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Projected quasiparticle perturbation theory

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The BCS and/or Hartree-Fock-Bogoliubov theories are extended by treating the effect of four quasiparticle states perturbatively. The approach is tested on the pairing Hamiltonian, showing that it combines the advantage of standard perturbation theory, valid at low pairing strength, and of nonperturbative approaches breaking the particle number, valid at higher pairing strength. Including the restoration of particle number further improves the description of pairing correlation. In the presented test, the agreement between the exact solution and the combined perturbative plus projection is almost perfect. The proposed method scales friendly when the number of particles increases and provides a simple alternative to other more complicated approaches.

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I. INTRODUCTION

Theories breaking explicitly the particle number, such as Bardeen-Cooper-Schrieffer (BCS) or Hartree-Fock-Bogoliubov (HFB) are the simplest efficient ways to describe pairing correlations in physical systems. However, these theories suffer from some limitations especially when the number of particles becomes rather small as is the case in mesoscopic systems such as nuclear physics [1] or condensed matter [2]. The main difficulty is the sharp transition from normal to superfluid phases as the pairing strength increases. The second difficulty is a systematic underestimation of pairing correlations that increases when the particle number decreases.

Recently, several approaches have been used to overcome these difficulties. When the number of particles is small enough, the exact solution of the pairing problem is accessible by direct diagonalization of the Hamiltonian [3–5] and/or using the secular equation originally proposed by Richardson [6–8]. Accurate description of the ground-state energy of superfluid systems with a larger particle number can be obtained using either quantum Monte Carlo technique (see for instance Refs. [9,10]) or extending quasiparticle theories using variation after projection approaches [11–22] (for recent applications see Refs. [23–25]). All of these methods are, however, rather involved and demanding in terms of computational power. The aim of the present work is to show that a perturbative approach can eventually provide a simpler and yet accurate alternative to treat the pairing problem.

In the following, standard perturbation theory is first recalled. It is then explained how to take advantage of both perturbative approaches and BCS-HFB theories. The importance of particle number restoration is finally highlighted.

II. STANDARD PERTURBATION THEORY

Our starting point here is similar to the one used in Refs. [9,26]. We assume a two-body pairing Hamiltonian given by

$$H = \sum_{i=1}^{\Omega} \varepsilon_i (a_i^\dagger a_i + a_{\bar{i}}^\dagger a_{\bar{i}}) + \sum_{i\neq j}^{\Omega} v_{ij} a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j \equiv H_0 + V. \quad (1)$$

Here, $(i, \bar{i})$ denotes a time-reversed pair. Such a Hamiltonian can be for instance constructed starting from a realistic self-consistent mean-field calculation providing single-particle energies and two-body matrix elements [10].

Here Ω denotes the maximal number of accessible levels for the pairs of particles. In the following, we will consider the specific case of equidistant levels with $\varepsilon_i = (i-1)\Delta\varepsilon$ with $\Delta\varepsilon = 1$ MeV and a number of particles $N = \Omega$.

As already noted some time ago [27] and recently discussed again [26,28], the two-body part V can be treated perturbatively to provide an accurate description of the pairing problem in the weak pairing interaction regime. Starting from the ground state $|\Phi_0\rangle$ of H_0, that corresponds to the Slater determinant obtained by occupying the lowest single-particle states, other excited states while other excited states $|\Phi_n\rangle$ of H_0 can be obtained by considering particle-hole (p-h), 2p-2h, ... excitations built on top of the $|\Phi_0\rangle$. Using second-order perturbation theory, the ground state energy of H reads

$$\mathbf{E}_0 = E_0 + E_0^{(2)}, \quad (2)$$

where $E_0 = 2\sum_{i=1,N_{\rm pair}} \varepsilon_i$ (with $N_{\rm pair} = N/2$) is the ground-state energy of H_0 while $E_0^{(2)}$ is the standard second-order correction, that can be found in textbook,

$$E_0^{(2)} = \sum_{n\neq 0} \frac{|\langle\Phi_0|V|\Phi_n\rangle|^2}{E_0 - E_n}. \quad (3)$$

