Improved treatment of ground-state correlations: Modified random phase approximation

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A method is proposed to improve the treatment of the ground-state correlations in a finite Fermi system compared with the standard random phase approximation (RPA) or earlier suggested renormalized RPA. The correlations lead to nonzero quasiparticle occupancies in the ground state. The method employs modified quasiparticles obtained by a canonical transformation of usual quasiparticles explicitly involving the quasiparticle occupation numbers. A set of equations is derived, which allows one to determine these occupation numbers along with the RPA modes. The formalism is illustrated with the Lipkin-Meshkov-Glick model, and a model for superconducting pairing at a finite temperature. With the new approach, the ground-state correlations are significantly reduced, the energy of the first excited state becomes closer to the exact solution around the region where the RPA collapses, and the superconducting gap monotonously decreases instead of the sharp phase transition. We discuss the effective equivalence of the interaction effects and variation of temperature for the ground-state correlations.

I. INTRODUCTION

One of the central issues in theory of many-body quantum systems, such as atomic nuclei, is the treatment of collective modes and their coupling to noncollective degrees of freedom. The collective modes are generated by the coherent motion of many quasiparticles beyond the mean-field approximation of independent quasiparticles. The microscopic treatment of the collective modes is routinely carried out within the framework of the random phase approximation (RPA) in the absence of superconducting pairing or quasiparticle RPA (QRPA) with pairing included. The RPA (or QRPA) equations are usually obtained within the quasiboson approximation, which violates the Pauli principle between the particle-hole (or quasiparticle) pairs considered as ideal bosons. In this way, only a part of ground-state correlations is accounted for. This leads to the collapse of the RPA at a critical point, where it yields an imaginary solution.

Several approaches were developed taking into account the ground-state correlations beyond the RPA to correct this inconsistency [1–5]. One of them is the renormalized RPA [1,5]. In this method, a set of RPA-like equations is solved self-consistently together with the equation for the single-particle (or quasiparticle) occupation numbers. The most complete form of the renormalized RPA is the so-called extended renormalized RPA proposed in [6]. It includes all possible ph, pp and hh transitions. This has been done by constructing the phonon operators, which include all the forward- and backward-going two quasiparticle amplitudes as well as the amplitudes describing the quasiparticle scattering. The presence of the quasiparticle occupation numbers n_j different from 0 brings in many new solutions associated with the new two quasiparticle poles $(\epsilon_j - \epsilon_{j'})$ in addition to the usual ones for the breaking of pairs, $(\epsilon_j + \epsilon_{j'})$. Now one has the nonvanishing terms $\propto (n_j - n_{j'})/[(\epsilon_j - \epsilon_{j'}) \pm \omega]$. The new formal solutions, classified by several authors as "spu-

rious," can be situated at very low energies (e.g., lower than the energy of the well-known first quadrupole state) if ϵ_j and $\epsilon_{j'}$ are close to each other.

In hot equilibrium Fermi systems, the quasiparticle occupation numbers can be described by the Fermi-Dirac distribution at a given temperature T. It is well known that the superconducting gap $\Delta(T)$, obtained as a solution of the finite-temperature BCS equation, collapses at a critical temperature $T_c \simeq 0.567\Delta(0)$ [7], which signals the phase transition from the superconducting state to the normal one. In macroscopic systems, the ground-state correlations are small so that the approximation of zero quasiparticle occupation numbers in the ground state is sufficiently accurate, and the sharp phase transition indeed takes place. In finite systems, such as nuclei, this is no longer valid. As a matter of fact, taking into account thermal fluctuations, it has been shown in a number of papers that the gap $\Delta(T)$ does not collapse, but decreases with increasing temperature, and remains finite even at rather high T [8–12]. On the other hand, a method using the particle number projection has also shown that the gap Δ does not vanish at high temperatures in finite Fermi systems [13]. Similar results follow from the exact solution of the nuclear pairing problem [14].

In the present work we propose a method to improve the treatment of the ground-state correlations. We preserve the contributions of all processes of creating or destructing quasiparticle pairs as well as those of quasiparticle scattering but eliminate at the same time the appearance of the extra poles. We also show that the same method can resolve the problem of the collapse of the BCS gap at finite temperature in finite systems.

The paper is organized as follows. The approach is developed within the framework of the QRPA in Sec. II, while its RPA limit is presented in the Appendix. Section III and IV discuss the application of this method to the exactly solvable Lipkin-Meshkov-Glick model, and a schematic model for the

superconducting gap at finite temperature, respectively. Conclusions are given in the last section.

II. THE MODIFIED QUASIPARTICLE RPA

A. Transformation to modified quasiparticles

We consider a system of fermions in a spherical mean field; the single-particle orbitals will be labeled by the angular momentum quantum numbers j and m. Assuming that the residual interaction contains a pairing part between the time conjugate orbitals, we perform the standard Bogoliubov canonical transformation from the particle operators, $a_{jm}^\dagger$ and a_{jm}, to the quasiparticle ones, $\alpha_{jm}^\dagger$ and α_{jm}. On top of that, we propose that the quasiparticles are modified by the correlations in the quasiparticle ground state according to the following secondary canonical transformation between the quasiparticle operators $\alpha_{jm}^\dagger$, α_{jm}, and the modified ones $\bar{\alpha}_{jm}^\dagger$, $\bar{\alpha}_{jm}$:

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

The inverse transformation to Eq. (1) is

$$\alpha_{jm}^\dagger = \sqrt{1-n_j}\,\bar{\alpha}_{jm}^\dagger - \sqrt{n_j}\,\bar{\alpha}_{j\tilde{m}}, \quad \alpha_{j\tilde{m}} = \sqrt{1-n_j}\,\bar{\alpha}_{j\tilde{m}} + \sqrt{n_j}\,\bar{\alpha}_{jm}^\dagger. \tag{2}$$

In Eqs. (1) and (2) the sign $^\sim$ stands for the time reversal operation, $a_{j\tilde{m}} = (-1)^{j-m} a_{j-m}$; n_j are the *quasiparticle* occupation numbers of orbitals j in the correlated ground state $|\bar{0}\rangle$,

$$n_j = \langle\bar{0}|\alpha_{jm}^\dagger \alpha_{jm}|\bar{0}\rangle \neq 0. \tag{3}$$

A transformation similar to Eq. (1) has been introduced in [15,16] at finite temperature T, where n_j takes the form of the Fermi-Dirac distribution with quasiparticle energy $\epsilon_j > 0$. The expectation value $\langle\bar{0}|\ldots|\bar{0}\rangle$ for the ground state is then substituted by the average over the grand canonical ensemble. In contrast to Refs. [15,16], no specific form for n_j is assumed here. The occupation numbers n_j will be found by solving self-consistently the modified QRPA equations derived below. Using the inverse transformation (2), we notice that in order to satisfy Eq. (3) it is necessary that

$$\langle\bar{0}|\bar{\alpha}_{jm}^\dagger \bar{\alpha}_{jm}|\bar{0}\rangle = 0. \tag{4}$$

Thus, the correlated ground state $|\bar{0}\rangle$ is the vacuum state with respect to the modified quasiparticle operators $\bar{\alpha}_{jm}^\dagger$ and $\bar{\alpha}_{jm}$.

