

Self-consistent quasiparticle random phase approximation for the description of superfluid Fermi systems

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Self-consistent quasiparticle random phase approximation (SCQRPA) is for the first time applied to a more level pairing case. Various filling situations and values for the coupling constant are considered. Very encouraging results in comparison with the exact solution of the model are obtained. The nature of the low-lying mode in SCQRPA is identified. The strong reduction of the number fluctuation in SCQRPA vs BCS is pointed out. The transition from superfluidity to the normal fluid case is carefully investigated.

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I. INTRODUCTION

One of the most spectacular quantum phenomena is the transition to the superconducting or superfluid state in interacting Fermi systems. This happens, e.g., in metals, liquid ³He, neutron stars, in finite nuclei, and it is actively searched for in systems of magnetically trapped atomic fermions. In most of these systems the canonical mean field approach of Bardeen, Cooper, and Schrieffer (BCS) with a couple of adjustable parameters works astonishingly well. However, in recent years there have been increasing attempts to describe the pairing phenomenon on completely microscopic grounds. To our knowledge, these attempts have mostly been carried out for nuclear systems. This stems, on the one hand, from the fact that phenomenological *NN* forces are on the market, which very well describe the nucleon-nucleon phase shifts in all channels and in a wide range of energies. On the other hand, the physics of neutron stars makes quantitative predictions of the pairing phenomenon in neutron matter indispensable, since superfluidity of neutron stars manifests itself only quite indirectly through, e.g., the phenomenon of neutron star glitches. The microscopic approaches to pairing, starting from a bare two-body interaction, are not very numerous. The simplest one is based on the BCS theory, using, however, in the gap equation the bare force and for the single-particle dispersion the one given by the Brückner theory. In this way one obtains, e.g., gap values in the ¹S₀ channel for neutron-neutron pairing which in infinite matter, as a function of the Fermi momentum k_F , have a typical bell-shaped form roughly dropping to zero around $k_F = 1.3 \text{ fm}^{-1}$ and culminating at $k_F = 0.8 \text{ fm}^{-1}$ to values of $\Delta = 2.5\text{--}3.0 \text{ MeV}$ for neutron and nuclear matter, respectively. This rather elementary approach has been extended in the past in various ways. The most ambitious procedure is probably the so-called correlated basis function approach [1]. However, more recently

self-consistent *T*-matrix approaches and extended Brückner theories with rearrangement terms have achieved a remarkable degree of sophistication [2]. The screening of the interaction was treated to lowest order in the density, resuming the random phase approximation (RPA) bubbles, in introducing self-consistent Landau parameters [3]. The outcome of all these investigations inevitably leads to a quite substantial reduction of pairing in not only neutron matter, but also in symmetric nuclear matter. The global reduction generally attains important values and often reaches factors close to 3. Such small values of the gap in infinite matter, however, pose a problem. Employing the local density approximation (LDA) to estimate from the infinite matter results the gap in finite nuclei [4], one finds with the simplified approach described above using the bare *NN* force, quite reasonable gap values for finite nuclei. Interestingly, in the gap equation, quite similar results are obtained with the Gogny D1S force [5] using the same procedure. However, with such strongly reduced gaps from the more sophisticated approaches mentioned above, one obtains much too small gaps in finite nuclei. Of course, this reasoning may be completely erroneous and the situation in finite nuclei may be very different from infinite matter. Nevertheless we find the above argumentation intriguing. On the other hand, we know that pairing is an extraordinarily subtle process, and employing theories that are in one or the other way uncontrolled may turn out to be a hazardous enterprise. In such a situation it is probably wise to investigate the problem from different angles using a variety of approaches.

In the past we have made very positive experience with an extension of RPA theory that we called self-consistent RPA (SCRPA) [6–8]. For instance, in a recent work this theory has been applied to the exactly solvable many-level pairing model in the precritical regime and very good agreement with the exact results for ground-state energy and the low-lying part of the spectrum was found [7,8]. This success has encouraged us to develop the SCRPA, formalism also for the fully developed superfluid regime. This is a not completely trivial extension of the SCRPA and we here apply it for the first time to the two-level pairing model. As we will see, the theory also gives very promising results in the superfluid phase. Since the self-consistent quasiparticle RPA

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(SCQRPA), as in general SCRPA theory, can be derived from a variational principle, which turns out to be very close to a Raleigh-Ritz variational theory, we believe that SCQRPA is a nonperturbative approach going in a certain systematic way beyond the mean field BCS theory, including, in a self-consistent way, correlations and quantum fluctuations. We believe that this microscopic approach can ultimately be used to calculate pairing properties of realistic Fermi systems starting from the bare force.

It should be mentioned that extensions of the RPA theory, based on the equation of motion (EOM) method, have by now a quite long history. They, to a great deal, have been developed in nuclear physics. It started out with the work of Hara who included the ground-state correlation in the Fermion occupation numbers [9]. More systematic was the subsequent work by Rowe and co-workers (see the review by Rowe [10]). The same theory was developed using the Green's function method by one of the present authors [6]. Independently, the method was also proposed by Röpke and co-workers using a graphical construction [11]. These authors named their method cluster-Hartree-Fock and it is equivalent to SCRPA. The latter approach has recently been further developed by Dukelsky and Schuck in a series of papers [7,8,12–15]. However, also other authors contributed actively to the subject [16–18]. For instance, in an early work Karadjov *et al.* [17] attempted, in a simplified version of SCRPA, the so-called renormalized RPA (*r*-RPA) to calculate collective nuclear states in a more fundamental way. In the same spirit, interesting results have been obtained for metallic clusters by Catara *et al.* [18]. A number of remarkable results have been obtained using SCRPA in nontrivial models where comparison with exact solutions was possible [8,12]. As already mentioned, for the exactly solvable many-level pairing model of Richardson [19], SCRPA provides very accurate results for the ground state and the low-lying part of the spectrum [7,8].

In detail our paper is organized as follows: in Sec. II the two-level pairing model is introduced; in Sec. III the SCQRPA formalism is presented; in Sec. IV numerical results are given and detailed discussions are presented. Comparison with other recent works is made in Sec. V; in Sec. VI the question of the second constraint on the particle number variance is invoked and applied to the seniority model. In Sec. VII, we will summarize the results and draw some conclusions. Finally, some useful mathematical relations and a second method for the calculation of occupation numbers are given in the appendixes.

II. THE MODEL

The two-level pairing model is an exactly solvable model extensively employed in nuclear physics to test many-body approximations. It was first used to test the standard particle-particle RPA (*pp*-RPA) [20] and its ability to describe ground-state correlations and vibrations in the normal phase as well as in the superfluid phase. The model is composed of two levels with equal degeneracy $2\Omega = 2J + 1$ (J is the spin of each level) and a single-particle energy splitting ϵ . The pairing Hamiltonian in this model space is

$$H = \frac{\epsilon}{2} \sum_j j \hat{N}_j - g \Omega \sum_{jj'} A_j^\dagger A_{j'}, \quad j = \pm 1, \quad (1)$$

where j takes the value 1 for the upper level and -1 for the lower level. \hat{N}_j and A_j^\dagger are the number and monopole pair operators of the level j , respectively,

$$A_j^\dagger = \frac{1}{\sqrt{\Omega}} \sum_{m=1}^{\Omega} a_{jm}^\dagger a_{j\bar{m}}^\dagger \quad (2)$$

and

$$\hat{N}_j = \sum_{m=1}^{\Omega} (a_{jm}^\dagger a_{jm} + a_{j\bar{m}}^\dagger a_{j\bar{m}}). \quad (3)$$

where a_{jm}^\dagger creates a particle in the level j with spin projection m and $a_{j\bar{m}} = (-1)^{J-m} a_{j-m}$. The operators obey the following commutations relations:

$$\begin{aligned} [A_j, A_{j'}^\dagger] &= \delta_{jj'} \left(1 - \frac{\hat{N}_j}{\Omega} \right), \\ [\hat{N}_j, A_{j'}^\dagger] &= \delta_{jj'} 2A_{j'}^\dagger, \\ [\hat{N}_j, A_{j'}] &= -\delta_{jj'} 2A_{j'}; \end{aligned} \quad (4)$$

thus, they define an SU(2) algebra for each level and the two level model satisfies an SU(2) \times SU(2) algebra.

For a system not at half-filling, the normalized states in the Hilbert subspace of the monopole pairs are

$$\begin{aligned} |n\rangle &= \frac{\Omega^{\tilde{\Omega}/2}}{\Omega!} \sqrt{\frac{(\Omega - \tilde{\Omega} + n)!(\Omega - n)!}{n!(\tilde{\Omega} - n)!}} (A_1^\dagger)^n (A_{-1}^\dagger)^{\tilde{\Omega} - n} |0\rangle, \\ &0 \leq n \leq \tilde{\Omega} \end{aligned} \quad (5)$$

where $\tilde{\Omega} = \Omega$ leads to the half-filling case, i.e., the lower level is filled for $g = 0$. The matrix Hamiltonian is tridiagonal of dimension $\tilde{\Omega} + 1$, with matrix elements

$$\begin{aligned} h_{n,n} &= \langle n | H | n \rangle \\ &= \epsilon(2n - \tilde{\Omega}) - g(2n\tilde{\Omega} - 2n^2 + \tilde{\Omega}\Omega - \tilde{\Omega}^2 + \tilde{\Omega}), \\ h_{n-1,n} &= \langle n-1 | H | n \rangle \\ &= -g \sqrt{n[\Omega - (n-1)](\Omega - \tilde{\Omega} + n)(\tilde{\Omega} - n + 1)}, \end{aligned} \quad (6)$$

where n is the number of pairs in the upper level and the number of particle is given by $N = 2\tilde{\Omega}$.

III. SELF-CONSISTENT QRPA

In a recent work [8] the SCRPA has been applied with very good success to the picket fence model in the nonsuperfluid phase. The extension to the superfluid phase is slightly

delicate and we here limit ourselves to the two-level model; however, considering arbitrary degeneracies and fillings of the levels. The objective in this section is to establish the equations for SCQRPA. A first application of SCQRPA has been performed in Ref. [14] for the case of the seniority model (one-level pairing model). We will later come back to this model. Here we want to consider the two-level pairing model with arbitrary filling and coupling strength in the SCQRPA approach, which already more or less shows the full complexity of more realistic many-level problems. As a first step, we have to transform the constrained Hamiltonian

$$H' = H - \mu \hat{N}, \quad (8)$$

where \hat{N} is the full particle number operator, to quasiparticle operators

$$\begin{pmatrix} \alpha_{jm}^\dagger \\ \alpha_{j\bar{m}} \end{pmatrix} = \begin{pmatrix} u_j & -v_j \\ v_j & u_j \end{pmatrix} \begin{pmatrix} a_{jm}^\dagger \\ a_{j\bar{m}} \end{pmatrix}, \quad (9)$$

$$\begin{pmatrix} a_{jm}^\dagger \\ a_{j\bar{m}} \end{pmatrix} = \begin{pmatrix} u_j & v_j \\ -v_j & u_j \end{pmatrix} \begin{pmatrix} \alpha_{jm}^\dagger \\ \alpha_{j\bar{m}} \end{pmatrix} \quad (10)$$

with

$$u_j^2 + v_j^2 = 1, \quad j = \pm 1. \quad (11)$$

We define new quasispin operators as

$$P_j^\dagger = \frac{1}{\sqrt{\Omega}} \sum_{m>0} \alpha_{jm}^\dagger \alpha_{j\bar{m}}^\dagger, \quad P_j = (P_j^\dagger)^\dagger \quad (12)$$

and the quasiparticle number operator in the level j is given by

$$\hat{N}_{q,j} = \sum_{m>0} (\alpha_{jm}^\dagger \alpha_{jm} + \alpha_{j\bar{m}}^\dagger \alpha_{j\bar{m}}). \quad (13)$$

The quasiparticle operators obey the following commutations relations:

$$\begin{aligned} [P_j, P_{j'}^\dagger] &= \delta_{jj'} \left(1 - \frac{\hat{N}_{q,j}}{\Omega} \right), \\ [\hat{N}_{q,j}, P_{j'}^\dagger] &= \delta_{jj'} 2P_{j'}^\dagger, \\ [\hat{N}_{q,j}, P_{j'}] &= -\delta_{jj'} 2P_{j'}. \end{aligned} \quad (14)$$

Then the Hamiltonian in the quasiparticle basis can be written as

$$H' = H'_{00} + H'_{11} + H'_{20} + H'_{22} + H'_{31} + H'_{40} + H'_{11-11}, \quad (15)$$

where for the sake of self-containedness of the paper we give the coefficients, in spite of the fact that they can be found in the literature [20]:

$$H'_{00} = h_0, \quad (16)$$

$$H'_{11} = h_1 \hat{N}_{q,1} + h_{-1} \hat{N}_{q,-1}, \quad (17)$$

$$H'_{20} = h_2 (P_1^\dagger + P_1) + h_{-2} (P_{-1}^\dagger + P_{-1}), \quad (18)$$

$$H'_{22} = h_3 P_1^\dagger P_1 + h_{-3} P_{-1}^\dagger P_{-1} + h_4 (P_1^\dagger P_{-1} + P_{-1}^\dagger P_1), \quad (19)$$

$$H'_{31} = h_5 (P_1^\dagger \hat{N}_{q,1} + \hat{N}_{q,1} P_1) + h_{-5} (P_{-1}^\dagger \hat{N}_{q,-1} + \hat{N}_{q,-1} P_{-1}) \quad (20)$$

$$\begin{aligned} &+ h_6 (P_1^\dagger \hat{N}_{q,-1} + \hat{N}_{q,-1} P_1) \\ &+ h_{-6} (P_{-1}^\dagger \hat{N}_{q,1} + \hat{N}_{q,1} P_{-1}), \end{aligned} \quad (21)$$

$$\begin{aligned} H'_{40} &= h_7 (P_1^\dagger P_1^\dagger + P_1 P_1) + h_{-7} (P_{-1}^\dagger P_{-1}^\dagger + P_{-1} P_{-1}) \\ &+ h_8 (P_1^\dagger P_{-1}^\dagger + P_{-1} P_1), \end{aligned} \quad (22)$$

$$H'_{11-11} = h_9 \hat{N}_{q,1}^2 + h_{-9} \hat{N}_{q,-1}^2 + h_{10} \hat{N}_{q,1} \hat{N}_{q,-1} \quad (23)$$

and

$$\begin{aligned} h_0 &= (\epsilon - 2\mu) \Omega v_1^2 - g \Omega (\Omega u_1^2 v_1^2 + v_1^4) - (\epsilon + 2\mu) \Omega v_{-1}^2 \\ &- g \Omega (\Omega u_{-1}^2 v_{-1}^2 + v_{-1}^4) - 2g \Omega^2 u_1 v_1 u_{-1} v_{-1}, \end{aligned}$$