In the specific case considered here [i.e., Eq. (1)] only 2p-2h states contribute to the second-order correction. More precisely, the states n could only differ from the ground state by one occupied pair above the Fermi sea (denoted by j) and one unoccupied pair below (denoted by i): $|\Phi_{i,j}\rangle = a_j^\dagger a_{\bar{j}}^\dagger a_{\bar{i}} a_i |\Phi_0\rangle$ and are eigenstates of H_0 with energy $E_{ij} = E_0 + 2(\varepsilon_j - \varepsilon_i)$. This leads to

$$E_0^{(2)} = -\frac{1}{2} \sum_{i=1,N_{\rm pair}} \sum_{j=N_{\rm pair}+1,N_{\rm max}} \frac{|v_{ij}|^2}{\varepsilon_j - \varepsilon_i}, \quad (4)$$

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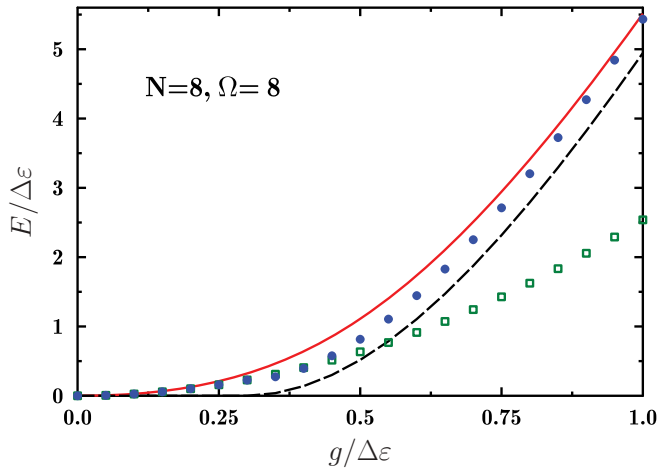

FIG. 1. (Color online) Illustration of the correlation energy as a function of the coupling strength for the case of $N = 8$ particles and $\Omega = 8$. The exact result solution (red solid curve), BCS (black dashed line), standard perturbation theory (green open squares), and Eq. (3) and QP^{2}T theory with second-order correction Eq. (14) (blue filled circles), are displayed.

with $N_{\rm pair} = N/2$ and $N_{\rm max} = \Omega/2$. This expression has been obtained in Ref. [28] using a different approach based on the Richardson-Gaudin equation. It is known [26,27] that standard perturbation theory provides an appropriate description in the weak coupling regime.

In Fig. 1, an example of standard perturbation theory (SPT) is presented for the $N = 8$ particles and constant coupling case (i.e., $v_{ij} = -g$). The correlation energy defined as the difference between the Hartree-Fock energy E_0 and the ground-state energy $\mathbf{E}_0$ obtained with STP are compared to the exact solution and BCS result. In the latter case, pairing correlation is nonzero only above the threshold value $g/\Delta\varepsilon \simeq 0.3$. As illustrated from Fig. 1, standard perturbation theory matches with the exact result below the threshold but significantly underestimates the correlation for larger g value. This aspect underlines the highly nonperturbative nature of the pairing quantum phase transition. On the contrary, one of the advantages of a theory such as BCS is the possibility to incorporate nonperturbative physics even in the strong interaction case by breaking the $U(1)$ symmetry associated to particle number conservation.

III. QUASIPARTICLE PERTURBATION THEORY

To provide a proper description of both the weak and strong pairing strength regimes, it seems quite natural to try to combine theories based on quasiparticles and perturbative approaches. This possibility has been explored in Refs. [29,30] mainly to discuss the removal of the dangerous diagram occurring in normal perturbation theory. Note that recently it has also been revisited as a possible tool to perform *ab initio* calculations in nuclei [31] based on Gorkov-Green function formalism [32]. In the following, it is assumed that the BCS-HFB approach has been applied in a preliminary study and that the Hamiltonian (1) is written in the canonical basis of the quasiparticle ground state. Then, the ground state takes the form

$$|\Phi_0\rangle = \prod_{i>0}(U_i + V_i a_i^\dagger a_{\bar{i}}^\dagger)|-\rangle, \tag{5}$$

and is the vacuum of the quasiparticle creation operators defined through

$$\beta_i^\dagger = U_i a_i^\dagger - V_i a_{\bar{i}}, \tag{6}$$

$$\beta_{\bar{i}}^\dagger = U_i a_{\bar{i}}^\dagger + V_i a_i. \tag{7}$$

In the BCS-HFB theory, the original hamiltonian is replaced by an effective Hamiltonian that is conveniently written as[1]

$$H_0 = E_0 + \sum_i E_i(\beta_i^\dagger \beta_i + \beta_{\bar{i}}^\dagger \beta_{\bar{i}}), \tag{8}$$

where E_0 is the BCS/HFB ground state energy, while E_i corresponds to the quasiparticle energy given by

$$E_i = \sqrt{(\varepsilon_i - \lambda)^2 + \Delta^2}, \tag{9}$$

where λ is the Lagrange multiplier used to impose the average particle number while Δ is the pairing gap (for a detailed discussion see Ref. [33]).