Using Eq. (2) we express the transformation from the original particle operators to the modified quasiparticle operators $\bar{\alpha}_{jm}^\dagger$, $\bar{\alpha}_{jm}$ as [15,16]

$$a_{jm}^\dagger = \bar{u}_j \bar{\alpha}_{jm}^\dagger + \bar{v}_j \bar{\alpha}_{j\tilde{m}}, \quad a_{j\tilde{m}} = \bar{u}_j \bar{\alpha}_{j\tilde{m}} - \bar{v}_j \bar{\alpha}_{jm}^\dagger, \tag{5}$$

with the coefficients $\bar{u}_j$ and $\bar{v}_j$ related to the conventional Bogoliubov coefficients u_j and v_j as

$$\bar{u}_j = u_j\sqrt{1-n_j} + v_j\sqrt{n_j}, \quad \bar{v}_j = v_j\sqrt{1-n_j} - u_j\sqrt{n_j}. \tag{6}$$

Because of Eq. (4), we find that the following expressions hold exactly in the correlated ground state:

$$\langle\bar{0}|[\bar{A}_{\lambda\mu}(jj'), \quad \bar{A}_{\lambda_1\mu_1}^\dagger(j_1 j_1')]|\bar{0}\rangle$$

$$= \delta_{\lambda\lambda_1}\delta_{\mu\mu_1}[\delta_{jj_1}\delta_{j'j_1'} - (-1)^{j+j'-\lambda}\delta_{jj_1'}\delta_{j'j_1}], \tag{7}$$

$$\langle\bar{0}|[\bar{B}_{\lambda\mu}^\dagger(jj'), \bar{B}_{\lambda_1\mu_1}(j_1 j_1')]|\bar{0}\rangle = 0,$$

where the standard notations are used for the operators of pair creation $\bar{A}_{\lambda\mu}^\dagger(jj')$ and scattering $\bar{B}_{\lambda\mu}(jj')$ of modified quasiparticles, namely,

$$\bar{A}_{\lambda\mu}^\dagger(jj') = \sum_{mm'} \langle jmj'm'|\lambda\mu\rangle \bar{\alpha}_{jm}^\dagger \bar{\alpha}_{j'm'}^\dagger,$$

$$\bar{B}_{\lambda\mu}(jj') = -\sum_{mm'} \langle jmj'm'|\lambda\mu\rangle \bar{\alpha}_{jm}^\dagger \bar{\alpha}_{j'\tilde{m}'}. \tag{8}$$

Using Eq. (2), we express the pair creation $A_{\lambda\mu}^\dagger(jj')$ and scattering $B_{\lambda\mu}(jj')$ operators in terms of their modified quasiparticle counterparts $\bar{A}_{\lambda\mu}^\dagger(jj')$ and $\bar{B}_{\lambda\mu}(jj')$ as

$$A_{\lambda\mu}^\dagger(jj') = \sqrt{(1-n_j)(1-n_{j'})}\,\bar{A}_{\lambda\mu}^\dagger(jj')$$

$$- \sqrt{n_j n_{j'}}\,\bar{A}_{\lambda\tilde{\mu}}(jj') + \sqrt{(1-n_j)n_{j'}}\,\bar{B}_{\lambda\mu}(jj')$$

$$+ \sqrt{n_j(1-n_{j'})}\,\bar{B}_{\lambda\tilde{\mu}}^\dagger(jj')$$

$$- \delta_{\lambda 0}\delta_{\mu 0}\delta_{jj'}\sqrt{2j+1}\,\sqrt{n_j(1-n_j)}, \tag{9}$$

$$B_{\lambda\mu}(jj') = \sqrt{(1-n_j)(1-n_{j'})}\,\bar{B}_{\lambda\mu}(jj') - \sqrt{n_j n_{j'}}\,\bar{B}_{\lambda\tilde{\mu}}^\dagger(jj')$$

$$- \sqrt{(1-n_j)n_{j'}}\,\bar{A}_{\lambda\mu}^\dagger(jj') - \sqrt{n_j(1-n_{j'})}\,\bar{A}_{\lambda\tilde{\mu}}(jj')$$

$$+ \delta_{jj'}\delta_{\lambda 0}\delta_{\mu 0}n_j\sqrt{2j+1}. \tag{10}$$

From Eqs. (7), (9), and (10) we find the following exact relations:

$$\langle\bar{0}|[A_{\lambda\mu}(jj'), A_{\lambda_1\mu_1}^\dagger(j_1 j_1')]|\bar{0}\rangle$$

$$= (1-n_j-n_{j'})\delta_{\lambda\lambda_1}\delta_{\mu\mu_1}$$

$$\times[\delta_{jj_1}\delta_{j'j_1'} - (-1)^{j+j'-\lambda}\delta_{jj_1'}\delta_{j'j_1}], \tag{11}$$

$$\langle\bar{0}|[B_{\lambda\mu}^\dagger(jj'), B_{\lambda_1\mu_1}(j_1 j_1')]|\bar{0}\rangle$$

$$= (n_{j'}-n_j)\delta_{\lambda\lambda_1}\delta_{\mu\mu_1}\delta_{jj_1}\delta_{j'j_1'}, \tag{12}$$

which recover the approximate commutation relations in the renormalized QRPA, see, e.g., Eqs. (A5) and (A6) of [6].

B. Modified phonons

We introduce the following modified phonon operators:

$$\bar{Q}^{\dagger}_{\lambda\mu i}=\frac{1}{2}\sum_{jj'}[\bar{X}^{(\lambda i)}_{jj'}\bar{A}^{\dagger}_{\lambda\mu}(jj')-\bar{Y}^{(\lambda i)}_{jj'}\bar{A}_{\lambda\tilde{\mu}}(jj')], \quad (13)$$

$$\bar{Q}_{\lambda\tilde{\mu}i}=\frac{1}{2}\sum_{jj'}[\bar{X}^{(\lambda i)}_{jj'}\bar{A}_{\lambda\tilde{\mu}}(jj')-\bar{Y}^{(\lambda i)}_{jj'}\bar{A}^{\dagger}_{\lambda\mu}(jj')].$$

Using Eqs. (1) and (8), we find that the modified phonon operators $\bar{Q}^{\dagger}_{\lambda\mu i}$ and $\bar{Q}_{\lambda\mu i}$ in (13) contain all the conventional two-quasiparticle parts $A^{\dagger}_{\lambda\mu}(jj')$, $A_{\lambda\tilde{\mu}}(jj')$, as well as the scattering parts $B_{\lambda\mu}(jj')$, and $B^{\dagger}_{\lambda\tilde{\mu}}(jj')$, namely,

$$\bar{Q}^{\dagger}_{\lambda\mu i}=\frac{1}{2}\sum_{jj'}[X^{(\lambda i)}_{jj'}A^{\dagger}_{\lambda\mu}(jj')-Y^{(\lambda i)}_{jj'}A_{\lambda\mu}(jj')$$
$$-Z^{(\lambda i)}_{jj'}B_{\lambda\mu}(jj')+W^{(\lambda i)}_{jj'}B^{\dagger}_{\lambda\tilde{\mu}}(jj')], \quad (14)$$