$$h_1 = \left(\frac{\epsilon}{2} - \mu \right) (u_1^2 - v_1^2) + g \Omega \left(2u_1^2 v_1^2 + \frac{v_1^4}{\Omega} \right)$$

$$+ 2g \Omega^2 u_1 v_1 u_{-1} v_{-1},$$

$$h_{-1} = - \left(\frac{\epsilon}{2} + \mu \right) (u_{-1}^2 - v_{-1}^2) + g \Omega \left(2u_{-1}^2 v_{-1}^2 + \frac{v_{-1}^4}{\Omega} \right)$$

$$+ 2g \Omega^2 u_{-1} v_{-1} u_1 v_1,$$

$$h_2 = \sqrt{\Omega} u_1 v_1 (\epsilon - 2\mu) - g \Omega \left\{ u_1 v_1 (u_1^2 - v_1^2) \sqrt{\Omega} + \frac{2u_1 v_1^3}{\sqrt{\Omega}} \right\}$$

$$- g \Omega \sqrt{\Omega} u_{-1} v_{-1} (u_1^2 - v_1^2),$$

$$\begin{aligned} h_{-2} &= -\sqrt{\Omega} u_{-1} v_{-1} (\epsilon + 2\mu) - g \Omega \left\{ u_{-1} v_{-1} (u_{-1}^2 \right. \\ &\left. - v_{-1}^2) \sqrt{\Omega} + \frac{2u_{-1} v_{-1}^3}{\sqrt{\Omega}} \right\} - g \Omega \sqrt{\Omega} u_1 v_1 (u_{-1}^2 - v_{-1}^2), \end{aligned}$$

$$h_3 = -g \Omega (u_1^4 + v_1^4),$$

$$h_4 = -g \Omega (u_1^2 u_{-1}^2 + v_1^2 v_{-1}^2),$$

$$h_5 = g \sqrt{\Omega} u_1 v_1 (u_1^2 - v_1^2),$$

$$h_6 = g \sqrt{\Omega} u_{-1} v_{-1} (u_{-1}^2 - v_{-1}^2),$$

$$h_7 = g \Omega u_1^2 v_1^2,$$

$$h_8 = g \Omega (u_1^2 v_{-1}^2 + u_{-1}^2 v_1^2),$$

$$h_9 = -g\Omega u_1^2 v_1^2,$$

$$h_{10} = -2g\Omega u_1 v_1 u_{-1} v_{-1}, \quad (24)$$

and $h_{-n} = h_n (1 \leftrightarrow -1)$ for $n=3,5,6,7,9$. Also, in this basis the full particle number operator is given by

$$\hat{N} = \sum_j \hat{N}_j, \quad j = \pm 1 \quad (25)$$

where

$$\hat{N}_j = (u_j^2 - v_j^2) \hat{N}_{q,j} + 2\Omega v_j^2 + 2u_j v_j \sqrt{\Omega} (P_j^\dagger + P_j). \quad (26)$$

The RPA excited states are, as usual, obtained as

$$|\nu\rangle = Q_\nu^\dagger |\text{RPA}\rangle, \quad (27)$$

where $|\text{RPA}\rangle$ is the correlated RPA ground-state defined via the vacuum condition

$$Q_\nu |\text{RPA}\rangle = 0. \quad (28)$$

In terms of the generators of the Hamiltonian $\hat{N}_{q,j}$, P_j^\dagger , and P_j , for the most general QRPA excitation operator, which can be viewed as a Bogoliubov transformation of fermion pair operators [35] we can write down the following expression:

$$Q_\nu^\dagger = \sum_{j=\pm 1} X_{j,\nu} \bar{P}_j^\dagger - Y_{j,\nu} \bar{P}_j, \quad \nu = 1, 2 \quad (29)$$

where we introduced the following notation:

$$\bar{P}_j = \frac{P_j}{\sqrt{1 - \frac{\langle \hat{N}_{q,j} \rangle}{\Omega}}}, \quad j = \pm 1 \quad (30)$$

guaranteeing that the RPA excited state (27) is normalized, i.e., $\langle \nu | \nu' \rangle = \langle \text{RPA} | [Q_\nu, Q_{\nu'}^\dagger] | \text{RPA} \rangle = \delta_{\nu,\nu'}$. The RPA amplitudes $X_{j,\nu}$ and $Y_{j,\nu}$ in Eq. (29) shall obey the following orthogonality relations:

$$\sum_{j=\pm 1} X_{j,\nu}^2 - Y_{j,\nu}^2 = 1, \quad \nu = 1, 2,$$

$$X_{-1,1} X_{-1,2} + X_{1,1} X_{1,2} - Y_{-1,1} Y_{-1,2} - Y_{1,1} Y_{1,2} = 0,$$

$$X_{1,2} Y_{1,1} + X_{-1,2} Y_{-1,1} - X_{1,1} Y_{1,2} - X_{-1,1} Y_{-1,2} = 0, \quad (31)$$

and the closure relations

$$\sum_{\nu=1,2} X_{j,\nu}^2 - Y_{j,\nu}^2 = 1, \quad j = \pm 1,$$

$$X_{-1,1} X_{1,1} + X_{-1,2} X_{1,2} - Y_{-1,1} Y_{1,1} - Y_{-1,2} Y_{1,2} = 0,$$

$$X_{1,1} Y_{-1,1} + X_{1,2} Y_{-1,2} - X_{-1,1} Y_{1,1} - X_{-1,2} Y_{1,2} = 0 \quad (32)$$

with which one can invert relation (29)

$$\begin{pmatrix} \bar{P}_1 \\ \bar{P}_{-1} \\ \bar{P}_1^\dagger \\ \bar{P}_{-1}^\dagger \end{pmatrix} = \begin{pmatrix} X_{1,1} & X_{1,2} & Y_{1,1} & Y_{1,2} \\ X_{-1,1} & X_{-1,2} & Y_{-1,1} & Y_{-1,2} \\ Y_{1,1} & Y_{1,2} & X_{1,1} & X_{1,2} \\ Y_{-1,1} & Y_{-1,2} & X_{-1,1} & X_{-1,2} \end{pmatrix} \begin{pmatrix} Q_1 \\ Q_2 \\ Q_1^\dagger \\ Q_2^\dagger \end{pmatrix}. \quad (33)$$

In analogy to Baranger [21] and Weigel and Winter [22] we obtain the SCQRPA equations in minimizing the following mean excitation energy:

$$\Omega_\nu = \frac{\langle [Q_\nu, [H', Q_\nu^\dagger]] \rangle}{\langle [Q_\nu, Q_\nu^\dagger] \rangle} \quad (34)$$

with respect to the RPA amplitudes $X_{j,\nu}$ and $Y_{j,\nu}$. The minimization leads straightforwardly to the following eigenvalue problem:

$$\begin{pmatrix} A_{1,1} & A_{1,2} & B_{1,1} & B_{1,2} \\ A_{2,1} & A_{2,2} & B_{2,1} & B_{2,2} \\ -B_{1,1} & -B_{1,2} & -A_{1,1} & -A_{1,2} \\ -B_{2,1} & -B_{2,2} & -A_{2,1} & -A_{2,2} \end{pmatrix} \begin{pmatrix} X_{1,\nu} \\ X_{-1,\nu} \\ Y_{1,\nu} \\ Y_{-1,\nu} \end{pmatrix} = \Omega_\nu \begin{pmatrix} X_{1,\nu} \\ X_{-1,\nu} \\ Y_{1,\nu} \\ Y_{-1,\nu} \end{pmatrix}, \quad (35)$$

where

$$A_{1,1} = \langle [\bar{P}_1, [H', \bar{P}_1^\dagger]] \rangle, \quad A_{1,2} = \langle [\bar{P}_1, [H', \bar{P}_{-1}^\dagger]] \rangle,$$

$$A_{2,1} = \langle [\bar{P}_{-1}, [H', \bar{P}_1^\dagger]] \rangle, \quad A_{2,2} = \langle [\bar{P}_{-1}, [H', \bar{P}_{-1}^\dagger]] \rangle,$$

$$B_{1,1} = -\langle [\bar{P}_1, [H', \bar{P}_1]] \rangle, \quad B_{1,2} = -\langle [\bar{P}_1, [H', \bar{P}_{-1}]] \rangle,$$

$$B_{2,1} = -\langle [\bar{P}_{-1}, [H', \bar{P}_1]] \rangle, \quad B_{2,2} = -\langle [\bar{P}_{-1}, [H', \bar{P}_{-1}]] \rangle, \quad (36)$$

and $\langle \dots \rangle$ stands for the expectation values in the RPA vacuum defined by Eq. (28). Explicitly, the RPA matrix elements are given by

$$\begin{aligned}
 A_{1,1} &= 2h_1 + h_3 \left\{ -\frac{2}{\Omega} \frac{\langle P_1^\dagger P_1 \rangle}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} + \frac{1 - \frac{2\langle \hat{N}_{q,1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,1}^2 \rangle}{\Omega^2}}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \right\} \\
 &\quad - \frac{2}{\Omega} \frac{1}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \{h_4 \langle P_{-1}^\dagger P_1 \rangle + 2h_7 \langle P_1 P_1 \rangle \\
 &\quad + h_8 \langle P_{-1} P_1 \rangle\} + 4h_9 \left\{ \frac{\langle P_1^\dagger P_1 \rangle + \langle P_1 P_1^\dagger \rangle}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \right. \\
 &\quad \left. + \frac{\langle \hat{N}_{q,1} \rangle - \frac{\langle \hat{N}_{q,1}^2 \rangle}{\Omega}}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \right\} + 2h_{10} \frac{\langle \hat{N}_{q,-1} \rangle - \frac{\langle \hat{N}_{q,1} \hat{N}_{q,-1} \rangle}{\Omega}}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}}, \\
 A_{1,2} &= A_{2,1} = h_4 \frac{1 - \frac{\langle \hat{N}_{q,1} \rangle + \langle \hat{N}_{q,-1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,1} \hat{N}_{q,-1} \rangle}{\Omega^2}}{\sqrt{\left(1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}\right) \left(1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}\right)}} \\
 &\quad + 4h_{10} \frac{\langle P_1 P_{-1}^\dagger \rangle}{\sqrt{\left(1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}\right) \left(1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}\right)}}, \\
 A_{2,2} &= 2h_{-1} + h_{-3} \left\{ -\frac{2}{\Omega} \frac{\langle P_{-1}^\dagger P_{-1} \rangle}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \right. \\
 &\quad \left. + \frac{1 - \frac{2\langle \hat{N}_{q,-1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,-1}^2 \rangle}{\Omega^2}}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \right\} \\
 &\quad - \frac{2}{\Omega} \frac{1}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \{h_4 \langle P_1^\dagger P_{-1} \rangle + 2h_{-7} \langle P_{-1} P_{-1} \rangle \\
 &\quad + h_8 \langle P_1 P_{-1} \rangle\} + 4h_{-9} \left\{ \frac{\langle P_{-1}^\dagger P_{-1} \rangle + \langle P_{-1} P_{-1}^\dagger \rangle}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \right. \\
 &\quad \left. + \frac{1 - \frac{2\langle \hat{N}_{q,-1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,-1}^2 \rangle}{\Omega^2}}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \right\}, \\
 B_{1,1} &= -\frac{2}{\Omega} \frac{1}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \{h_3 \langle P_1 P_1 \rangle + h_4 \langle P_{-1} P_1 \rangle \\
 &\quad + h_8 \langle P_{-1}^\dagger P_1 \rangle\} + 8h_9 \frac{\langle P_1 P_1 \rangle}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \\
 &\quad + 2h_7 \left\{ -\frac{1}{\Omega} \frac{\langle P_1^\dagger P_1 \rangle + \langle P_1 P_1^\dagger \rangle}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \right. \\
 &\quad \left. + \frac{1 - \frac{2\langle \hat{N}_{q,1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,1}^2 \rangle}{\Omega^2}}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \right\}, \\
 B_{1,2} &= B_{2,1} = h_8 \frac{1 - \frac{\langle \hat{N}_{q,1} \rangle + \langle \hat{N}_{q,-1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,1} \hat{N}_{q,-1} \rangle}{\Omega^2}}{\sqrt{\left(1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}\right) \left(1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}\right)}} \\
 &\quad + 4h_{10} \frac{\langle P_{-1} P_1 \rangle}{\sqrt{\left(1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}\right) \left(1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}\right)}}, \\
 B_{2,2} &= -\frac{2}{\Omega} \frac{1}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \{h_{-3} \langle P_{-1} P_{-1} \rangle + h_4 \langle P_1 P_{-1} \rangle \\
 &\quad + h_8 \langle P_1^\dagger P_{-1} \rangle\} + 8h_{-9} \frac{\langle P_{-1} P_{-1} \rangle}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \\
 &\quad + 2h_{-7} \left\{ -\frac{1}{\Omega} \frac{\langle P_{-1}^\dagger P_{-1} \rangle + \langle P_{-1} P_{-1}^\dagger \rangle}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \right. \\
 &\quad \left. + \frac{1 - \frac{2\langle \hat{N}_{q,-1} \rangle}{\Omega} + \frac{\langle \hat{N}_{q,-1}^2 \rangle}{\Omega^2}}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \right\}. \tag{37}
 \end{aligned}$$

Using Eq. (33) and condition (28), the expectation values of type $\langle P_j^\dagger P_{j'} \rangle$, $\langle P_j P_{j'}^\dagger \rangle$, $\langle P_j^\dagger P_{j'}^\dagger \rangle$, and $\langle P_j P_{j'} \rangle$ are readily expressed by the RPA amplitudes $X_{j,\nu}$ and $Y_{j,\nu}$. For example, one obtains

$$\begin{aligned} \langle P_j P_{j'} \rangle &= \langle P_j^\dagger P_{j'}^\dagger \rangle \\ &= (X_{j,1} Y_{j',1} + X_{j,2} Y_{j',2}) \\ &\quad \times \sqrt{\left(1 - \frac{\langle \hat{N}_{q,j} \rangle}{\Omega}\right) \left(1 - \frac{\langle \hat{N}_{q,j'} \rangle}{\Omega}\right)}, \end{aligned} \quad (38)$$

and similarly for the other expectation values.

