\alpha}_{j-m},$$

$$(-)^{j-m} a_{j-m} = (-)^{j-m} \overline{u}_j \overline{\alpha}_{j-m} - \overline{v}_j \overline{\alpha}^\dagger_{jm}, \tag{A27}$$

where

$$\overline{u}_j = u_j \sqrt{1-n_j} + v_j \sqrt{n_j}, \quad \overline{v}_j = v_j \sqrt{1-n_j} - u_j \sqrt{n_j}. \tag{A28}$$

Using the secondary Bogoliubov transformation (73) to express $A^\dagger_{j_\pi j_\nu}(JM)$ and $A_{j_\pi j_\nu}(JM)$ in terms of $\overline{A}^\dagger_{j_\pi j_\nu}(JM)$, $\overline{A}_{j_\pi j_\nu}(JM)$, $\overline{B}^\dagger_{j_\pi j_\nu}(JM)$, and $\overline{B}_{j_\pi j_\nu}(JM)$ [see Eqs. (9) and (10) of Ref. [13]], we find that Eqs. (A12) and (A21) hold in the correlated ground state (A26) if $\overline{B}^\dagger_{j_\pi j_\nu}(JM)$ and $\overline{B}_{j_\pi j_\nu}(JM)$ commute, while $\overline{A}^\dagger_{j_\pi j_\nu}(JM)$ and $\overline{A}_{j_\pi j_\nu}(JM)$ obey the same commutation relation (A8) with respect to the correlated ground state $|\overline{\mathrm{RPA}}\rangle$. Therefore, the set of equations to define the energy and amplitudes $\overline{X}^{(Ji)}_{j_\pi j_\nu}$ and $\overline{Y}^{(Ji)}_{j_\pi j_\nu}$ of the modified $\pi\nu$-phonon excitation have the same form as of the usual QRPA ones. This set of equations is called the modified QRPA equations. The amplitudes $\overline{X}^{(Ji)}_{j_\pi j_\nu}$ and $\overline{Y}^{(Ji)}_{j_\pi j_\nu}$ obey the same normalization condition as in Eq. (A10), namely,

$$\sum_{j_\pi j_\nu} [\overline{X}^{(Ji)}_{j_\pi j_\nu} \overline{X}^{(J'i')}_{j_\pi j_\nu} - \overline{Y}^{(Ji)}_{j_\pi j_\nu} \overline{Y}^{(J'i')}_{j_\pi j_\nu}] = \delta_{JJ'} \delta_{ii'}. \tag{A29}$$

The set of modified QRPA equations should be solved simultaneously with the normalization condition (A29) and the equation for $n_j$. The latter is evaluated from Eq. (A18) as

$$n_j = \sum_{Ji} \frac{2J+1}{2j+1} \sum_{j'} D_{jj'} [\mathcal{Y}^{(Ji)}_{jj'}]^2, \tag{A30}$$

where $\mathcal{Y}^{(Ji)}_{jj'}$ is expressed in terms of $\overline{X}^{(Ji)}_{jj'}$ and $\overline{Y}^{(Ji)}_{jj'}$ as (see Eq. (16) of Ref. [13])

$$\mathcal{Y}^{(Ji)}_{jj'} = \overline{X}^{(Ji)}_{jj'} \sqrt{(1-n_j)(1-n_{j'})} + \overline{Y}^{(Ji)}_{jj'} \sqrt{n_j n_{j'}}. \tag{A31}$$

Because of the renormalization factors $\sqrt{(1-n_j)(1-n_{j'})}$ and $\sqrt{n_j n_{j'}}$ the modified QRPA can avoid the collapse in a way similar to that of the renormalized QRPA. Using the same secondary Bogoliubov transformation (73), it is easy to see that the modified QRPA phonon operators contain all the operators $A^\dagger_{j_\pi j_\nu}(JM)$ and $A_{j_\pi j_\nu}(JM)$, and $B^\dagger_{j_\pi j_\nu}(JM)$ and $B_{j_\pi j_\nu}(JM)$ in its definition (see Eq. (13) of Ref. [13]). This feature allows the modified QRPA to restore the Ikeda sum rule as shown below.

The quantity $S^- - S^+$ is calculated within the modified QRPA as

$$
\begin{aligned}
(\mathcal{S}^- - \mathcal{S}^+)_{\mathrm{MRPA}}
&= \sum_i |\langle \overline{\mathrm{RPA}} | \overline{Q}_{JMi} \beta^- | \overline{\mathrm{RPA}} \rangle|^2 \\
&\quad - \sum_i |\langle \overline{\mathrm{RPA}} | \overline{Q}_{JMi} \beta^+ | \overline{\mathrm{RPA}} \rangle|^2 \\
&= \left| \sum_{j_\pi j_\nu} q_{j_\pi j_\nu} (\overline{u}_{j_\pi} \overline{v}_{j_\nu} \overline{X}_{j_\pi j_\nu} + \overline{v}_{j_\pi} \overline{u}_{j_\nu} \overline{Y}_{j_\pi j_\nu}) \right|^2 \\
&\quad - \left| \sum_{j_\pi j_\nu} q_{j_\nu j_\pi} (\overline{v}_{j_\pi} \overline{u}_{j_\nu} \overline{X}_{j_\pi j_\nu} + \overline{u}_{j_\pi} \overline{v}_{j_\nu} \overline{Y}_{j_\pi j_\nu}) \right|^2 \\
&= \sum_{j_\pi j_\nu} |q_{j_\pi j_\nu}|^2 (\overline{v}^2_{j_\nu} - \overline{v}^2_{j_\pi}) \\
&= 2(2J+1) \left[ \sum_{j_\nu} \Omega_{j_\nu} \overline{v}^2_{j_\nu} - \sum_{j_\pi} \Omega_{j_\pi} \overline{v}^2_{j_\pi} \right] \\
&= (2J+1)(N-Z),
\end{aligned} \tag{A32}
$$

making use of the normalization condition (A29), Eq. (A28) for $\overline{v}_j$ in terms of $u_j$ and $v_j$, and MBCS Eq. (79) for particle number. We have just proved that the modified QRPA restores the Ikeda sum rule.

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