$$\bar{Q}_{\lambda\tilde{\mu}i}=\frac{1}{2}\sum_{jj'}[X^{(\lambda i)}_{jj'}A_{\lambda\tilde{\mu}}(jj')-Y^{(\lambda i)}_{jj'}A^{\dagger}_{\lambda\mu}(jj')$$
$$-Z^{(\lambda i)}_{jj'}B^{\dagger}_{\lambda\tilde{\mu}}(jj')+W^{(\lambda i)}_{jj'}B_{\lambda\mu}(jj')], \quad (15)$$

where

$$X^{(\lambda i)}_{jj'}=\bar{X}^{(\lambda i)}_{jj'}\sqrt{(1-n_j)(1-n_{j'})}+\bar{Y}^{(\lambda i)}_{jj'}\sqrt{n_j n_{j'}},$$

$$Y^{(\lambda i)}_{jj'}=\bar{Y}^{(\lambda i)}_{jj'}\sqrt{(1-n_j)(1-n_{j'})}+\bar{X}^{(\lambda i)}_{jj'}\sqrt{n_j n_{j'}}, \quad (16)$$

$$Z^{(\lambda i)}_{jj'}=\bar{X}^{(\lambda i)}_{jj'}\sqrt{(1-n_j)n_{j'}}-\bar{Y}^{(\lambda i)}_{jj'}\sqrt{n_j(1-n_{j'})},$$

$$W^{(\lambda i)}_{jj'}=\bar{Y}^{(\lambda i)}_{jj'}\sqrt{(1-n_j)n_{j'}}-\bar{X}^{(\lambda i)}_{jj'}\sqrt{n_j(1-n_{j'})}. \quad (17)$$

Equations (14) and (15) show that the modified operators $\bar{Q}^{\dagger}_{\lambda\mu i}$ and $\bar{Q}_{\lambda\mu i}$ in Eq. (13) have the general structure of the extended renormalized QRPA phonon operators discussed in [6].

Due to the vacuum expectation of the commutation relations (7), we obtain the usual QRPA-like orthonormalization for the modified phonon amplitudes $\bar{X}^{(\lambda i)}_{jj'}$ and $\bar{Y}^{(\lambda i)}_{jj'}$,

$$\sum_{jj'}[\bar{X}^{\lambda i}_{jj'}\bar{X}^{\lambda_1 i_1}_{jj'}-\bar{Y}^{\lambda i}_{jj'}\bar{Y}^{\lambda_1 i_1}_{jj'}]=2\delta_{\lambda\lambda_1}\delta_{ii_1}, \quad (18)$$

so that the modified phonon operators $\bar{Q}^{\dagger}_{\lambda\mu i}$ and $\bar{Q}_{\lambda\mu i}$ are ideal bosons with respect to the new vacuum state

$$\langle\bar{0}|[\bar{Q}_{\lambda\mu i},\bar{Q}^{\dagger}_{\lambda_1\mu_1 i_1}]|\bar{0}\rangle=\delta_{\lambda\lambda_1}\delta_{\mu\mu_1}\delta_{ii_1}. \quad (19)$$

Therefore, within a model Hamiltonian including a residual two-body interaction, the equations of motion for the modified phonon operators $\bar{Q}^{\dagger}_{\lambda\mu i}$ and $\bar{Q}_{\lambda\mu i}$ have exactly the same form as the usual QRPA equations. Since the latter have ana-

lytic solutions for separable interactions, we can illustrate the results considering the Hamiltonian as in Eqs. (A1) and (A2) of Ref. [6].

Using the canonical transformations (5) and (13), we express this Hamiltonian in terms of $\bar{Q}^{\dagger}_{\lambda\mu i}$, $\bar{Q}_{\lambda\mu i}$, $\bar{B}_{\lambda\mu}(jj')$, and $\bar{B}^{\dagger}_{\lambda\tilde{\mu}}(jj')$. Applying the standard procedure of deriving the QRPA equation for separable interactions, we obtain the dispersion relation for the phonon energy ω as

$$1-k^{(\lambda)}\bar{F}(\omega)=0, \quad (20)$$

where

$$\bar{F}(\omega)=\frac{1}{2\lambda+1}\sum_{jj'}(q^{(\lambda)}_{jj'})^2\frac{(\bar{u}^{(+)}_{jj'})^2(\bar{\epsilon}_j+\bar{\epsilon}_{j'})}{(\bar{\epsilon}_j+\bar{\epsilon}_{j'})^2-\omega^2}. \quad (21)$$

In Eqs. (20) and (21), $k^{(\lambda)}$ is the coupling parameter of the separable interaction for multipolarity λ; $q^{(\lambda)}_{jj'}$ is the single-particle matrix element corresponding to the separable interaction $(q^{(\lambda)}\cdot q^{(\lambda)})$; $\bar{\epsilon}_j\equiv\sqrt{(E_j-\bar{E}_F)^2+\bar{\Delta}^2}$ is the modified quasiparticle energy with the modified superconducting pairing gap $\bar{\Delta}$, single-particle energy E_j and the modified Fermi energy $\bar{E}_F$. The function $\bar{u}^{(+)}_{jj'}$ is a combination of the modified Bogoliubov coherence factors (6)

$$\bar{u}^{(+)}_{jj'}\equiv\bar{u}_j\bar{v}_{j'}+\bar{v}_j\bar{u}_{j'}=[\sqrt{(1-n_j)(1-n_{j'})}-\sqrt{n_j n_{j'}}]u^{(+)}_{jj'}$$
$$-[\sqrt{(1-n_j)n_{j'}}+\sqrt{n_j(1-n_{j'})}]v^{(-)}_{jj'}, \quad (22)$$

where $u^{(+)}_{jj'}=u_j v_{j'}+v_j u_{j'}$, $v^{(-)}_{jj'}=u_j u_{j'}-v_j v_{j'}$. For simplicity, we do not specify the neutron and proton components as well as the isoscalar and isovector parts of the multipole interaction.

The equations for the modified paring gap $\bar{\Delta}$ and the modified Fermi energy $\bar{E}_F$ have exactly the same form as the BCS equations, where the coefficients u_j and v_j are replaced with $\bar{u}_j$ and $\bar{v}_j$ from Eq. (6). In terms of the usual Bogoliubov coefficients, u_j and v_j, the equations have the form

$$\bar{\Delta}=G\sum_j\Omega_j\bar{u}_j\bar{v}_j=G\sum_j\Omega_j[(1-2n_j)u_j v_j$$
$$-\sqrt{n_j(1-n_j)}(u_j^2-v_j^2)], \quad (23)$$

$$N=2\sum_j\Omega_j\bar{v}_j^2=2\sum_j\Omega_j[(1-2n_j)v_j^2+n_j]$$
$$-4\sum_j\Omega_j\sqrt{n_j(1-n_j)}u_j v_j, \quad (24)$$

where N is the particle number, the pairing matrix elements are approximated by the constant G, and $\Omega_j=j+1/2$. Once the modified phonon energy $\omega_{\lambda i}$ is found as the solution of Eq. (20), the amplitudes $\bar{X}^{(\lambda i)}_{jj'}$ and $\bar{Y}^{(\lambda i)}_{jj'}$ are calculated as

$$\bar{X}_{jj'}^{(\lambda i)} = \frac{q_{jj'}^{(\lambda)} \bar{u}_{jj'}^{-(+)}}{\bar{\epsilon}_j + \bar{\epsilon}_{j'} - \omega_{\lambda i}} \bar{M}_{\lambda i}, \quad \bar{Y}_{jj'}^{(\lambda i)} = \frac{q_{jj'}^{(\lambda)} \bar{u}_{jj'}^{-(+)}}{\bar{\epsilon}_j + \bar{\epsilon}_{j'} + \omega_{\lambda i}} \bar{M}_{\lambda i},$$