Before we discuss how to express the expectation values $\langle \hat{N}_{q,j} \rangle$, $\langle \hat{N}_{q,j}^2 \rangle$, and $\langle \hat{N}_{q,j} \hat{N}_{q,j'} \rangle$ as functions of the amplitudes $X_{j,\nu}$ and $Y_{j,\nu}$, we want to give the equations for the determination of the Bogoliubov amplitudes u_j , v_j of Eqs. (9) and (10). As usual they are determined from the minimization of the ground-state energy [13,23]

$$\frac{\partial \langle H' \rangle}{\partial u_j} + \frac{\partial \langle H' \rangle}{\partial v_j} \frac{\partial v_j}{\partial u_j} \equiv \langle [H', \bar{P}_j^\dagger] \rangle = 0, \quad j = \pm 1, \quad (39)$$

where H' is given by Eq. (15). It is worth noticing that the second of relation (39) is equivalent to $\langle [H', Q_\nu^\dagger] \rangle = \langle [H', Q_\nu] \rangle = 0$ with $\nu = 1, 2$. This relation is very suggestive, since, with Eq. (33), it holds true in the exact case. When Eq. (39) is evaluated with a BCS ground-state then this leads to the usual BCS equations. However, here we use the correlated RPA ground state and then the mean field equations couple back to the RPA amplitudes $X_{j,\nu}$ and $Y_{j,\nu}$. Explicitly these equations lead to

$$2\xi_j u_j v_j + \Delta_j (v_j^2 - u_j^2) = 0, \quad j = \pm 1, \quad (40)$$

which together with Eq. (11) can be written as

$$\begin{pmatrix} \xi_j & \Delta_j \\ \Delta_j & -\xi_j \end{pmatrix} \begin{pmatrix} u_j \\ v_j \end{pmatrix} = E_j \begin{pmatrix} u_j \\ v_j \end{pmatrix}, \quad E_j = \sqrt{\xi_j^2 + \Delta_j^2} \quad (41)$$

with the standard solution

$$\begin{aligned} u_j^2 &= \frac{1}{2} \left(1 + \frac{\xi_j}{\sqrt{\xi_j^2 + \Delta_j^2}} \right), \\ v_j^2 &= \frac{1}{2} \left(1 - \frac{\xi_j}{\sqrt{\xi_j^2 + \Delta_j^2}} \right) \end{aligned} \quad (42)$$

from where follows the gap equation

$$\Delta_i = \sum_j \tilde{g}_{ij} u_j v_j = \frac{1}{2} \sum_j \tilde{g}_{ij} \frac{\Delta_j}{\sqrt{\xi_j^2 + \Delta_j^2}}, \quad i, j = \pm 1, \quad (43)$$

where the renormalized single-particle energies are

$$\begin{aligned} \xi_j &= \left(j \frac{\epsilon}{2} - g v_j^2 \right) + \frac{g}{1 - \frac{\langle \hat{N}_{q,j} \rangle}{\Omega}} (u_{-j}^2 - v_{-j}^2) \langle \langle P_j^\dagger P_{-j}^\dagger \rangle \rangle \\ &\quad + \langle \langle P_j^\dagger P_{-j} \rangle \rangle - \mu, \quad j = \pm 1 \end{aligned} \quad (44)$$

and the renormalized interaction is given by

$$\tilde{g} = \begin{pmatrix} \tilde{g}_{1,1} & \tilde{g}_{1,-1} \\ \tilde{g}_{-1,1} & \tilde{g}_{-1,-1} \end{pmatrix}, \quad (45)$$

with

$$\begin{aligned} \tilde{g}_{1,1} &= g\Omega - \frac{g}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}} \left\{ 2(\langle \langle P_1^\dagger P_1^\dagger \rangle \rangle + \langle \langle P_1^\dagger P_1 \rangle \rangle) + \langle \hat{N}_{q,1} \rangle \right. \\ &\quad \left. - \frac{\langle \hat{N}_{q,1}^2 \rangle}{\Omega} \right\}, \\ \tilde{g}_{1,-1} &= g\Omega - g \frac{\langle \hat{N}_{q,-1} \rangle - \frac{\langle \hat{N}_{q,1} \hat{N}_{q,-1} \rangle}{\Omega}}{1 - \frac{\langle \hat{N}_{q,1} \rangle}{\Omega}}, \\ \tilde{g}_{-1,1} &= g\Omega - g \frac{\langle \hat{N}_{q,1} \rangle - \frac{\langle \hat{N}_{q,1} \hat{N}_{q,-1} \rangle}{\Omega}}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}}, \\ \tilde{g}_{-1,-1} &= g\Omega - \frac{g}{1 - \frac{\langle \hat{N}_{q,-1} \rangle}{\Omega}} \left\{ 2(\langle \langle P_{-1}^\dagger P_{-1}^\dagger \rangle \rangle + \langle \langle P_{-1}^\dagger P_{-1} \rangle \rangle) \right. \\ &\quad \left. + \langle \hat{N}_{q,-1} \rangle - \frac{\langle \hat{N}_{q,-1}^2 \rangle}{\Omega} \right\}. \end{aligned} \quad (46)$$

We see that the mean field equations have exactly the same mathematical structure as in the BCS case, however, with renormalized vertices and single-particle energies involving the RPA amplitudes. We, therefore, explicitly see that the mean field equations are coupled to the quantum fluctuations.

Let us now come to the elaboration of the quasiparticle occupation numbers and their variances. The determination of those quantities is one of the difficulties in the SCQRPA approach [8,13,23]. However, this problem has found an elegant solution in the early works of Ref. [24] (see also Ref. [25]). In the same way, we derived expressions of the quasiparticle occupation numbers and their variances as expansions in the operators P_j^\dagger and P_j up to any order in a systematic way. The detailed derivation is given in Appendix B. We here present a different method that shows some inter-

esting aspects and will lead to the same result. Using the bosonic representation of the quasispin operators of our model, we can write

$$\begin{aligned}\hat{N}_{q,j} &= 2B_j^\dagger B_j, \\ P_j^\dagger &= B_j^\dagger \left(1 - \frac{1}{\Omega} B_j^\dagger B_j \right)^{1/2}, \\ P_j &= (P_j^\dagger)^\dagger = \left(1 - \frac{1}{\Omega} B_j^\dagger B_j \right)^{1/2} B_j,\end{aligned}\quad (47)$$

where one can show that these operators in this representation always obey the commutation rules of angular momentum (14). We also can invert this relation, and we obtain

$$\begin{aligned}B_j^\dagger &= P_j^\dagger \left(1 - \frac{1}{\Omega} B_j^\dagger B_j \right)^{-1/2}, \\ B_j &= \left(1 - \frac{1}{\Omega} B_j^\dagger B_j \right)^{-1/2} P_j.\end{aligned}\quad (48)$$

With Eq. (48) $\hat{N}_{q,j}$ can be expressed as

$$\begin{aligned}\hat{N}_{q,j} &= 2B_j^\dagger B_j = 2P_j^\dagger \left(1 - \frac{1}{\Omega} B_j^\dagger B_j \right)^{-1} P_j \\ &= 2P_j^\dagger \left(1 - \frac{1}{2\Omega} \hat{N}_{q,j} \right)^{-1} P_j.\end{aligned}\quad (49)$$

Therefore, we obtained a recursive relation for $\hat{N}_{q,j}$, and using it we can derive an expansion for $\hat{N}_{q,j}$. By successive replacement of $\hat{N}_{q,j}$ in the right-hand side of Eq. (49), one finds the following expansion:

$$\begin{aligned}\hat{N}_{q,j} &= 2P_j^\dagger \left(1 - \frac{1}{\Omega} P_j^\dagger P_j \right)^{-1} P_j \\ &= 2P_j^\dagger P_j + \frac{2}{\Omega} P_j^\dagger \sum_{n=0}^{\infty} \left(\frac{P_j P_j^\dagger}{\Omega} \right)^n P_j^2 \\ &= 2P_j^\dagger P_j + \frac{2}{\Omega} P_j^\dagger \sum_{n=0}^{\infty} \left(\frac{\Omega P_j^\dagger P_j - \hat{N}_{q,j} + \Omega}{\Omega^2} \right)^n P_j^2 \\ &= 2P_j^\dagger P_j + \frac{2}{\Omega} P_j^\dagger \sum_{n=0}^{\infty} \left(\frac{1}{\Omega} \right)^n P_j^2 + \dots \\ &= 2P_j^\dagger P_j + \frac{2}{\Omega-1} P_j^\dagger P_j^2 + \dots.\end{aligned}\quad (50)$$

It should be noted that the first term in Eq. (50) becomes already exact for $J=1/2$ and, including the second term, it is also exact for $J=3/2$, etc.

For $\hat{N}_{q,j}^2$, we can use the Casimir relation,

$$\Omega P_j^\dagger P_j + \frac{\hat{N}_{q,j}^2}{4} - \frac{\Omega+1}{2} \hat{N}_{q,j} = 0.\quad (51)$$

It is equivalent to use the expansion of $\hat{N}_{q,j}^2$ obtained as the square of $\hat{N}_{q,j}$,

$$\hat{N}_{q,j}^2 = 4P_j^\dagger P_j + \frac{4(\Omega+1)}{(\Omega-1)} P_j^\dagger P_j^2 + \dots\quad (52)$$

In the same way, we use Eq. (50) to obtain an expansion for $\hat{N}_{q,1} \hat{N}_{q,-1}$, but it is sufficient to use the term of the first order of this expansion, to obtain

$$\hat{N}_{q,1} \hat{N}_{q,-1} = 4P_1^\dagger P_1 P_{-1}^\dagger P_{-1} + \dots\quad (53)$$

In principle the expansion (50) can be pushed to higher order, however, it quickly becomes quite cumbersome and in practice we always will stop at second order. In any case the expansion is finite with maximal $J+1/2$ terms. It is natural that such an expansion exists since there is a duality between the pair of operators $B_j^\dagger, B_j \leftrightarrow P_j^\dagger, P_j$. There is the choice either to bosonize the problem, then everything is expressed in terms of B_j^\dagger and B_j operators; or else one stays with the fermion pair operators and everything is expressed in terms of P_j^\dagger and P_j . In Ref. [26] the former route was chosen, here we choose the latter one. One should mention that a truncation of the series (50) also entails some violation of the Pauli principle, but one may notice that the series is very fast converging and that already the lowest order correctly contains two limits: $J=1/2$, as already mentioned, and $J \rightarrow \infty$, since then $P_j^\dagger \rightarrow B_j^\dagger$ and the lowest order is also correct see Eq. (47). With these remarks in mind we go ahead. By the inversion of the QRPA excitation operator Q_ν^\dagger , the expectation values of these expressions are immediately given in terms of the RPA amplitudes $X_{j,\nu}$ and $Y_{j,\nu}$, as one can see in Appendix A, where we give some details concerning the calculation of expectation values of these expressions in the RPA ground state.

Our system of SCQRPA equations is now fully closed and we can proceed to its solution. First let us, however, shortly come back to the limit of standard QRPA. This we will do for the symmetric case, i.e., $N=2\Omega$. This case is obtained in evaluating all expectation values in all interaction kernels with the BCS ground state or else putting $Y_{j,\nu}=0$ and $\sum_\nu X_{j,\nu}^2 = 1$ for $j=\pm 1$. The matrix elements are then

$$\begin{aligned}A_{1,1} &= A_{2,2} = g\Omega - \frac{\Delta^2}{2g\Omega^2} + \frac{\Delta^2}{2g\Omega}, \\ A_{1,2} &= A_{2,1} = -\frac{\Delta^2}{2g\Omega}, \\ B_{1,1} &= B_{2,2} = -\frac{\Delta^2}{2g\Omega^2} + \frac{\Delta^2}{2g\Omega}, \\ B_{1,2} &= B_{2,1} = g\Omega - \frac{\Delta^2}{2g\Omega},\end{aligned}\quad (54)$$

where the gap equation in the BCS theory leads to the solution in the symmetric case

$$\Delta = \sqrt{g^2 \Omega^2 - \frac{\xi^2}{4}}, \quad (55)$$

together with

$$u_1^2 = v_{-1}^2 = \frac{1}{2} \left(1 + \frac{\xi}{2g\Omega} \right),$$

$$v_1^2 = u_{-1}^2 = \frac{1}{2} \left(1 - \frac{\xi}{2g\Omega} \right),$$

$$\mu = -\frac{g}{2}, \quad (56)$$

where ξ is defined as $\xi = 2\epsilon\Omega/(2\Omega - 1)$. For the positive eigenvalues of the RPA matrix, we obtain

$$\Omega_1^{QRPA} = 0, \quad (57a)$$

$$\Omega_2^{QRPA} = \sqrt{4\Delta^2 - \frac{2\Delta^2}{\Omega}}. \quad (57b)$$

As usual, the other two eigenvalues are $-\Omega_\nu^{QRPA}$ with $\nu = 1, 2$. These results are well known [20,27]. We have repeated them here for completeness and stressing the point that in QRPA, because of the spontaneously broken particle number symmetry, one obtains a Goldstone mode $\Omega_1^{QRPA} = 0$. We again would like to stress the point that this is the case only if we evaluate Eq. (54) with the solution u_j, v_j given by the mean field equations (40) which for $\sum_\nu X_{j,\nu}^2 = 1, Y_{j,\nu} = 0$ reduce to the usual BCS equations. We explicitly showed it here for the symmetric case but the same scenario holds true for cases away from half-filling.

IV. RESULTS AND DISCUSSION

We first recall that the phase transition point in the BCS theory for the two-level pairing model is produced at $g_c = \epsilon/(2\Omega - 1)$, where ϵ is the single-particle energy splitting and Ω is the pair degeneracy of each level. In the following, the graphs are plotted, as usual, as a function of the variable $V = g\Omega/2\epsilon$, and refer to the case with level spin $J = 11/2$, i.e., $\Omega = 6$ and single-particle energy $\epsilon = 2$ (in arbitrary units). This latter value for J has been chosen for easier comparison with the results of Ref. [26] which will be given in Sec. V.

Let us first discuss the case with $N = 12$, i.e., the lower level is filled in the absence of correlations. We call this the half-filled or symmetric case. In Fig. 1 we show in the upper panel the excitation energies. Let us consider the well known scenario of the standard RPA. Before the phase transition to the superfluid phase, we work with the unconstrained Hamiltonian. One obtains two eigenvalues with the interpretation of differences of ground-state energies, differing by two units in mass $2\mu^\pm = \pm(E_0^{N\pm 2} - E_0^N)$. They are evidently related to the chemical potential and in *pp*-RPA they are given by

$$\Omega_a = 2\mu^+ = -g + \sqrt{g + \epsilon} \sqrt{\epsilon + g(1 - 2\Omega)}, \quad (58a)$$

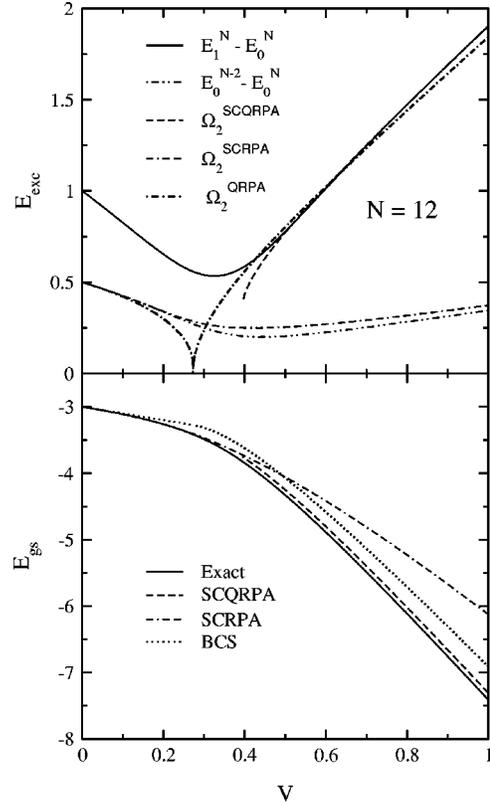


FIG. 1. Ground-state energy E_{gs} and excitation energy of the first 0^+ state E_{exc} as a function of the variable $V = g\Omega/2\epsilon$ described in the text and for particle number $N = 12$ (energies are divided by 2ϵ). The spin of the levels is $J = 11/2$. The results refer to exact calculations (solid line and double-dot dashed line), BCS (dotted line), RPA and QRPA (dot-dashed line), SCQRPA (dashed line), and SCRPA (double-dash dotted line). (Note that SCRPA and SCQRPA solutions coexist over a wide range of V values.)

$$\Omega_r = -2\mu^- = g + \sqrt{g + \epsilon} \sqrt{\epsilon + g(1 - 2\Omega)}, \quad (58b)$$

where Ω_a and Ω_r correspond to the addition and removal phonons of the *pp*-RPA, respectively. In Fig. 1 the case $-2\mu^-$ is shown and we will discuss the case $2\mu^+$ separately below in Fig. 8. We see on the graph the usual result, namely, that $-2\mu^-$ drops to zero at the phase transition point (strictly speaking only in the large Ω limit). After the phase transition point we work with the constrained Hamiltonian (15) in the BCS quasiparticle representation. The QRPA eigenvalue (57b) is also shown in Fig. 1. The Goldstone mode (57a) at zero energy corresponds to a rotation in gauge space whereas the second eigenvalue corresponds to the “ β vibration” of the nucleus with N particles [28]. This difference in interpretation is also well borne out in the SCQRPA in comparison with the exact solution. We see that in the transition region SCRPA shows a tremendous improvement over RPA and that SCRPA follows the exact value of $-2\mu^-$ even far beyond the phase transition point (as defined by the BCS theory) where no RPA solution exists. It is also to be noticed that the sharp phase transition seen in RPA-QRPA is an artifact of the theory and that in reality the phase transition is completely washed out due to the finite-

ness of the system. The fact that the “spherical” SCRPA solution coexists with the “deformed” SCQRPA solution over a wide parameter range representing different energy states of the system is a quite unique situation. In all other model cases where we have investigated the “spherical-deformed” transition the spherical solution ceased to converge numerically [29] beyond a certain critical coupling. This, however, is no proof that the spherical solution does not also exist far in the deformed region representing physical states. It may be that in those works, simply the method for the numerical solution was not sophisticated enough. This is a point to be investigated in the future. In the superfluid (deformed) region SCQRPA still is superior to QRPA but the improvement is less spectacular. This stems from the fact that the transformation to BCS quasiparticles effectively accounts for some supplementary correlations in QRPA and thus the differences with exact and SCQRPA solutions become less important than in the nonsuperfluid regime. A feature that is to be remarked in Fig. 1 is the fact that SCRPA and SCQRPA do not smoothly match in the transition region, whereas RPA and QRPA have a certain continuity at the transition point. However, we see that SCRPA and SCQRPA describe two physically very distinct states that do not have any contact in the exact case neither and therefore it is not astonishing that SCRPA and SCQRPA do not join. This mismatch has as a consequence that there also exists a rupture in the ground-state energy as a function of interaction as is seen in the lower panel of Fig. 1. Again SCQRPA results improve strongly over BCS ground-state energies in the deformed region.

So far we have omitted the discussion of two items of the case considered in Fig. 1 which are slightly subtle. The first is the fact that the QRPA shows two eigenvalues: the β vibration and the Goldstone mode at zero energy (the pair rotation mode), whereas we have not shown the corresponding low energy mode of SCQRPA. Below we will discuss this issue. The second point is that we have not shown in Fig. 1 the QRPA values for the ground-state energies. We show this separately in an enlarged scale around the transition point in Fig. 2. We there see that QRPA overbinds in the transition region, but that, further to the right of the transition region, the QRPA values are closer to the exact solution than the ones from SCQRPA. This is a paradoxical result that systematically repeats itself for all other configurations we will consider below. However, the seemingly “better agreement” is an artifact of the QRPA which has already been encountered in others cases [29]. We want to argue as follows: SCQRPA is in itself a well defined theory, resulting from the variational principle (34) for two-body correlation functions. One also can consider it as a Hartree-Fock-Bogoliubov (HFB) approach for fermion pairs. The Pauli principle is respected in an optimal way, since at no point a bosonization of fermion pair operators is introduced and the Pauli principle is only violated in the truncation of Eq. (50) which is a very fast converging series. However, any approximation to the full SCQRPA scheme necessarily violates (mildly) the Pauli principle and consequently simulates more energy gain than there should be. Since, for the present model case, the SCQRPA ground-state energy is systematically above the ex-

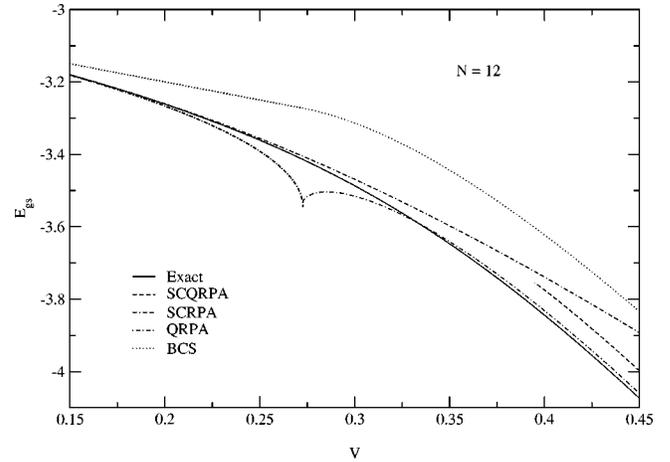


FIG. 2. An enlargement on the ground-state energy E_{gs} as a function of the variable $V=g\Omega/2\epsilon$ described in the text and for particle number $N=12$ (energies are divided by 2ϵ). The spin of the levels is $J=11/2$. The results refer to exact calculations (solid line), BCS (dotted line), RPA and QRPA (dot-dashed line), SCQRPA (dashed line), and SCRPA (double-dash dotted line).

act one (under binding), it may happen that, when the Pauli principle constraint is released in going from SCQRPA to QRPA, the corresponding gain in energy is such that, accidentally, the QRPA ground-state energy practically coincides with the exact values over a wide range of parameters. We think that this is what happens in this model not only for the configuration in Fig. 1, but systematically for all types of degeneracies and all fillings. We will not discuss this issue for the other cases any more in this work. We again should mention that we have found such fortuitous coincidences already in other works [29]. However, in more realistic cases ones usually finds that the standard RPA strongly overbinds with respect to the exact values (see, e.g., Ref. [30]).

Let us now discuss situations where either the lower or upper levels are only partially filled. As in the one-level pairing case, these configurations always show a nontrivial BCS solution, i.e., they are always in the superfluid regime independent of V . Let us look at Fig. 3 with $J=11/2$ and $N=8$ that is the lower level partially filled for $V=0$. In the upper panel the high-lying eigenvalue of the SCQRPA equations is shown against the exact value. We see that there is some improvement of SCQRPA with respect to QRPA but it is not spectacular. It is similar to the case of Fig. 1 where, in the superfluid region, the improvement, for reasons already explained above, is modest. For the ground-state energy there is quite strong improvement over the BCS theory. The QRPA result is not shown, but the situation is the same as already explained above. The cases $J=11/2$, $N=4$, and $N=14$ shown in Figs. 4 and 5 are qualitatively similar.

Let us now come to the low-lying eigenvalue of SCQRPA which in QRPA corresponds to the zero-energy eigenvalue (Goldstone or spurious mode). In Fig. 6 we show the low lying eigenvalue for the case $J=11/2$ and $N=10$. We see that this eigenvalue follows very precisely the difference $2(\mu^+ - \mu^-) = E_0^{N+2} + E_0^{N-2} - 2E_0^N$ of the two chemical potentials $2\mu^+ = E_0^{N+2} - E_0^N$ and $2\mu^- = E_0^N - E_0^{N-2}$ as obtained

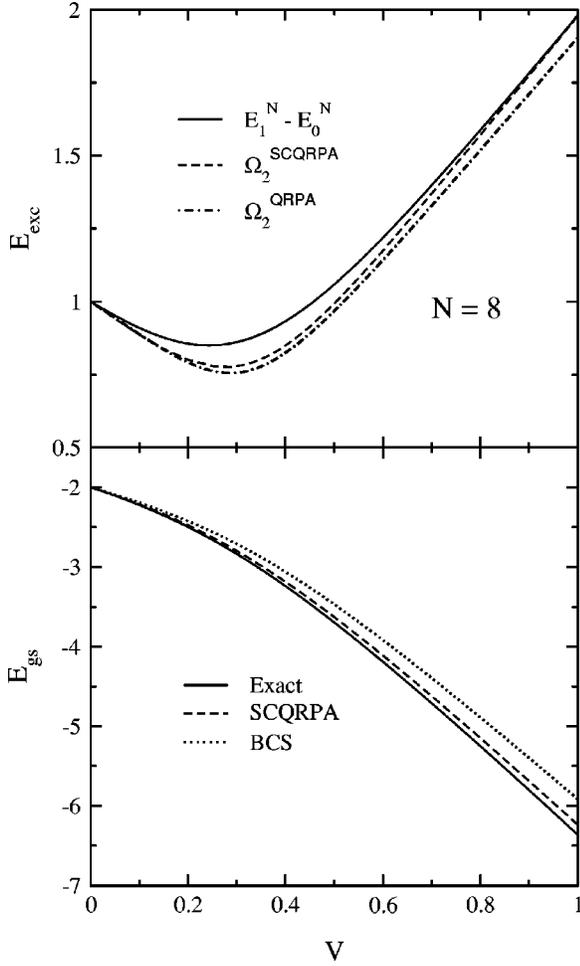


FIG. 3. As in Fig. 1 but for $N=8$.

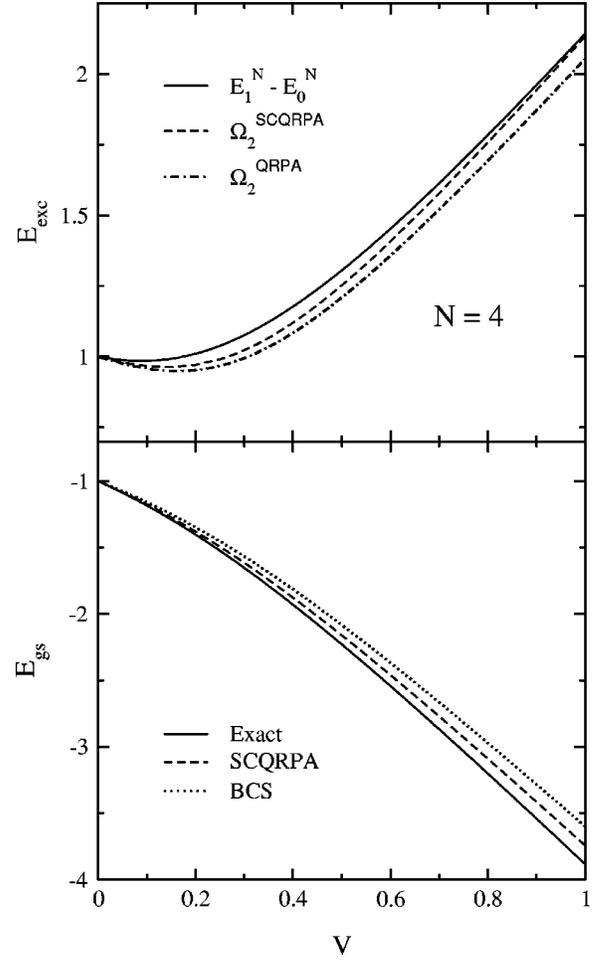


FIG. 4. As in Fig. 1 but for $N=4$.

from the exact calculation. This identification makes indeed sense: since we are in the symmetry broken phase, the SCQRPA system cannot distinguish between $N \pm 2$ states. For large N , both $2\mu^+$ and $2\mu^-$ tend individually to Goldstone modes but for finite N it definitely is reasonable to define the difference between $2\mu^+$ and $2\mu^-$ as the low-lying excitation, and it is this combination that shows up as low-lying mode in the SCQRPA calculation. This is confirmed in looking at other configurations: in Fig. 7 we show the case $J=11/2$, $N=4$ and in fact we find analogous scenarios for all configurations we investigated, besides one: this is the symmetric case with $J=11/2$, $N=12$. In the Fig. 8 we see that the picture is slightly different from the rest of the cases. This stems from the fact that in the symmetric case we have a transition from the superfluid to the nonsuperfluid regime, which is absent in the other partially filled cases. We also see that the values for $2\mu^+$ and $2\mu^-$ are very asymmetric; $2\mu^+$ apparently taking the role of the Goldstone mode alone. Also the agreement of the low-lying SCQRPA solution Ω_1 is slightly less good than in all other cases.

Let us also add some remarks why in SCQRPA there is, contrary to QRPA, no exact Goldstone mode at zero energy. This is relatively easy to understand: in quasiparticle representation the number operator is given by Eqs. (25) and (26). One can check that in QRPA the terms $\alpha^\dagger \alpha$, if they were

included, completely decouple of the QRPA equations. Therefore, in QRPA, it is as if one had used the full particle number operator and therefore a particular solution of the QRPA equations is $Q^\dagger \equiv \hat{N}$ and with $[H, \hat{N}] = 0$ we get the zero eigenvalue in the EOM approach. This argumentation is no longer true in SCQRPA where the terms $\hat{N}_{q,j}$ Eq. (26), of the number operator contribute in principle to SCQRPA. However, we cannot include them in the RPA operator because these are Hermitian pieces leading to non-normalizable eigenstates. Therefore $Q^\dagger = \hat{N}$, as a particular solution, only holds in QRPA but not in other cases such as SCQRPA. However as a benefit, we see in the preceding figures that we can identify the finite value of Ω_1 with a particular rotational frequency in the gauge space of the exact solution of the problem. The finite energy comes because of the finite particle number in the system. On the other hand, in realistic situation, one can include in the RPA operator terms of the form $\alpha_k^\dagger \alpha_{k'}$, for $k \neq k'$ [14]. Only the Hermitian operators $\alpha_k^\dagger \alpha_k$ have to be excluded for the reason already mentioned. These components correspond in an infinite system to momentum transfer zero and they are thus of zero measure. Therefore, in an infinite system, we have again full restoration of symmetry.