(25)

with

$$\bar{M}_{\lambda i} = \left\{ \sum_{jj'} [q_{jj'}^{(\lambda)}]^2 [\bar{u}_{jj'}^{-(+)}]^2 \left[\frac{1}{(\bar{\epsilon}_j + \bar{\epsilon}_{j'} - \omega_{\lambda i})^2} \right. \right.$$

$$\left. \left. - \frac{1}{(\bar{\epsilon}_j + \bar{\epsilon}_{j'} + \omega_{\lambda i})^2} \right] \right\}^{-1/2}.$$

(26)

In a general case of a nonseparable interaction, we do not have the dispersion equation (20) and the analytic expressions for $\bar{X}_{jj'}^{(\lambda i)}$ and $\bar{Y}_{jj'}^{(\lambda i)}$ as in Eq. (25). Instead, we obtain a set of equations, which has to be solved by diagonalization to find the RPA eigenvectors $\{\bar{X}_{jj'}^{(\lambda i)}, \bar{Y}_{jj'}^{(\lambda i)}\}$, and the eigenvalues $\omega_{\lambda i}$. Equations (20), (21), (25), and (26) have the same form as their counterparts in the QRPA. The number of solutions (normal modes) is also the same because the number of two quasiparticle poles $(\bar{\epsilon}_j + \bar{\epsilon}_{j'})$ remains unchanged. In this way, the problem of "spurious" solutions, which may occur due to the new poles $\epsilon_j - \epsilon_{j'}$ within the extended QRPA [6] is eliminated here. The new features are in the coefficients $\bar{u}_{jj'}^{(+)}$ (22) instead of $u_{jj'}^{(+)}$, and in the modified quasiparticle energies $\bar{\epsilon}_j$ instead of the usual ϵ_j. Since $\bar{u}_{jj'}^{(+)}$ as well as Eqs. (23) and (24) contain the unknown quasiparticle occupation numbers n_j, we discuss below the way to determine it.

C. Quasiparticle occupation numbers

We define n_j using the procedure of the extended renormalized QRPA proposed in [6], according to which we obtained Eq. (A7) of Ref. [6] for the ground state correlation factor $\bar{D}_{jj'}$. Using Eq. (16), we express the right hand side of (A7) of Ref. [6] in terms of the modified phonon amplitudes $\bar{X}_{jj'}^{(\lambda i)}$ and $\bar{Y}_{jj'}^{(\lambda i)}$ as

$$\bar{D}_{jj'} \equiv 1 - n_j - n_{j'} = 1$$

$$- \sum_{\lambda i} \sum_{j''} \{ \bar{D}_{jj''} [\bar{Y}_{jj''}^{(\lambda i)} \sqrt{(1-n_j)(1-n_{j''})}$$

$$+ \bar{X}_{jj''}^{(\lambda i)} \sqrt{n_j n_{j''}}]^2 + \bar{D}_{j''j'} [\bar{Y}_{j''j'}^{(\lambda i)} \sqrt{(1-n_{j''})(1-n_{j'})}$$

$$+ \bar{X}_{j''j'}^{(\lambda i)} \sqrt{n_{j''} n_{j'}}]^2 \}.$$

(27)

The set of Eqs. (20), (23)–(25), and (27) should be solved self-consistently for determining the modified BCS gap $\bar{\Delta}$, Fermi energy $\bar{E}_F$, phonon energies $\omega_{\lambda i}$, the amplitudes $\bar{X}_{jj'}^{(\lambda i)}$ and $\bar{Y}_{jj'}^{(\lambda i)}$, as well as the quasiparticle occupation numbers n_j. We refer to Eqs. (23) and (24) as the modified BCS equation, and Eq. (20) supplemented with Eqs. (21), (22), (25)–(27) as the modified QRPA equation.

In numerical calculations, these equations can be solved iteratively as follows. Starting from the usual BCS equation ($n_j = 0$), one obtains the quasiparticle energies ϵ_j, the gap Δ, and the Fermi energy E_F. Using them, one solves the modified RPA equation to find $\omega_{\lambda i}$, $\bar{X}_{jj'}^{(\lambda i)}$, $\bar{Y}_{jj'}^{(\lambda i)}$, and the quasiparticle occupation numbers n_j. The latter are inserted into the modified BCS equations (23) and (24) to determine $\bar{\Delta}$, $\bar{E}_F$, and $\bar{\epsilon}_j$. These values are used to solve the modified RPA equation again, and the procedure is repeated until the required convergence is reached.

III. A TESTING GROUND: THE LIPKIN-MESHKOV-GLICK MODEL

In this section we compare the exact solutions of the Lipkin-Meshkov-Glick (LMG) model [17] with those obtained with the use of various approximations (RPA, renormalized RPA, and modified RPA). The model considers a system of N fermions distributed in two levels each having a 2Ω-fold degeneracy; the levels are separated by energy E. In the noninteracting system the lower level is occupied by N particles, i.e., $2\Omega = N$. The model is described by the Hamiltonian

$$H = EJ_0 - \frac{1}{2} V(J_+^2 + J_-^2) - \frac{1}{2} V_1 (J_+ J_- + J_- J_+), \quad (28)$$

where the operators

$$J_0 = \frac{1}{2} \sum_{m=1}^{N} (a_{+m}^\dagger a_{+m} - a_{-m}^\dagger a_{-m}),$$

$$J_+ = \sum_{m=1}^{N} a_{+m}^\dagger a_{-m}, \quad J_- = (J_+)^\dagger \quad (29)$$

are the usual SU(2) generators, satisfying the commutation relations

$$[J_+, J_-] = 2J_0, \quad [J_0, J_\pm] = \pm J_\pm. \quad (30)$$

The quasispin J is an exact constant of motion while its projection $M \equiv J_0$ is not conserved because of the processes of pair transfer between the levels generated by the coupling constant V. The exact eigenenergies $\mathcal{E}_i$ of this general version of the LMG model are found by diagonalizing the tridiagonal matrix, whose nonvanishing elements in the space of states $|J,M\rangle$ with $-J \leq M \leq J$ $(J = \Omega = N/2)$ are

$$\langle J,M|H|J,M\rangle = EM - V_1[J(J+1) - M^2],$$

$$\langle J,M \pm 2|H|J,M\rangle$$

$$= -\frac{1}{2} V \sqrt{(J \mp M)[J^2 - (M \pm 1)^2](J \pm M + 2)}. \quad (31)$$