Other quantities that are interesting to be calculated

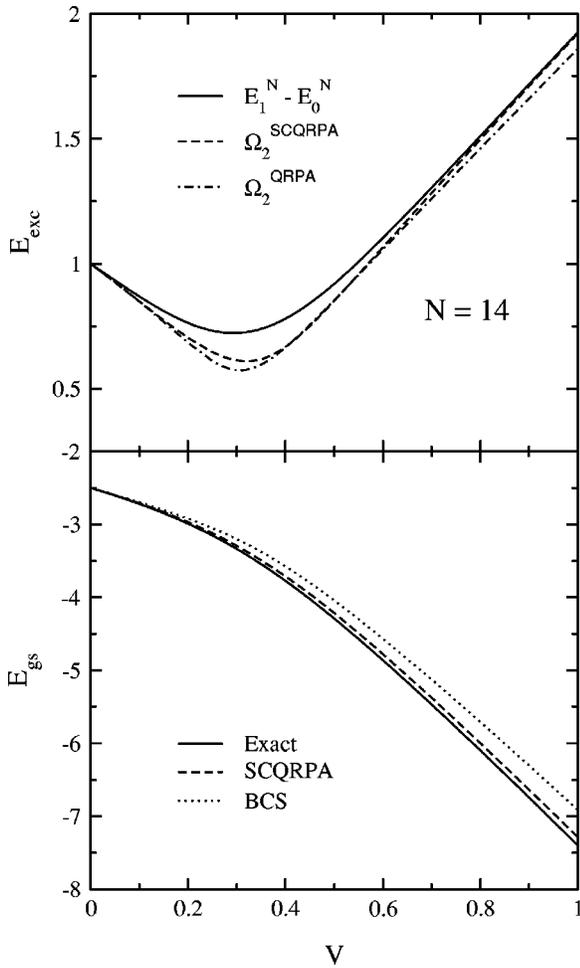


FIG. 5. As in Fig. 1 but for $N=14$.

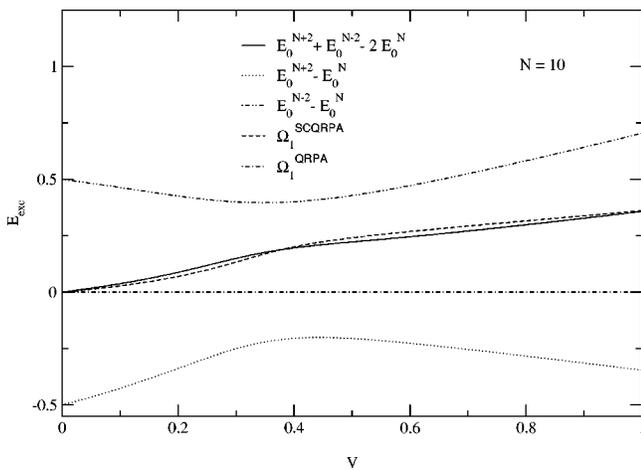


FIG. 6. Excitation energy of the soft (spurious) mode (energies are divided by 2ϵ) as a function of the variable $V=g\Omega/2\epsilon$ described in the text and for particle number $N=10$. The spin of the levels is $J=11/2$. The results refer to exact calculations (solid line, dotted line, and double-dot dashed line), RPA and QRPA (dot-dashed line), QRPA (dot-dashed line), and SCQRPA (dashed line).

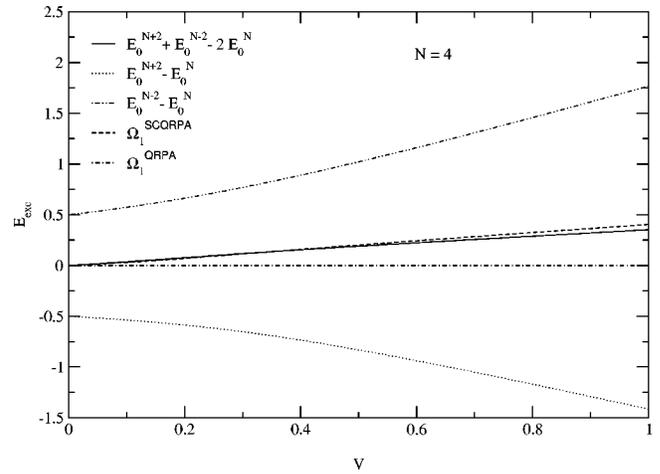


FIG. 7. As in Fig. 6 but for $N=4$.

within the SCQRPA formalism are the chemical potentials directly from differences of ground-state energies. For example, in Figs. 9 and 10 we show $\mu^\pm = \pm \frac{1}{2}(E_0^{N\pm 2} - E_0^N)$ where the individual ground-state energies are obtained directly from separate SCQRPA calculations. We see for $J=11/2$ and $N=4$ and 8 that the agreement between SCQRPA results and exact values is excellent, and in any case a strong improvement over BCS theory can be noticed. The same is true for the chemical potential μ as obtained from $\mu = \frac{1}{2}(\mu^+ + \mu^-)$ in the exact calculation. The latter, which is an average chemical potential, should be identified with the Lagrange multiplier μ used for restoring the symmetry of the good particle number (8) in BCS and SCQRPA. This identification is shown in each upper panel in Figs. 9–11. In Fig. 11 we show the results for μ and μ^\pm for the symmetric case $J=11/2$ and $N=12$. We see that again the same remarks as for the asymmetric cases hold true. However, we notice the

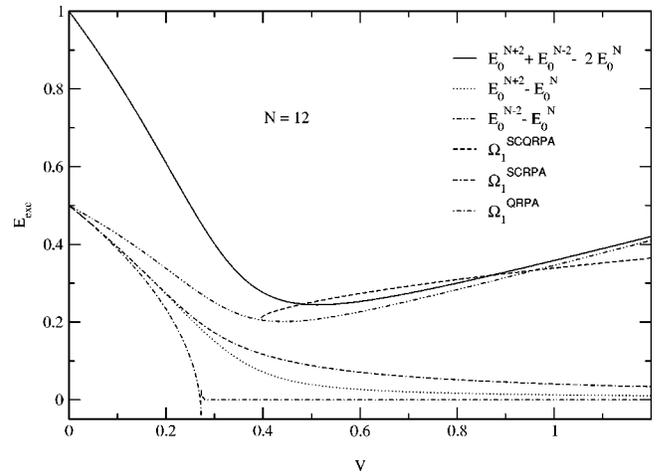


FIG. 8. Excitation energy of the soft (spurious) mode (energies are divided by 2ϵ) as a function of the variable $V=g\Omega/2\epsilon$ described in the text and for particle number $N=12$. The spin of the levels is $J=11/2$. The results refer to exact calculations (solid line, dotted line, and double-dot dashed line), RPA and QRPA (dot-dashed line), SCQRPA (dashed line), and SCRPA (double-dash-dot line).

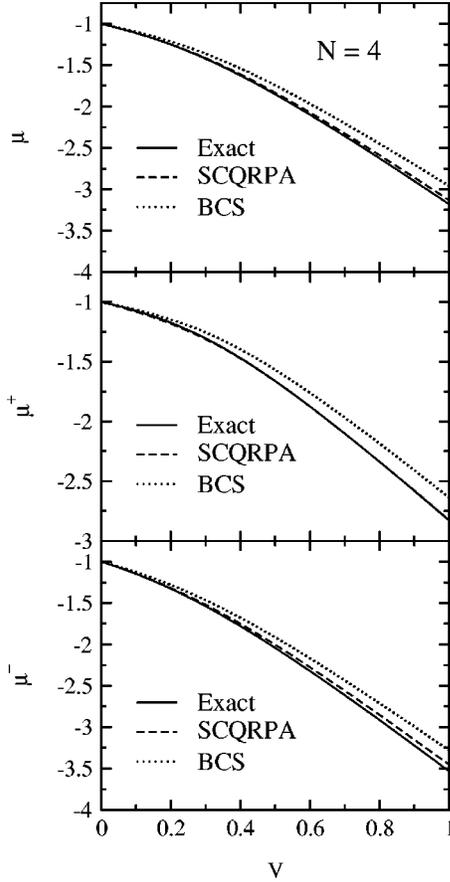


FIG. 9. Comparison between SCQRPA, BCS, and exact results for the chemical potentials $\mu = \frac{1}{2}(\mu^+ + \mu^-)$ and $\mu^\pm = \pm \frac{1}{2}(E_0^{N\pm 2} - E_0^N)$, for particle number $N=4$. The spin of the levels is $J = 11/2$. The results refer to exact calculations (solid line), SCQRPA (dashed line), and BCS (dotted line).

particular situation that for μ the exact, BCS, and SCQRPA solutions coincide exactly. This has to do with the specific symmetries in the half-filled case.

It is also interesting to show the chemical potentials $2\mu^+$ and $2\mu^-$ in a symmetric way as done in Ref. [31]. This also gives us the occasion to study the accuracy of our approximation (50) and (53) for the occupation numbers. Let us first of all say that we have here a quite unusual situation for SCRPA: as already mentioned, the solution in the spherical, i.e., nonsuperfluid basis, exists far into the superfluid regime. Usually in other models the solution of SCRPA in the spherical basis can be found up to interaction values slightly beyond the mean field transition point but here very reasonable values for the chemical potentials $2\mu^\pm$ are obtained for all values of V as seen in Fig. 12. This was also found in the work by Passos *et al.* [31]. It should be mentioned, however, that maintaining the spherical basis gives much less good results for the ground-state energy as seen in Fig. 1. Indeed after the transition point the ground state energy values deviate quite strongly from the exact results. In Fig. 12 we calculate the expectation values $\langle \hat{N}_i \rangle$ and $\langle \hat{N}_i \hat{N}_j \rangle$ with the exact RPA ground state [15]

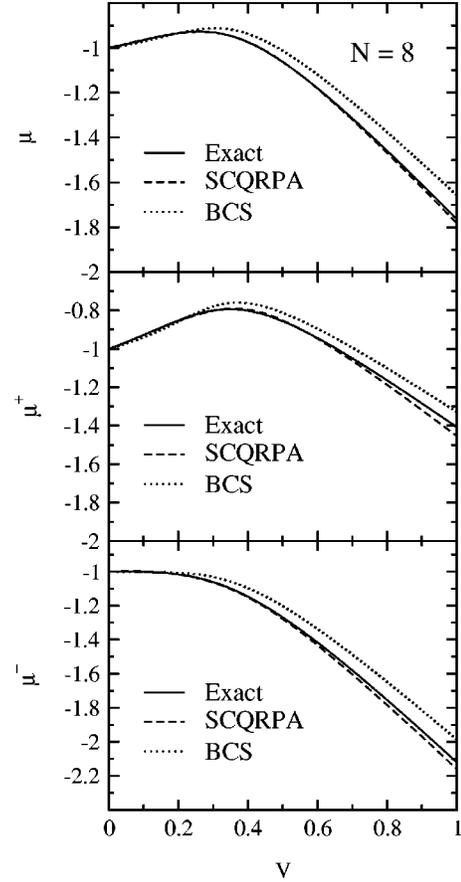


FIG. 10. As in Fig. 9 but for $N=8$.

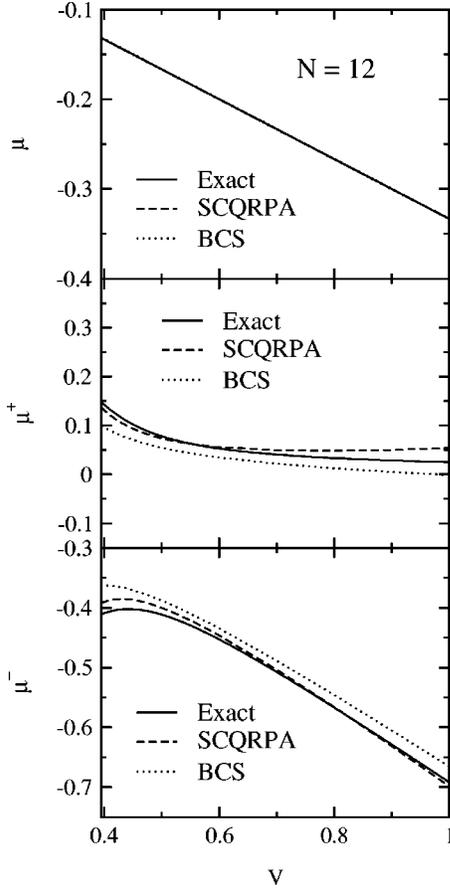
$$|RPA\rangle = \sum_{l=0}^{\Omega} \left(\frac{Y}{X} \right)^l (A_1^\dagger)^l (A_{-1}^\dagger)^{\Omega-l} |-\rangle, \quad (59)$$

where X, Y are the RPA amplitudes, defined with the addition (P) and removal (R) phonons of the particle-particle RPA and satisfying the normalization condition $X^2 - Y^2 = 1$. This gives the broken lines. If we calculate the same values from our limited expansion (50) then the dotted lines are obtained. We see that beyond the transition point the solution becomes extremely sensitive to approximations. Indeed our approximated values deviate quite a bit from the ones calculated with the full wave function $|RPA\rangle$.

The occupation numbers are particularly sensitive to the correct treatment of correlations are. For example, for the particle number in the upper level we obtain

$$\langle \hat{N}_1 \rangle = (u_1^2 - v_1^2) \langle \hat{N}_{q,1} \rangle + 2\Omega v_1^2 \quad (60)$$

and the result is shown in Fig. 13 for the superfluid and nonsuperfluid regimes. Once again we see that the change around the phase transition is not continuous. Still with SCQRPA one notices a tremendous improvement over standard QRPA for which the amplitudes diverge at the critical point. Indeed it is just in such quantities as occupation numbers where the full superiority of SCQRPA over its linearized version of QRPA is fully borne out. Before finishing this section, we will explain how we proceeded to make the


 FIG. 11. As in Fig. 9 but for $N=12$.

QRPA and RPA calculation of $\langle \hat{N}_{q,1} \rangle$ in both regions, normal and superfluid. We use the first order of the bosonic expansion of the $\hat{N}_{q,1}$, i.e., the first order of the expansion shown in Eq. (50), where it is sufficient to put $P_1^\dagger = B_1^\dagger$. Thus, with the commutation rules (14), we find

$$\langle \hat{N}_{q,1} \rangle = \frac{2(Y_{1,1}^2 + Y_{1,2}^2)}{\left[1 + \frac{2}{\Omega}(Y_{1,1}^2 + Y_{1,2}^2) \right]}. \quad (61)$$

In linearizing this expression, we obtain

$$\langle \hat{N}_{q,1} \rangle = 2(Y_{1,1}^2 + Y_{1,2}^2). \quad (62)$$

It is interesting to detail this calculation, since it is useful to see analytically the QRPA and RPA results for the particle number in the upper level close the transition point. It is well known that the two excitation modes in the RPA method converge to zero at the transition point, then the corresponding RPA amplitudes tend to infinity, which explains the divergence of $\langle \hat{N}_1 \rangle$. In the superfluid zone, we mention that we neglected the RPA amplitudes corresponding to the Goldstone (spurious) mode when we make the calculation of $\langle \hat{N}_1 \rangle$.

A constant concern for superfluidity or superconductivity in finite systems is that the quasiparticle transformation (9)

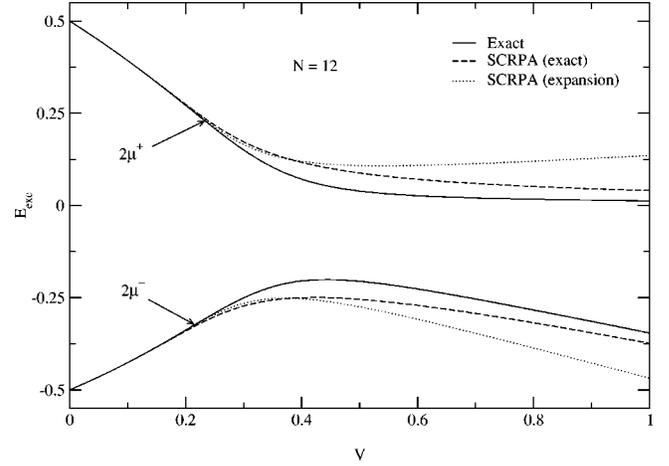


FIG. 12. Excitation energies $2\mu^+$ (upper lines) and $2\mu^-$ (energies are divided by 2ϵ) as a function of the variable $V=g\Omega/2\epsilon$ described in the text and for $N=12$. The spin of the levels is $J=11/2$. The full lines correspond to the exact results, the broken lines to SCRPA with occupation numbers calculated with the wave function (59), and dotted lines to SCRPA with occupation numbers.

does not preserve good particle number. Even though one fixes particle number in the mean with the help of a Lagrange multiplier, the contamination of expectation values with components that have wrong particle number can be quite important. This is for instance the case for atomic nuclei. That is why, very early, one has thought of how to improve the BCS theory with respect to particle number conservation. One quite popular approach is to project the BCS wave function on good particle number. An approximation to this relatively heavy scheme is the approximate particle number projection by Lipkin and Nogami [32]. It is therefore interesting to investigate how much SCQRPA improves on the spread in particle number. We therefore will calculate

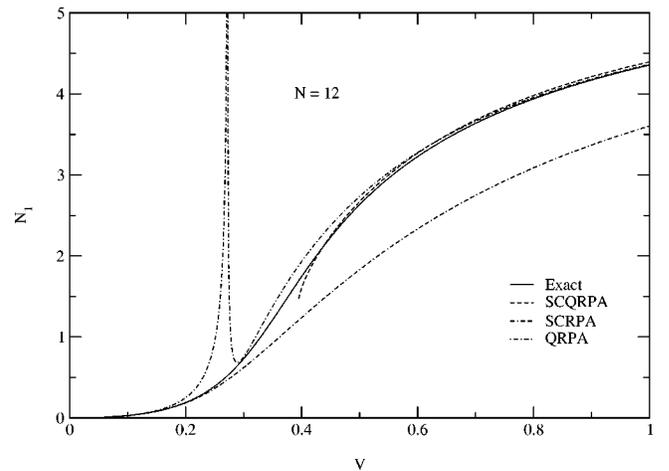


FIG. 13. Particle number in the upper level N_1 as a function of the variable $V=g\Omega/2\epsilon$ described in the text and for $N=12$. The spin of the levels is $J=11/2$. The results refer to exact calculations (solid line), SCQRPA (dashed line), SCRPA (double-dash dotted line), and QRPA (dot-dashed line).

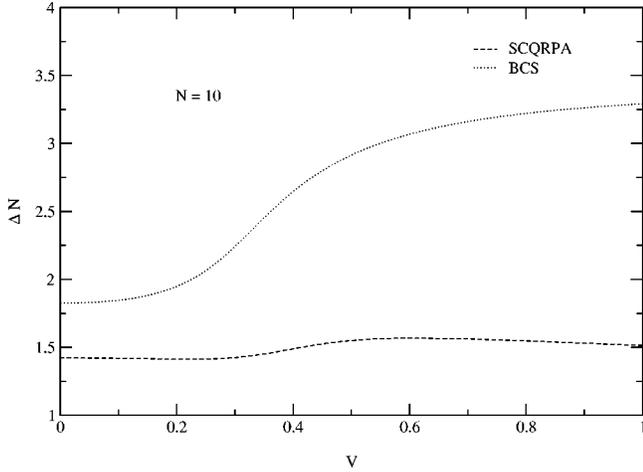


FIG. 14. Variance as a function of the variable $V=g\Omega/2\epsilon$ described in the text and for particle number $N=10$. The spin of the levels is $J=11/2$. The results refer to SCQRPA calculations (dashed line) and BCS (dotted line).

$$(\Delta N)^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 \quad (63)$$

with $\hat{N} = \hat{N}_1 + \hat{N}_{-1}$ being the particle number operator and \hat{N}_j given by Eq. (26) within SCQRPA. The terms involving bilinear forms in P_j^\dagger , P_j are as usual directly expressed by the RPA amplitudes and for the quasiparticle occupation number operators we use Eqs. (50)–(53). Then ΔN can be calculated and the results for various configurations are shown in Figs. 14–16. We see that the spread in particle number is strongly reduced over BCS values reaching typical factors 2–3. We, however, see that ΔN even in SCQRPA acquires nonvanishing sizable values. This is an expression that particle number is not completely restored. We will see in Sec. VI how one eventually can improve on this. We also tried to evaluate ΔN in standard QRPA in applying a lowest-order bosonization of the expression. However, due to the non-normalizable Goldstone mode we ran into troubles with this procedure and could not reach a definite conclusion on this point.

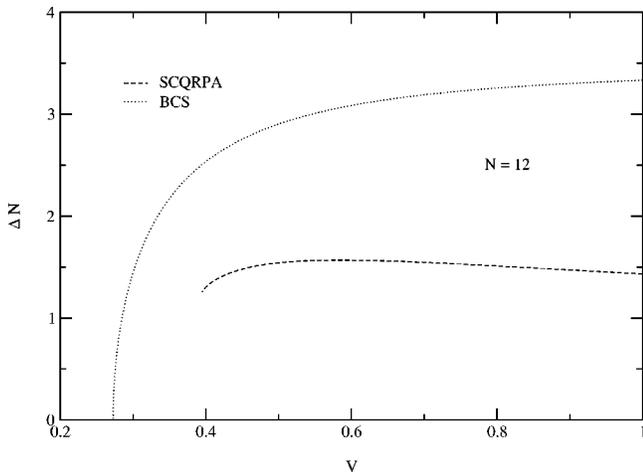


FIG. 15. As in Fig. 14 but $N=12$.

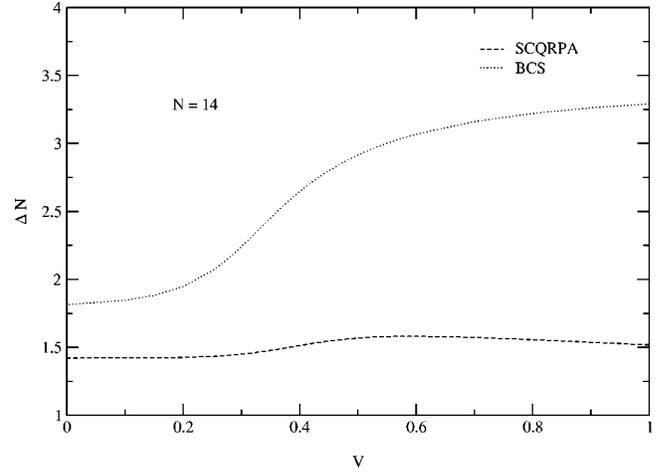


FIG. 16. As in Fig. 14 but $N=14$.

Another interesting aspect that can be studied with our model is the question whether the pairing correlations, with respect to BCS, have been enhanced or weakened due to the SCQRPA correlations. To this end we define the following quantal expression for the correlation function:

$$C = \frac{1}{\Omega} \sum_{j=\pm 1} \left(\langle A_j^\dagger A_j \rangle - \frac{1}{4\Omega^2} \langle \hat{N}_j \rangle \langle \hat{N}_j \rangle \right). \quad (64)$$

This expression reduces to the following expression when evaluated with the BCS ground state:

$$C_{BCS} = \sum_{j=\pm 1} u_j^2 v_j^2. \quad (65)$$

Often Eq. (64) is given in a nondiagonal form [33], but having difficulties to express nondiagonal densities with SCQRPA amplitudes we will not consider the nondiagonal form here. We therefore evaluate Eq. (64) in three approximations: we can express Eq. (64) in terms of P_j^\dagger , P_j , and $\hat{N}_{q,j}$ operators and then take the expectation value with the SCQRPA ground state. Equations (33), (50), and (52) then allow us to express C in terms of the SCQRPA amplitudes $X_{j,v}$, $Y_{j,v}$. We will call this C_{SCQRPA} . We also evaluate Eq. (65) in the standard BCS approximation which is Eq. (64). However, we also calculate Eq. (65) with u_j , v_j amplitudes from the renormalized BCS (r -BCS) theory, i.e., from Eq. (42) with Δ_j solution of Eq. (43). The results are shown in Figs. 17 and 18 for $N=12$ and $N=14$, respectively (the case $N=10$ gives exactly same results as $N=14$). We see that r -BCS gives less correlations with respects to BCS. Eventually this suppression of pairing can be put into analogy with gap suppression in infinite neutron matter from renormalized theories [3] (see discussion in the Introduction). However, the suppression of pairing correlation in r -BCS is misleading in our model, since, on the contrary, the full SCQRPA gives mostly an

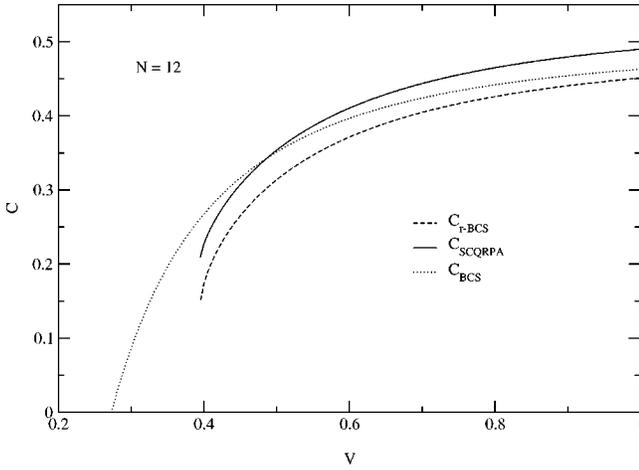


FIG. 17. Correlation function \mathcal{C} as a function of the variable $V = g\Omega/2\epsilon$ described in the text and for particle number $N=12$. The spin of the levels is $J=11/2$. The results refer to SCQRPA (solid line), renormalized BCS, (dashed line) and standard BCS (dotted line).

enhancement of pair correlations with respect to BCS. It is not obvious whether this conclusion can be taken over to the infinite matter case. It may, however, be indicated that the renormalized gap equations from screening (RPA)-type correlations should be carefully treated consistently with the evaluation of a two-body correlation function before definite conclusions can be reached.

V. COMPARISON WITH OTHER RECENT WORKS

The two-level pairing model has recently served as a testing ground for various generalizations of the BCS theory. The work that comes closest to the present is the one of Sambataro and Dinh Dang [26]. Instead of treating quasiparticle pair operators directly as we do here, they bosonize them (with a method developed in Ref. [26]) and expand the Hamiltonian (1) in terms of these bosons up to fourth order. A Bogoliubov transformation of the boson operators quite

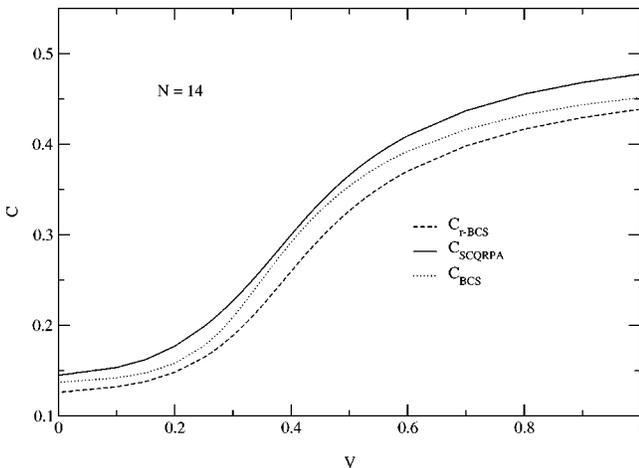


FIG. 18. As in Fig. 17 but $N=14$.

analogous to our Bogoliubov transformation of fermion pair operators (9) is then performed and the corresponding non-linear Hartree-Fock-Bogoliubov equation is written down. Again these are quite analogous to our SCQRPA equations. The coefficients of quasiparticle transformation are obtained, as usual, by minimizing the ground-state energy [see also our procedure (39)] with respect to the transformation coefficients. As in our case, equations are obtained which couple back to the bosonic HFB, i.e., the RPA amplitudes. The coupled system of equations for fermionic and bosonic transformation amplitudes is then solved self-consistently. For better comparison, we actually, on purpose, have chosen most of the configurations in J and N the same as in Ref. [26]. Since in Ref. [26] $J=11/2$, which is a rather high degeneracy of the levels, the fermion pair operators are quite collective and a bosonization certainly is a valid procedure. Not unexpectedly, therefore, the results of the present work are very close to those presented in Ref. [26]. A detailed comparison shows that our results are systematically closer to the exact ones by a very small amount. This may be due to the fact that we never bosonize and treat the fermion pair commutation rules exactly but the difference is too small for drawing any definite conclusion. In Ref. [26], Sambataro and Dinh Dang show an explicit comparison of results referring to the symmetric case with $J=19/2$. We also can make such a comparison for the ground-state energy referring to the same configuration. It is given in Table I, where we show the results for four different many-body approaches: our approach (SCQRPA), approach of Sambataro and Dinh Dang (BF-RPA) [26], standard QRPA [27], and the BCS method [28]. Of course, we recall that in our approach, we use the self-consistent particle-particle RPA in the normal fluid zone, while, in the superfluid region, we use the generalized version of SCRPA that is SCQRPA. In order to accentuate the differences one would have to go to configurations with much lower degeneracies where the constraints from the Pauli principle become much more severe. For example, the SCRPA approach has been applied to the case $J=1/2$ with $N=2$ in Ref. [8] and the exact result was recovered. It would be interesting to see how the approach with the bosonization [26] performs in that case. In spite of being very similar, in general, to the work in Ref. [26] we have solved and considered several additional problems that remained open in Ref. [26]. In the first place, this concerns the low-lying eigenvalue of SCQRPA. No interpretation of this important root was given in Ref. [26]. We, however, suppose that the results in Ref. [26] for this state (no numerical values have been given) can be equally interpreted as the difference $2(\mu^+ - \mu^-)$ as in our case. Another quantity that was not considered in Ref. [26] is the number fluctuation. Again we believe that corresponding values would be close to the ones found here. Also the transition to the nonsuperfluid regime has not been treated in Ref. [26]. However, probably all these aspects will be quite similar in both approaches as long as the bosonization of the fermion pair operators is valid. We think, however, that it does not cost much to avoid bosonization altogether as with the SCQRPA approach.