The phonon operators for the model are

$$Q^\dagger = XJ_+ - YJ_-, \quad \mathcal{Q}^\dagger = \mathcal{X} \frac{J_+}{\sqrt{D}} - \mathcal{Y} \frac{J_-}{\sqrt{D}},$$

$$\bar{Q}^{\dagger} = \bar{X}\bar{J}_{+} - \bar{Y}\bar{J}_{-} , \qquad (32)$$

in the RPA, renormalized RPA, and modified RPA, respectively. The factor $D = 1/(1+2\mathcal{Y}^2)$ is defined according to Refs. [5,6]. The orthonormalization condition for the renormalized phonon amplitudes $\mathcal{X}$ and $\mathcal{Y}$, and the modified phonon amplitudes $\bar{X}$ and $\bar{Y}$ are the same as that for the RPA phonon amplitudes X and Y, namely,

$$N(\mathcal{X}^2 - \mathcal{Y}^2) = N(\bar{X}^2 - \bar{Y}^2) = N(X^2 - Y^2) = 1. \qquad (33)$$

After some algebra, we obtain the analytic solutions for the normal frequencies ω of the RPA, ω_{ren} of the renormalized RPA, and ω_{mod} of the modified RPA equations as

$$\omega = \pm E \sqrt{(1-\chi_1)^2 - \chi^2},$$

$$\omega_{\text{ren}} = \pm E \sqrt{(1-\chi_1 D)^2 - \chi^2 D^2}, \qquad (34)$$

$$\omega_{\text{mod}} = \pm \bar{E} \sqrt{(1-\bar{\chi}_1 \bar{u}^{(+)})^2 - \bar{\chi}^2 [\bar{u}^{(+)}]^2},$$

where

$$\chi = NV/E, \quad \chi_1 = NV_1/E, \quad \bar{\chi} = \chi[\bar{u}^{(+)}],$$

$$\bar{\chi}_1 = \chi_1 \bar{u}^{(+)}, \quad \bar{E} = E\bar{u}^{(+)}, \qquad (35)$$

with

$$\bar{u}^{+} = 1 - 2n = \bar{D} = \frac{1}{1 + 2[n\bar{X} + (1-n)\bar{Y}]^2}, \qquad (36)$$

see Eq. (27). The expressions of the phonon amplitudes are

$$X = \left[\frac{1}{2N} \frac{E(1-\chi_1) + \omega}{\omega} \right]^{1/2}, \quad Y = \left[\frac{1}{2N} \frac{E(1-\chi_1) - \omega}{\omega} \right]^{1/2}, \qquad (37)$$

$$\mathcal{X} = \left[\frac{1}{2N} \frac{E(1-\chi_1 D) + \omega_{\text{ren}}}{\omega_{\text{ren}}} \right]^{1/2},$$

$$\mathcal{Y} = \left[\frac{1}{2N} \frac{E(1-\chi_1 D) - \omega_{\text{ren}}}{\omega_{\text{ren}}} \right]^{1/2}, \qquad (38)$$

$$\bar{X} = \left[\frac{1}{2N} \frac{\bar{E}(1-\bar{\chi}_1 \bar{u}^{(+)}) + \omega_{\text{mod}}}{\omega_{\text{mod}}} \right]^{1/2},$$

$$\bar{Y} = \left[\frac{1}{2N} \frac{\bar{E}(1-\bar{\chi}_1 \bar{u}^{(+)}) - \omega_{\text{mod}}}{\omega_{\text{mod}}} \right]^{1/2}, \qquad (39)$$

for the three versions of the RPA, respectively. We note that, in the conventional form of the renormalized RPA considered here [5], the quasiparticle energy ϵ_j is not renormalized. A full renormalized RPA should include such renormalization due to the nonzero quasiparticle occupancies n_j. The renormalized BCS equation has then the form identical to the finite-temperature BCS equation [7] but with the occupation
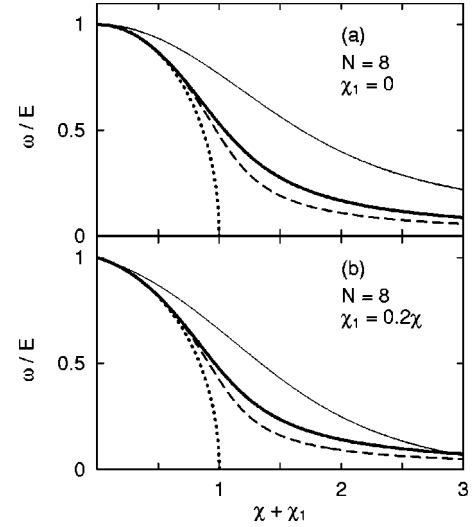

FIG. 1. Normalized excitation energies as a function of the interaction $\chi + \chi_1$ for $N=8$ particles: exact solution, thin solid line; RPA, dotted line; renormalized RPA, dashed line; and modified RPA, thick solid line.

numbers n_j found by solving self-consistently the set of renormalized BCS+RPA equations.

Shown in Fig. 1 are the exact excitation energy $\mathcal{E}_1 - \mathcal{E}_0$ and the frequencies ω, ω_{ren}, and ω_{mod} (in units of the level spacing E) as functions of the interaction strength $\chi + \chi_1$ for $N=8$ particles. The energy $\mathcal{E}_0$ is the lowest exact eigenvalue of the Hamiltonian (28), while $\mathcal{E}_1$ is the energy of the lowest excited state. The calculations have been carried out for (a) $\chi_1 = 0$, the standard LMG model and (b) $\chi_1 = 0.2 \chi$. The RPA solution collapses at $\chi + \chi_1 = 1$. In contrast to that, the frequencies for the renormalized RPA, modified RPA, and exact solution monotonously decrease with the increasing interaction strength $\chi + \chi_1$. The excitation energy obtained within the modified RPA is larger, and closer to the exact solution than that of the renormalized RPA at a given interaction. With increasing χ_1 the lowest level and the one above it in the exact solution start to cross. This corresponds to the transition from the spherical scheme to the deformed one. Therefore, below we will concentrate on the standard version of the LGM model with $\chi_1 = 0$.

The normalized excitation energies ω_{exact}/E, ω/E, ω_{ren}/E, and ω_{mod}/E, obtained for $N=16, 24, 50$, and 100 are plotted in Fig. 2 as a function of the interaction χ. The energy obtained with the modified RPA is always closer to the exact energy at $\chi \lesssim \chi_c$, where χ_c is the value of the interaction parameter, at which the exact solution crosses with that of the modified RPA. The values of χ_c are found to be around 1.86, 1.48, 1.2, and 1.1 for $N=16, 24, 50$, and 100, respectively. The difference between the energy obtained within the modified RPA and that of the renormalized RPA decreases with the increasing particle number N so that, at asymptotically large N ($N>100$), the solutions given by all three versions of the RPA become rather close to the exact one. This indicates that the ground-state correlations are small in large systems, where the RPA works well.