TABLE I. Results for the ground-state energy (in arbitrary units) vs the variable $V = g\Omega/2\epsilon$ described in the text. The spin of the levels is $J = 19/2$ and the number of particles is $N = 20$.

V	Exact	SCQRPA	BF-RPA	QRPA	BCS
-0.50	-18.55446	-18.55410	-18.55360	-18.56890	-18.00000
-0.45	-18.66849	-18.66821	-18.66784	-18.67924	-18.20000
-0.40	-18.78706	-18.78686	-18.78660	-18.79474	-18.40000
-0.35	-18.91072	-18.91058	-18.91040	-18.91592	-18.60000
-0.30	-19.04010	-19.04001	-19.03990	-19.04338	-18.80000
-0.25	-19.17600	-19.17594	-19.17588	-19.17787	-19.00000
-0.20	-19.31939	-19.31936	-19.31933	-19.32031	-19.20000
-0.15	-19.47153	-19.47151	-19.47150	-19.47188	-19.40000
-0.10	-19.63406	-19.63405	-19.63405	-19.63415	-19.60000
-0.05	-19.80919	-19.80919	-19.80919	-19.80919	-19.80000
0.00	-20.00000	-20.00000	-20.00000	-20.00000	-20.00000
0.05	-20.21101	-20.21101	-20.21101	-20.21102	-20.20000
0.10	-20.44921	-20.44918	-20.44917	-20.44953	-20.40000
0.15	-20.72625	-20.72599	-20.72593	-20.72899	-20.60000
0.20	-21.06339	-21.06130	-21.06100	-21.08080	-20.80000
0.25	-21.50260	-21.48733	-21.48640	-21.64174	-21.00000
0.30	-22.12491	-22.03638	-22.03620	-22.13484	-21.37193
0.35	-23.03321	-22.80453	-22.77899	-22.99299	-22.21880
0.40	-24.24609	-23.99588	-23.97001	-24.21285	-23.37895
0.45	-25.68929	-25.42829	-25.39821	-25.65779	-24.74795
0.50	-27.29077	-27.01885	-26.98390	-27.25633	-26.26316

Also in the work by Passos *et al.* [31] the SCRPA method was applied to the present model. However, only the nonsuperfluid formulation, i.e., SCRPA, was studied. The results are quite analogous to ours. In addition, in Ref. [31] a further approximation, half way between RPA and SCRPA, the so-called r -RPA where only the single-particle occupation numbers are allowed to be affected by ground-state correlation, has been considered. The astonishing finding there was that the exact occupation numbers are almost perfectly reproduced over the whole range of the coupling constant with r -RPA but not with SCRPA that undershoots the correlations. This was interpreted in Ref. [31] as a positive feature of r -RPA over SCRPA. We cannot follow this conclusion from our experience with SCRPA in this and other works [8]. As we outlined above, any relaxation of the severe constraints of the Pauli principle respected in SCRPA will inevitably lead to more correlations as there should be. It can happen by accident that one relaxes the Pauli principle just by the right amount that one falls more or less on the exact values. This is what happened for the QRPA ground-state energy discussed above and apparently it is also what happens for the occupation numbers in r -RPA. However, we think this result cannot be generalized and for other models or physical situations the scenario may be completely different. The only really trust worthy theory is the full SCRPA approach, since it can be derived from a variational principle. If the results are not good, one must improve on SCRPA (i.e., include, e.g., higher configurations) and not approximate it.

In the work by Hagino and Bertsch [27] the QRPA approach is advocated. This in the spirit to have a numerically viable alternative to projected BCS and the method by

Nogami and Lipkin [32]. It is certainly true that in realistic cases SCRPA is numerically very demanding, though probably not impossible to solve with modern computers. Then, of course, in a first step it is worthwhile to investigate standard QRPA. This is for instance true if one intends to do large scale calculations for a great number of nuclei [27]. However, one should always remember that standard QRPA may have quite important failures, which certainly will be most prominent in situations where the system is close to a phase transition.

VI. THE QUESTION OF A SECOND CONSTRAINT ON THE PARTICLE NUMBER VARIANCE

As we have seen above, with respect to BCS the SCQRPA reduces the spread in particle number by an important factor. However, the variance ΔN is still appreciable and one can ask the question whether or not it is possible to further improve the theory on this point. A natural idea that comes to mind is that instead of fixing only $\langle \hat{N} \rangle = N$, one could at the same time fix $\langle \hat{N} \hat{N} \rangle = N^2$ with a second Lagrange multiplier. Since in SCQRPA the number of variational parameters is largely increased with respect to BCS, one could imagine that there is indeed enough freedom for constraining the particle number fluctuation to zero. The Hamiltonian to be considered is therefore

$$H' = H - \mu_1 \hat{N} - \mu_2 \hat{N}^2. \quad (66)$$

Let us immediately give our conclusion: in the two-level pairing case we could not find a solution to this problem. The system of nonlinear equations with the two constraints μ_1 and μ_2 is quite complex and in spite of considerable numerical effort we did not succeed in getting converged solution. We were not able to decide whether the difficulty is purely numerical or there is a principal problem. In fact we were at first encouraged by results we obtained in the one-level pairing case (the seniority model). The outcome of employing the second constraint was that the one-level model was solved exactly. In spite of being a somewhat trivial model that certainly limits the conclusions, it may be interesting to sketch the procedure. The Hamiltonian to be considered is now

$$H = -g\Omega A^\dagger A \quad (67)$$

in analogy to Eq. (2) $A^\dagger = 1/\sqrt{\Omega} \sum_{m>0} a_m^\dagger a_{-m}^\dagger$, and where we put the origin of energy at the single-particle level. As in the two-level case we transform to quasiparticles and with only one level the SCQRPA equation reduces to a (2×2) eigenvalue problem, with A and B in analogy to the two-level case. Also the generalized mean field equations are in analogy to the two-level case.

In addition to the SCQRPA equations we have two further equations that, in principle, allow us to find the Lagrange multipliers μ_1 and μ_2 (see, however, below),

$$N = \langle \hat{N} \rangle = (u^2 - v^2) \langle \hat{N}_q \rangle + 2\Omega v^2, \quad (68a)$$

$$\begin{aligned} N^2 = \langle \hat{N}^2 \rangle &= (u^2 - v^2)^2 \langle \hat{N}_q^2 \rangle + 8\Omega u^2 v^2 \left(1 - \frac{\langle \hat{N}_q \rangle}{\Omega} \right) (XY + Y^2) \\ &+ 4\Omega v^2 (u^2 + \Omega v^2) + 4v^2 (\Omega (u^2 - v^2) \\ &- u^2) \langle \hat{N}_q \rangle. \end{aligned} \quad (68b)$$

We see that Eqs. (68) reduce to the standard expressions, once, as in the HFB approximation, we pose $Y = \langle \hat{N}_q \rangle = \langle \hat{N}_q^2 \rangle = 0$. In the case of the seniority model the number equation (68a) in the HFB approximation determines the amplitudes u, v and then no freedom is left to impose $\Delta N = \sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2} = 0$. However, in the more general approach of SCQRPA there is more freedom, and one we will be able to satisfy the relation $\Delta N = 0$ as well. For \hat{N}_q and \hat{N}_q^2 we have the same relation as in Eqs. (50) and (52). Again the system of equations is therefore closed.

Usually the number equations (68a) and (68b) are to be used for the determination of the chemical potential μ_1 and the second Lagrange multiplier μ_2 and the mean field equations for the amplitudes u, v and X, Y . In the present case it is, however, more convenient to invert the role of the mean field and number equations, since Eqs. (68) do not depend on

the Lagrange multipliers and therefore readily allow us to determine v^2 and Y^2 as a function of the particle number N . Inversely the two mean field equations SCQRPA and generalized BCS turn out to be linear in μ_1 and μ_2 and, for instance, one can deduce that SCQRPA equations directly yield

$$\mu_2 = \frac{g}{4}, \quad (69)$$

independent of the particle number N . Considering, the well known exact expression for the ground-state energy E_0 of the model [28] we realize from $\mu_2 = \partial^2 E_0 / \partial N^2$ that this is the exact value for the second Lagrange multiplier μ_2 . For the chemical potential μ_1 we obtain

$$\begin{aligned} \mu_1 = (g - 4\mu_2) \left\{ (\Omega - 1)v^2 + (1 - 2v^2) \left(XY + Y^2 \right. \right. \\ \left. \left. + \frac{1}{2} \frac{\langle \hat{N}_q \rangle - \frac{\langle \hat{N}_q^2 \rangle}{\Omega}}{1 - \frac{\langle \hat{N}_q \rangle}{\Omega}} \right) \right\} - \frac{g}{2} \Omega - 2\mu_2, \end{aligned} \quad (70)$$

with relation (69) this gives $\mu_1 = -g/2(\Omega + 1)$ which again is the exact value. Furthermore, one obtains that $A = B = 0$ and therefore the RPA eigenvalue $E = 0$. This means that, as in standard QRPA, SCQRPA yields a Goldstone mode at zero energy. This feature signifies that the particle number symmetry is exactly restored.

It is well known that the restoration of good particle number implies in this very simple model case that the model is solved exactly [28]. We have already seen that one obtains the exact values for μ_1 and μ_2 . One can show that one also obtains the exact value for the ground-state energy (and therefore for the whole band of ground-state energies). This goes as follows. For the expectation value of H of Eq. (67) in the RPA ground state, using the analogous relations (28) and (33) for this case and the quasiparticle representation for H , we can write

$$\begin{aligned} E_0 = \langle H \rangle &= -\frac{g}{2} (\Omega + 1) \{ (1 - 2v^2) \langle \hat{N}_q \rangle + 2\Omega v^2 \} \\ &+ \frac{g}{4} \{ (1 - 2v^2)^2 \langle \hat{N}_q^2 \rangle + [4v^2 (\Omega (1 - 2v^2) - 1 \\ &+ v^2) - 8(1 - v^2)v^2 (XY + Y^2)] \langle \hat{N}_q \rangle \\ &+ 8\Omega (1 - v^2)v^2 (XY + Y^2) \\ &+ 4\Omega v^2 (1 - v^2 + \Omega v^2) \}. \end{aligned} \quad (71)$$

In this expression we have used the Casimir relation for this case $4Y^2(\Omega - \langle \hat{N}_q \rangle) = 2(\Omega + 1)\langle \hat{N}_q \rangle - \langle \hat{N}_q^2 \rangle$ that follows from Eq. (51). Using the expression for N and N^2 of Eqs. (68a) and (68b) once more, we see that the exact expression is recovered. It should be mentioned that because of the simplicity of the model, also the Lipkin-Nogami approach [32] solves the model exactly.

VII. CONCLUSION

In this work we extended for the first time the self-consistent RPA theory (SCQRPA) to the superfluid case for a model with more than one level. Indeed in Ref. [14] SCQRPA was already applied to the seniority model but this only allowed one to study rotation in gauge space whereas intrinsic excitations (β vibrations) are absent in the 0^+ sector of the seniority model. We have considered the two-level version of the pairing Hamiltonian with arbitrary degeneracies and fillings of the levels. We mostly considered the case $J=11/2$ for the upper and lower levels. This configuration was chosen in order to have a better comparison with the work by Sambataro and Dinh Dang [26], which in many aspects is quite analogous to ours. Indeed SCQRPA can be considered as a Bogoliubov transformation among quasiparticle pair operators $\alpha^\dagger \alpha^\dagger$ and $\alpha \alpha$, whereas in Ref. [26] the quasiparticle pair operators were replaced by ideal bosons $\alpha^\dagger \alpha^\dagger \sim B^\dagger$, and then a Bogoliubov transformation among these boson operators was applied while the pairing Hamiltonian was also bosonized up to fourth order. For such collective pairs as are formed in $J=11/2$ shells, a bosonization seems indeed valid and as expected our results are very close to the ones given in Ref. [26], even though they are consistently slightly better. This could be due to the fact that in SCQRPA one never bosonizes, and rather all constraints from Pauli principle are fully kept. However, we do not want to attribute much importance to these differences that only could become relevant for cases where a bosonization fails. On the other hand in our work, considerably more issues were studied. In the first place, this concerns the physical interpretation and identification of the low-lying state in SCQRPA. This state corresponds to the Goldstone mode in standard QRPA. However, in SCQRPA for finite N this state comes at finite energy and reproduces very precisely the difference $2(\mu^+ - \mu^-)$ of the chemical potentials of the exact solution. We also evaluated the fluctuation ΔN of the particle number and showed that, with respect to the fluctuation in BCS theory, there is a strong improvement. However, the particle number symmetry is still not entirely restored. Also for other quantities, SCQRPA is always superior to the BCS and QRPA approaches as explained in the main text. In fact the situation with respect to the particle number symmetry is somewhat particular and not encountered in other cases of spontaneously broken symmetries. For example, in the case of rotation the angular momentum operator L_z has no contributions that are Hermitian in the deformed basis, and then the Goldstone mode also comes in the case of SCRPA [34]. In order to improve on the restoration of the particle number symmetry we also investigated the possibility of fixing $\langle \hat{N}^2 \rangle = N^2$ with a second Lagrange multiplier. Whereas in the

one-level pairing model we could show analytically that this solves the model exactly, in the two-level model we could not find a numerical solution of the system of equations. It remained unclear whether this is due to some fundamental problem or just a numerical difficulty.

We also discuss carefully in this work the transition from the nonsuperfluid regime to the superfluid one. We, for instance, pointed out that the transition from SCRPA to SCQRPA is not continuous and in fact in both regimes quite different physical excitations are described. This also can be seen looking at the ground-state energies as a function of the coupling constant. In the transition region there is no continuous transition between the SCRPA and SCQRPA values but it is definitively seen that the SCRPA values for the ground-state energies deviate quite strongly from the exact values after the phase transition, whereas SCQRPA stays close to them.

In conclusion we can say that we have applied with very promising success for the first time SCQRPA to a more level pairing situation, where, at least for the 0^+ sector, all the complexity of a more realistic situation is present. It could be interesting to extend this work to the description of ultra-small superconducting metallic grains for which the many-level picket fence model seems appropriate [8].

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APPENDIX A: SOME USEFUL MATHEMATICAL RELATIONS

We will explain how we express the quasiparticle occupation number for each level j as a function of the RPA amplitudes. We start with the expectation value of (50) in the RPA state, we can write

$$\langle \hat{N}_{q,j} \rangle \approx 2\langle P_j^\dagger P_j \rangle + \frac{2}{\Omega - 1} \langle P_j^{\dagger 2} P_j^2 \rangle. \quad (\text{A1})$$

Using Eqs. (28) and (33) we find

$$\langle P_j^{\dagger 2} P_j^2 \rangle = K_{j,1} + K_{j,2} \langle P_j^\dagger P_j \rangle + K_{j,3} \langle P_j P_j^\dagger \rangle + K_{j,4} \langle P_j^\dagger P_j^\dagger \rangle, \quad (\text{A2})$$

where

$$K_{j,1} = \left(1 + \frac{2}{\Omega} \right) \{ (X_{j,1} Y_{j,1} + X_{j,2} Y_{j,2})^2 + 2(Y_{j,1}^2 + Y_{j,2}^2)^2 \},$$

$$\begin{aligned}
 K_{j,2} &= -\frac{2}{\Omega^2} \{2(X_{j,1}Y_{j,1} + X_{j,2}Y_{j,2})^2 + 3(Y_{j,1}^2 + Y_{j,2}^2)^2\}, \\
 K_{j,3} &= -\frac{2}{\Omega^2} \{(X_{j,1}Y_{j,1} + X_{j,2}Y_{j,2})^2 + 3(Y_{j,1}^2 + Y_{j,2}^2)^2\}, \\
 K_{j,4} &= -\frac{6}{\Omega^2} (X_{j,1}Y_{j,1} + X_{j,2}Y_{j,2})(Y_{j,1}^2 + Y_{j,2}^2). \quad (\text{A3})
 \end{aligned}$$

$$\begin{aligned}
 \langle \hat{N}_{q,j} \rangle &\simeq 2(Y_{j,1}^2 + Y_{j,2}^2) \left(1 - \frac{\langle \hat{N}_{q,j} \rangle}{\Omega} \right) + \frac{2}{(\Omega-1)} K_{j,1} \\
 &+ \frac{2}{(\Omega-1)} \{K_{j,2}(Y_{j,1}^2 + Y_{j,2}^2) + K_{j,3}(X_{j,1}^2 + X_{j,2}^2) \\
 &+ K_{j,4}(X_{j,1}Y_{j,1} + X_{j,2}Y_{j,2})\} \left(1 - \frac{\langle \hat{N}_{q,j} \rangle}{\Omega} \right). \quad (\text{A4})
 \end{aligned}$$

Expressing the remaining expectation values by $X_{j,\nu}$, $Y_{j,\nu}$ amplitudes, we obtain

Therefore, we can express $\langle \hat{N}_{q,j} \rangle$ as function of the RPA amplitudes,

$$\langle \hat{N}_{q,j} \rangle \simeq \frac{2(Y_{j,1}^2 + Y_{j,2}^2) + \frac{2}{(\Omega-1)} \{K_{j,1} + \Omega[K_{j,2}(Y_{j,1}^2 + Y_{j,2}^2) + K_{j,3}(X_{j,1}^2 + X_{j,2}^2) + K_{j,4}(X_{j,1}Y_{j,1} + X_{j,2}Y_{j,2})]\}}{1 + \frac{2}{\Omega}(Y_{j,1}^2 + Y_{j,2}^2) + \frac{2}{(\Omega-1)} \{K_{j,2}(Y_{j,1}^2 + Y_{j,2}^2) + K_{j,3}(X_{j,1}^2 + X_{j,2}^2) + K_{j,4}(X_{j,1}Y_{j,1} + X_{j,2}Y_{j,2})\}}. \quad (\text{A5})$$

In the same way, we express $\langle \hat{N}_{q,i}^2 \rangle$ and $\langle \hat{N}_{q,1}\hat{N}_{q,-1} \rangle$ as follows:

$$\langle \hat{N}_{q,i}^2 \rangle = 2(\Omega + 1) \langle \hat{N}_{q,i} \rangle - 4\Omega(Y_{j,1}^2 + Y_{j,2}^2) \left(1 - \frac{\langle \hat{N}_{q,j} \rangle}{\Omega} \right) \quad (\text{A6})$$

and

$$\langle \hat{N}_{q,1}\hat{N}_{q,-1} \rangle \simeq 4 \langle P_1^\dagger P_1 P_{-1}^\dagger P_{-1} \rangle \simeq \frac{4M}{1 - \frac{4}{\Omega^2}(Y_{1,1}^2 + Y_{1,2}^2)(Y_{-1,1}^2 + Y_{-1,2}^2)}, \quad (\text{A7})$$

where M is a constant depending of the RPA amplitudes, and is given by

$$\begin{aligned}
 M &= (Y_{1,1}^2 + Y_{1,2}^2)(Y_{-1,1}^2 + Y_{-1,2}^2) + \left(1 + \frac{2}{\Omega} \right) \{ (Y_{-1,1}X_{1,1} + Y_{-1,2}X_{1,2})(X_{-1,1}Y_{1,1} + X_{-1,2}Y_{1,2}) + (Y_{-1,1}Y_{1,1} + Y_{-1,2}Y_{1,2}) \\
 &\times (X_{-1,1}X_{1,1} + X_{-1,2}X_{1,2}) \} - \frac{2}{\Omega} [(Y_{-1,1}X_{1,1} + Y_{-1,2}X_{1,2})(X_{-1,1}X_{1,1} + X_{-1,2}X_{1,2}) \langle P_1^\dagger P_1 \rangle + (Y_{-1,1}Y_{1,1} + Y_{-1,2}Y_{1,2}) \\
 &\times (X_{-1,1}Y_{1,1} + X_{-1,2}Y_{1,2}) \langle P_1 P_1 \rangle + \{ (Y_{-1,1}X_{1,1} + Y_{-1,2}X_{1,2})(X_{-1,1}Y_{1,1} + X_{-1,2}Y_{1,2}) + (Y_{-1,1}Y_{1,1} + Y_{-1,2}Y_{1,2})(X_{-1,1}X_{1,1} \\
 &+ X_{-1,2}X_{1,2}) \} (2 \langle P_1^\dagger P_1 \rangle + \langle P_1 P_1 \rangle) + (Y_{-1,1}^2 + Y_{-1,2}^2)(X_{-1,1}Y_{1,1} + X_{-1,2}Y_{1,2}) \langle P_1^\dagger P_{-1}^\dagger \rangle + (Y_{-1,1}^2 + Y_{-1,2}^2)(Y_{-1,1}Y_{1,1} \\
 &+ Y_{-1,2}Y_{1,2}) \langle P_1^\dagger P_{-1} \rangle + \frac{1}{2}(Y_{1,1}^2 + Y_{1,2}^2)(Y_{-1,1}^2 + Y_{-1,2}^2)(\langle \hat{N}_{q,1} \rangle + \langle \hat{N}_{q,-1} \rangle)]. \quad (\text{A8})
 \end{aligned}$$

APPENDIX B: METHOD FOR CALCULATION OF $\hat{N}_{q,j}^k$

In this appendix, we will present our method inspired from Ref. [24] (see also Ref. [25]) for the derivation of the quantities of type $\hat{N}_{q,j}^k$ in the case of the two-levels pairing model. At first, we recall that in this model the operators $\hat{N}_{q,j}$, $P_{q,j}^\dagger$, and $P_{q,j}$ close the SU(2) algebra for each level j .

Consequently the two-level model fulfills an SU(2) \times SU(2) algebra. Thanks to this special group structure, it is easy to find a complete orthonormalized basis for the Hilbert subspace corresponding to each level j ,

$$|n_j\rangle = \sqrt{\frac{\Omega^{n_j}(\Omega - n_j)!}{\Omega! n_j!}} P_j^{\dagger n_j} |-\rangle, \quad j = \pm 1, \quad (\text{B1})$$

where $n_j=0,1,\dots,\Omega$. Using this basis, we can express the identity operator relative to each level j as

$$1_j = \sum_{n_j=0}^{\Omega} |n_j\rangle\langle n_j|$$

$$= |-\rangle\langle -| + \sum_{n_j=1}^{\Omega} \frac{\Omega^{n_j}(\Omega-n_j)!}{\Omega!n_j!} P_j^{\dagger n_j} |-\rangle\langle -| P_j^{n_j}, \quad j = \pm 1; \quad (\text{B2})$$

therefore, we can express the projector $|-\rangle\langle -|$ as follows:

$$|-\rangle\langle -| = 1_j - \sum_{n_j=1}^{\Omega} \frac{\Omega^{n_j}(\Omega-n_j)!}{\Omega!n_j!} P_j^{\dagger n_j} |-\rangle\langle -| P_j^{n_j}. \quad (\text{B3})$$

One sees that Eq. (B3) produces an expansion of the form

$$|-\rangle\langle -| = \sum_{m_j=0}^{\Omega} \beta_{m_j} P_j^{\dagger m_j} P_j^{m_j}, \quad (\text{B4})$$

if we substitute Eq. (B4) in both the lhs and rhs of Eq. (B3), we obtain the coefficients β_{m_j} ,

$$\beta_0 = 1, \quad \beta_{m_j} = - \sum_{l=0}^{m_j-1} \frac{\Omega^{m_j-l}(\Omega-m_j+l)!}{\Omega!(m_j-l)!} \beta_l. \quad (\text{B5})$$

For example, the first terms β_{m_j} are explicitly given by

$$\beta_0 = 1,$$

$$\beta_1 = -1,$$

$$\beta_2 = \frac{\Omega-2}{2(\Omega-1)},$$

$$\beta_3 = - \frac{\Omega^2-6\Omega+12}{6(\Omega-1)(\Omega-2)}. \quad (\text{B6})$$

However, to calculate the quantities $\hat{N}_{q,j}$ and $\hat{N}_{q,j}^2$, one can expand these operators as

$$\hat{N}_{q,j}^k = \sum_{l_j=1}^{\Omega} \alpha_{l_j}^{(k)} P_j^{\dagger l_j} P_j^{l_j}, \quad j = \pm 1. \quad (\text{B7})$$

For all operators of the form $\hat{N}_{q,j}^k$, using the fact that

$$\hat{N}_{q,j}|n_j\rangle = 2n_j|n_j\rangle, \quad (\text{B8})$$

we can calculate

$$\hat{N}_{q,j}^k = \sum_{n_j=0}^{\Omega} \hat{N}_{q,j}^k |n_j\rangle\langle n_j| \quad (\text{B9a})$$

$$= \sum_{n_j=0}^{\Omega} (2n_j)^k |n_j\rangle\langle n_j| \quad (\text{B9b})$$

$$= \sum_{n_j=0}^{\Omega} \frac{\Omega^{n_j}(\Omega-n_j)!}{\Omega!n_j!} (2n_j)^k P_j^{\dagger n_j} |-\rangle\langle -| P_j^{n_j}. \quad (\text{B9c})$$

By inserting Eq. (B4) in the rhs of Eq. (B9c) and substituting Eq. (B7) into the lhs of Eq. (B9c), we obtain

$$\hat{N}_{q,j}^k = \sum_{n_j=0}^{\Omega} \frac{\Omega^{n_j}(\Omega-n_j)!}{\Omega!n_j!} (2n_j)^k \sum_{m_j=0}^{\Omega} \beta_{m_j} P_j^{\dagger n_j} P_j^{\dagger m_j} P_j^{m_j} P_j^{n_j},$$

$$\sum_{l_j=1}^{\Omega} \alpha_{l_j}^{(k)} P_j^{\dagger l_j} P_j^{l_j}$$

$$= \sum_{n_j=1}^{\Omega} \frac{\Omega^{n_j}(\Omega-n_j)!}{\Omega!n_j!} (2n_j)^k \sum_{m_j=0}^{\Omega} \beta_{m_j} P_j^{\dagger n_j+m_j} P_j^{n_j+m_j}$$

$$= \sum_{l_j=1}^{\Omega} \sum_{m_j=0}^{l_j-1} \frac{\Omega^{l_j-m_j}(\Omega-l_j+m_j)!}{\Omega!(l_j-m_j)!}$$

$$\times [2(l_j-m_j)]^k \beta_{m_j} P_j^{\dagger l_j} P_j^{l_j}. \quad (\text{B10})$$

Therefore, by identification, from Eq. (B10) it is easy to get the coefficients $\alpha_{l_j}^{(k)}$,

$$\alpha_{l_j}^{(k)} = \sum_{m_j=0}^{l_j-1} \frac{\Omega^{l_j-m_j}(\Omega-l_j+m_j)!}{\Omega!(l_j-m_j)!} [2(l_j-m_j)]^k \beta_{m_j}. \quad (\text{B11})$$

To calculate $\hat{N}_{q,j}$ we put $k=1$ in (B7), and find

$$\hat{N}_{q,j} = \sum_{l_j=1}^{\Omega} \alpha_{l_j}^{(1)} P_j^{\dagger l_j} P_j^{l_j}, \quad (\text{B12})$$

with

$$\alpha_{l_j}^{(1)} = \sum_{m_j=0}^{l_j-1} \frac{\Omega^{l_j-m_j}(\Omega-l_j+m_j)!}{\Omega!(l_j-m_j)!} [2(l_j-m_j)] \beta_{m_j}. \quad (\text{B13})$$

The first coefficients $\alpha_{l_j}^{(1)}$ are explicitly given by

$$\alpha_1^{(1)} = 2,$$

$$\alpha_2^{(1)} = \frac{2}{\Omega-1},$$

$$\alpha_3^{(1)} = \frac{4}{(\Omega-1)(\Omega-2)},$$

$$\alpha_4^{(1)} = \frac{2(5\Omega - 6)}{(\Omega - 1)^2(\Omega - 2)(\Omega - 3)}. \quad (\text{B14})$$

Therefore, for $\hat{N}_{q,j}$ we can write

$$\begin{aligned} \hat{N}_{q,j} = & 2P_j^\dagger P_j + \frac{2}{\Omega - 1} P_j^{\dagger 2} P_j^2 + \frac{4}{(\Omega - 1)(\Omega - 2)} P_j^{\dagger 3} P_j^3 \\ & + \frac{2(5\Omega - 6)}{(\Omega - 1)^2(\Omega - 2)(\Omega - 3)} P_j^{\dagger 4} P_j^4 + \dots. \end{aligned} \quad (\text{B15})$$

In the same way, it is very easy using this method to find an expansion for $\hat{N}_{q,j}^2$; it is sufficient to put $k=2$ in Eq. (B7) and calculate $\alpha_j^{(2)}$. We find

$$\begin{aligned} \hat{N}_{q,j}^2 = & 4P_j^\dagger P_j + \frac{4(\Omega + 1)}{\Omega - 1} P_j^{\dagger 2} P_j^2 + \frac{8(\Omega + 1)}{(\Omega - 1)(\Omega - 2)} P_j^{\dagger 3} P_j^3 \\ & + \frac{4(\Omega + 1)(5\Omega - 6)}{(\Omega - 1)^2(\Omega - 2)(\Omega - 3)} P_j^{\dagger 4} P_j^4 + \dots. \end{aligned} \quad (\text{B16})$$

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