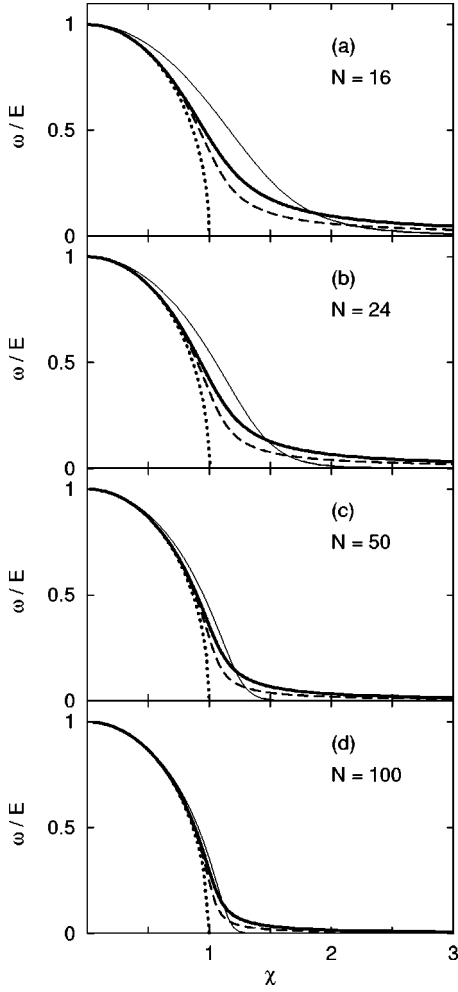The difference between the correlated ground state and

FIG. 2. Normalized excitation energies as a function of the interaction χ ($\chi_1 = 0$) for various particle numbers N. Notations are the same as in Fig. 1.

the BCS vacuum is given by the square of the backward-going amplitude, i.e., Y^2, $\mathcal{Y}^2$, and $\bar{Y}^2$ of the RPA, renormalized RPA, and modified RPA, respectively. Being proportional to the expectation value of the boson number operator in the ground state, these quantities can serve as a measure for the ground-state correlations [18]; they are shown in Fig. 3 as a function of χ for several particle numbers N. At χ below around 0.5 the results of the RPA, renormalized RPA, and modified RPA practically coincide. At larger values of the interaction, the ground-state correlations become too strong within the RPA so that Y^2 collapses at $\chi = 1$. At the instability point, the RPA overestimates the ground-state correlations by a factor of 18 compared to the renormalized RPA, and by a factor of 30 compared to the modified RPA at $N = 4$; these factors are reduced about twice when the particle number N is doubled. At $\chi > 1$, only the results obtained with the renormalized RPA and modified RPA remain, whereas the ground-state correlations for the modified RPA are about thrice weaker than those for the renormalized RPA at large χ.

The quasiparticle occupation number n at energy E can be fitted well with a Fermi-Dirac distribution n
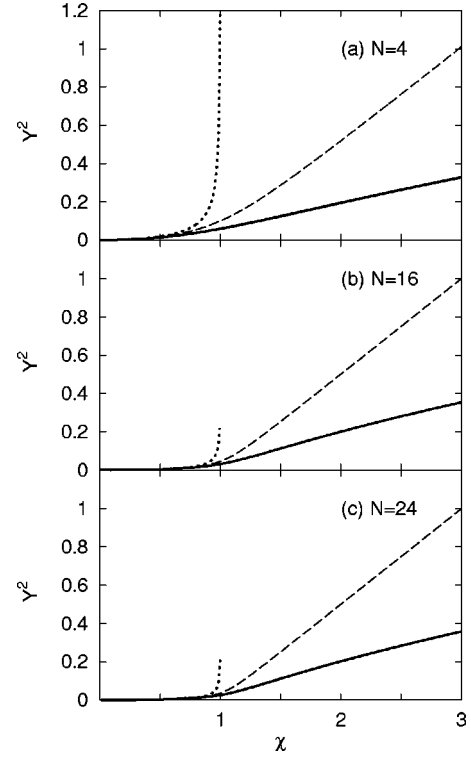

FIG. 3. Squared backward-going amplitudes Y^2 of RPA (dotted line), $\mathcal{Y}^2$ of renormalized RPA (dashed line), and $\bar{Y}^2$ of modified RPA (solid line) as a function of the interaction χ for various particle numbers N.

$= 1/[\exp(E/T_{\text{eff}}) + 1]$ at an effective temperature T_{eff}. The temperature T_{eff} is derived directly from this distribution as

$$T_{\text{eff}} = E\left[\ln\left(\frac{1}{n} - 1 \right) \right]^{-1}. \qquad (40)$$

The values of T_{eff}/E are plotted in Fig. 4 versus the interaction parameter χ. It is seen from this figure that the validity region of the RPA corresponds to $T_{\text{eff}} \lesssim 0.4 \times E$ (MeV) at $N = 4$, which is reduced to $T_{\text{eff}} \lesssim 0.2 \times E$ (MeV) at $N = 100$. At large χ the dependence of T_{eff} on χ is independent of N. At $\chi \gtrsim 6$, where ω/E is practically zero, it can be well approximated with a simple relation
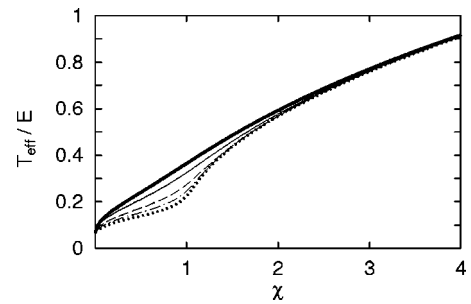

FIG. 4. Effective temperature as a function of χ. The thick solid, thin solid, dashed, dash-dotted, and dotted lines denote the results obtained for $N = 4$, 8, 24, 50, and 100, respectively.

$$T_{\text{eff}} = \frac{1}{2} E(\sqrt{\chi} - 0.1). \tag{41}$$

The relationship between the interaction and the effective temperature also demonstrates that the study of the effect of the ground-state correlations beyond the RPA on various nuclear characteristics as a function of interaction at zero temperature is essentially equivalent to the study of the ground-state correlations as a function of temperature at a fixed interaction. This observation is important for the study of thermodynamics of small many-body systems. Various phenomena related to the fluctuations of nuclear degrees of freedom can be in fact understood as thermal effects at an effective temperature [19,20]. The emergence of quantum liquid features with a typical particle distribution corresponding to some temperature in a finite isolated strongly interacting system was studied in the shell-model framework for nuclei [12,21], atoms [22] and model systems of fermions [23] or bosons [24]. This gives rise to a new point of view at the statistical description of thermal equilibrium in a small finite system where the interaction plays a role of the effective heat bath [25]. One of the relevant nuclear characteristics is the superconducting gap, which will be considered in the following section.

IV. A SCHEMATIC MODEL FOR SUPERCONDUCTING GAP AT FINITE TEMPERATURE

In this section we compare the solution of the modified BCS approximation, Eqs. (23) and (24), with that of the standard finite-temperature BCS equation [7]:

$$\Delta = \sum_j \Omega_j (1 - 2n_j) u_j v_j,$$

$$N = \sum_j \Omega_j \left[1 - \frac{E_j - E_F}{\epsilon_j} (1 - 2n_j) \right], \tag{42}$$

where the quasiparticle occupation numbers n_j are described by the Fermi-Dirac distribution $n_j = 1/[\exp(\epsilon_j/T) + 1]$ at a temperature T with $\epsilon_j = \sqrt{(E_j - E_F)^2 + \Delta^2}$, and $E_j = E_j^0 - G v_j^2$; G is the pairing constant.

The schematic model is studied in two versions, a two-level version (a), and a version with a realistic level scheme (b). The version (a) considers N particles distributed in two Ω_j-fold levels and interacting via a pairing force with the strength G. We choose the energies of the lower and upper levels to be -2.5 and 2.5 MeV, respectively, $G = 0.6$ MeV, and $\Omega = 5$ ($j = 9/2$). This gives the constraint for the particle number $N < 10$.

The gaps, normalized to their corresponding values at zero temperature, were obtained from Eqs. (23) and (42). The results for the version (a) are plotted as a function of T/T_c at several values of the particle number N in Fig. 5. The finite-temperature BCS gap (a dotted line) collapses at $T = T_c$, which is equal to 0.86, 1.02, 1.04, and 1 MeV at $N = 2$, 4, 6, and 8, respectively. For the ratio $c = T_c/\Delta(0)$ of the critical temperature to the BCS gap at $T = 0$ we found
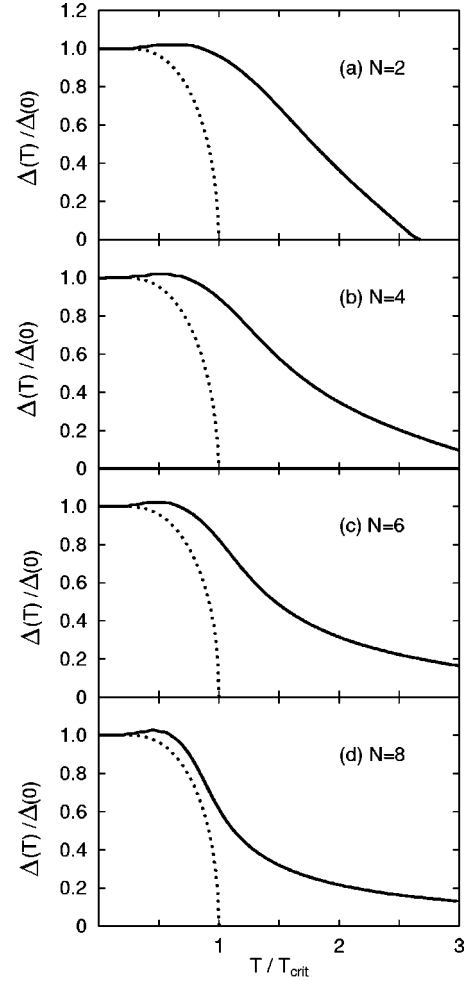

FIG. 5. Pairing gap (normalized to its value at zero temperature) as a function of temperature (normalized to T_c) for various particle numbers N. The modified gap $\bar{\Delta}(T)$ is plotted as a solid line, while the usual finite-temperature BCS gap $\Delta(T)$ is represented by a dotted line.

$c = 0.567$, 0.528, 0.507, and 0.529 at $N = 2$, 4, 6, and 8, respectively. These numbers are close to the value 0.567 predicted by the BCS theory for infinite systems [7].

The vanishing pairing gap in the finite-temperature BCS theory is a signature of the phase transition from the superconducting state to the normal one. In finite systems, such as nuclei, the ground state may differ significantly from the BCS one. This effect of the ground state correlations is seen in the behavior of the modified gap $\bar{\Delta}(T)$ from Eq. (23) as a function of temperature (solid line). For $N = 2$ the modified gap $\bar{\Delta}(T)$ still vanishes but at $\bar{T}_c \approx 2.2$ MeV that is much higher than $T_c = 0.86$ MeV in the finite-temperature BCS theory. As the particle number N increases, the value of $\bar{T}_c$ is also sharply increasing. At $N > 4$ the phase transition point is practically washed out. The modified gap $\bar{\Delta}(T)$ decreases with increasing T, but remains finite up to very high temperature $T > 6$ MeV. It also becomes closer to the finite-temperature BCS gap at $T < T_c$. These features are robust being observed in calculations using different sets of the parameters, namely, (i) $G = 0.6$ MeV, $E = 3$ MeV, and (ii) G
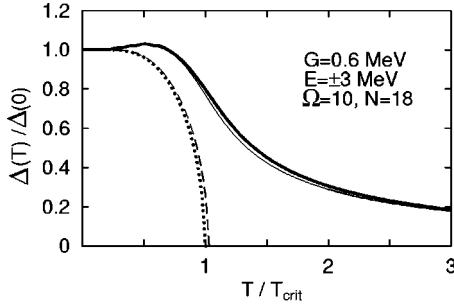
FIG. 6. Pairing gap (normalized to its value at zero temperature) as a function of temperature (normalized to T_c) obtained using the parameter set (i) (see text) at $N=18$. The notations for the modified gap $\bar{\Delta}(T)$ and the usual finite-temperature BCS gap $\Delta(T)$ are the same as in Fig. 5. The corresponding values of these gaps (but obtained without the correction) $-G\bar{v}_j^2$ and $-Gv_j^2$ are shown by thin solid and dashed lines, respectively.

$=0.8$ MeV, $E=6$ MeV, with the degeneracy $\Omega=10$ ($N<20$). The whole behavior is analogous to that found in the large scale shell model diagonalization [12].

We also notice that, in the self-consistent solutions, the shifts $-Gv_j^2$ (or $-G\bar{v}_j^2$) of the single-particle energy $E_j=E_j^0-Gv_j^2$ (or $\bar{E}_j=E_j^0-G\bar{v}_j^2$) give rather small contributions to the gap, especially at larger N as seen in Fig. 6, which is obtained for $N=18$ using the parameter set (i) above. The gap at $T=0$, with this shift taken into account, is 1.74 MeV, which is only 0.2% smaller than that obtained neglecting this shift. The value of T_c decreases only by about 3% compared to the value of 0.84 MeV when this shift is omitted. For simplicity, we ignore this small shift in the calculations below with the version (b) of this model since here the neutron number N_ν is 70.

In version (b), we consider a realistic nucleus ^{120}Sn, which has an open neutron shell. The single-particle energies for this nucleus are calculated with the Woods-Saxon potential. The neutron single-particle energies span a space of 24 levels between -33 and 17 MeV. Using a pairing strength $G=0.13$ MeV ($=15.6/A$ MeV), the BCS neutron pairing gap at $T=0$ is found to be $\Delta_\nu(0)=1.42$ MeV in agreement with the experimental value at the neutron number $N_\nu=70$ [26]. Shown in Fig. 7 is the neutron pairing gap for this nucleus as a function of temperature. The usual finite-temperature BCS gap $\Delta_\nu(T)$ decreases sharply with increas-
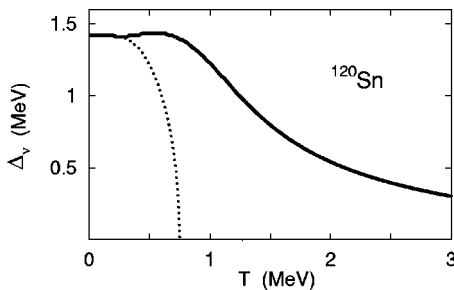

FIG. 7. Neutron pairing gap for ^{120}Sn as a function of temperature. The notations are the same as in Fig. 5.

ing T and vanishes at $T_c=0.75$ MeV. The modified gap $\bar{\Delta}_\nu(T)$ remains nearly constant up to $T=T_c$, then decreases with increasing T, but never disappears. At $T=1$ MeV, the modified gap is still about 87% of its value at $T=0$. Even at a temperature as high as $T=3$ MeV, $\bar{\Delta}_\nu(T)$ is still around 0.3 MeV. Therefore, the pairing gap cannot be neglected in the calculations of properties of hot open-shell nuclei at $T \leqslant 2$ MeV.

V. CONCLUSIONS

The central issue in the present work is that the ground-state correlations modify the quasiparticle and collective excitations. This effect is taken into account via the secondary canonical transformation from quasiparticle operators to modified quasiparticle ones. The coefficients of this transformation, $\sqrt{1-n_j}$ and $\sqrt{n_j}$, include the mean quasiparticle occupation numbers n_j that are different from zero because of the ground-state correlations. Based on this transformation a modified BCS+QRPA theory is developed. The derived set of modified equations must be solved self-consistently to define the modified pairing gap $\bar{\Delta}$, the Fermi energy $\bar{E}_F$, the energies of the modified phonons ω_{mod}, the phonon amplitudes $\bar{X}$ and $\bar{Y}$, as well as the quasiparticle occupation numbers n_j. The equation for n_j is derived making use of the ground-state correlation factor obtained within the renormalized QRPA. The major merit of this method is that it separates the collective solutions associated with only the creation of two quasiparticles from those arising from the scattering quasiparticles, retaining the effect of the latter in the excitation operator.

The formalism is illustrated with two well-known schematic models, which are frequently used in the literature, namely the two-level LMG model with the ph interaction and the model with a monopole pairing interaction. The analysis of the numerical results obtained in these models allows us to make the following conclusions.

(1) As compared to the renormalized RPA [1,5], the modified RPA indeed offers an improved treatment of the ground-state correlations beyond the RPA. The energy of the first excited state obtained with the modified RPA is closer to the exact energy than that of the renormalized RPA within the validity region of the RPA and around the point where the RPA collapses. This is a consequence of the fact that the "spurious" poles in the RPA equations are eliminated, and the significant part of the ground-state correlations is taken into account by the new canonical transformation so that the remaining correlations within the modified RPA are significantly weaker than that of the renormalized RPA near the RPA instability point and beyond it.

(2) The behavior of the quasiparticle occupation numbers as a function of interaction parameter can be well approximated by a Fermi-Dirac distribution at a given temperature. From here an effective temperature has been deduced as a function of the interaction parameter. This shows that the effect of ground-state correlations as a function of interaction at zero temperature can be equivalently treated as a function of effective temperature at fixed interaction giving a new

argument in favor of treating the interparticle interaction in a small closed system as an agent playing the role of an effective heat bath.

(3) Within the modified finite-temperature BCS approximation, the proposed method increases the temperature of the phase transition point from the superconducting state to the normal one in finite systems until smearing out completely this phase transition. This has been done without using any approximate particle number projection. The pairing gap in open-shell nuclei does not vanish even at high temperatures, therefore, it cannot be neglected in the study of hot nuclei at least up to $T \simeq 2$ MeV. These analyses show that the modified RPA is a method that properly accounts for an essential part of the ground state correlations and can resolve self-consistently and simultaneously a number of problems typical for the conventional approximations.

ACKNOWLEDGMENTS

APPENDIX: THE MODIFIED RPA

In the absence of the superconducting pairing and with the interaction limited only to the particle-hole (ph) channel, the modified QRPA equation is reduced to the modified RPA equation. Using the usual canonical Bogoliubov transformation between original particles and quasiparticles, one can see that the quasiparticle occupation numbers n_j (3) are related to the single-particle occupation numbers

$$f_j \equiv \langle \bar{0} | a_{jm}^{\dagger} a_{jm} | \bar{0} \rangle \tag{A1}$$

as $f_p = n_p$, $f_h = 1 - n_h$. Ignoring the ground-state correlations beyond the RPA leads to $n_p = n_h = 0$, which restores the usual Hartree-Fock (HF) single-particle occupation numbers $f_p^{HF} = 0$, $f_h^{HF} = 1$. Function $\bar{F}(\omega)$ in Eq. (21) takes the form

$$\bar{F}(\omega) = \frac{1}{2\lambda + 1} \sum_{ph} [q_{ph}^{(\lambda)}]^2 [\sqrt{(1-f_p)f_h}$$
$$- \sqrt{f_p(1-f_h)}]^2 \frac{(E_p - E_h)}{(E_p - E_h)^2 - \omega^2}, \tag{A2}$$

which should be compared with the corresponding expressions within the RPA

$$F(\omega) = \frac{1}{2\lambda + 1} \sum_{ph} [q_{ph}^{(\lambda)}]^2 \frac{(E_p - E_h)}{(E_p - E_h)^2 - \omega^2}, \tag{A3}$$

and within the renormalized RPA

$$F_{\text{ren}}(\omega) = \frac{1}{2\lambda + 1} \sum_{ph} [q_{ph}^{(\lambda)}]^2 \frac{(f_h - f_p)(E_p - E_h)}{(E_p - E_h)^2 - \omega^2}. \tag{A4}$$

The expression within the extended renormalized RPA coincides with Eq. (A4) in this case [6]. The modified phonon amplitudes $\bar{X}_{ph}^{(\lambda i)}$ and $\bar{Y}_{ph}^{(\lambda i)}$ have the form

$$\bar{X}_{ph}^{(\lambda i)} = \frac{q_{ph}^{(\lambda)} [\sqrt{(1-f_p)f_h} - \sqrt{f_p(1-f_h)}]}{E_p - E_h - \omega_{\lambda i}} \bar{M}_{\lambda i}, \tag{A5}$$

$$\bar{Y}_{ph}^{(\lambda i)} = \frac{q_{ph}^{(\lambda)} [\sqrt{(1-f_p)f_h} - \sqrt{f_p(1-f_h)}]}{E_p - E_h + \omega_{\lambda i}} \bar{M}_{\lambda i},$$

with

$$\bar{M}_{\lambda i} = \left\{ \sum_{ph} [q_{ph}^{(\lambda)}]^2 [\sqrt{(1-f_p)f_h} \right.$$
$$- \sqrt{f_p(1-f_h)}]^2 \left[\frac{1}{(E_p - E_h - \omega_{\lambda i})^2} \right.$$
$$\left. \left. - \frac{1}{(E_p - E_h + \omega_{\lambda i})^2} \right] \right\}^{-1/2}. \tag{A6}$$

The ground-state correlation factor $\bar{D}_{ph}^A \equiv f_h - f_p$ satisfies the equation

$$\bar{D}_{ph} = 1 - \sum_{\lambda i} \left\{ \sum_{p'} \bar{D}_{p'h} [\bar{Y}_{p'h}^{(\lambda i)} \sqrt{(1-f_{p'})f_h} \right.$$
$$+ \bar{X}_{p'h}^{(\lambda i)} \sqrt{f_{p'}(1-f_h)}]^2$$
$$\left. + \sum_{h'} \bar{D}_{ph'}^A [\bar{Y}_{ph'}^{(\lambda i)} \sqrt{(1-f_p)f_{h'}} + \bar{X}_{ph'}^{(\lambda i)} \sqrt{f_p(1-f_{h'})}]^2 \right\}. \tag{A7}$$

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