For even systems, excited states of H_0 are two-quasiparticle (2QP), four-quasiparticle (4QP), ... excitations with respect to the ground state. The original Hamiltonian H contains many terms that are neglected in H_0 [1] and that are responsible from the deviation between the quasiparticle and the exact solution. However, noting that

$$H|\Phi_0\rangle = \left(H_0 - \sum_{i\neq j} v_{ij} U_i^2 V_j^2 \beta_i^\dagger \beta_{\bar{i}}^\dagger \beta_j^\dagger \beta_{\bar{j}}^\dagger\right)|\Phi_0\rangle, \tag{10}$$

it can be anticipated that the main source of discrepancy is due to the coupling of Φ_0 with the 4QP states. Some arguments showing that 4QP states should improved the description of pairing especially in the weak coupling regime have been given in Ref. [34].

Below, perturbation theory is applied assuming that H_0 [Eq. (8)] is the unperturbed Hamiltonian while the perturbation V is given by

$$V = -\sum_{i\neq j} v_{ij} U_i^2 V_j^2 \beta_i^\dagger \beta_{\bar{i}}^\dagger \beta_j^\dagger \beta_{\bar{j}}^\dagger. \tag{11}$$

V couples the ground state with the 4QP states, defined as (for $i > j$)

$$|\Phi_{i,j}\rangle = \beta_i^\dagger \beta_{\bar{i}}^\dagger \beta_j^\dagger \beta_{\bar{j}}^\dagger |\Phi_0\rangle \tag{12}$$

and associated to the unperturbed energy

$$E_{ij} = E_0 + 2(E_i + E_j). \tag{13}$$

The present approach, that is a direct extension of standard perturbation theory, is called hereafter quasiparticle perturbation theory (QP^{2}T). Using Eq. (3), the second order correction

[1]Note that here, it is implicitly assumed that H is replaced by $H - \lambda N$

to the ground state energy is equal to:

$$E_0^{(2)} = -\frac{1}{2}\sum_{i>j} v_{ij}^2 \frac{\left(U_i^2 V_j^2 + U_j^2 V_i^2\right)^2}{E_i + E_j}. \quad (14)$$

This correction properly extends Eq. (4) from the normal to the superfluid phase. Indeed at the threshold value of g (i.e., when $\Delta \to 0$) the 4QP states identify with 2p-2h excitations while

$$E_i + E_j \to |\varepsilon_i - \lambda| + |\varepsilon_j - \lambda| = \varepsilon_i - \varepsilon_j, \quad (15)$$

and the standard perturbation theory case is recovered.

The result obtained with the QP^{2}T approach at second order in perturbation (14) are displayed in Fig. 1 with filled circles. Note that below the BCS threshold, standard perturbation theory is used. The present approach can be regarded as a rather academic exercise but it turns out to provide a very simple way to extend mean-field theory based on quasiparticle states. In particular, it avoids the threshold problem of the latter and improves the description of correlation in the intermediate and strong coupling case.

IV. EFFECT OF THE RESTORATION OF PARTICLE NUMBER

Similarly to the original quasiparticle theory, the energy deduced from the QP^{2}T contains a spurious contribution coming from the fact that the perturbed state does not preserve the particle number. Indeed, using standard formulas, to second order in perturbation, the ground state expresses as

$$\begin{aligned} |\Psi_0\rangle &= \left|\Psi_0^{(0)}\right\rangle + \left|\Psi_0^{(1)}\right\rangle + \left|\Psi_0^{(2)}\right\rangle \cdots \\ &= |\Phi_0\rangle + \sum_{i>j} c_{ij} |\Phi_{i,j}\rangle + \cdots \end{aligned} \quad (16)$$

where $|\Psi_0^{(i)}\rangle$, $i = 0, 1, \ldots$ denotes the contribution to the state at i^{th} order in perturbation and where

$$c_{ij} = -\frac{v_{ij}}{2}\frac{\left(U_i^2 V_j^2 + U_j^2 V_i^2\right)}{E_i + E_j}. \quad (17)$$

Above the BCS threshold, neither $|\Phi_0\rangle$ nor $|\Phi_{i,j}\rangle$ are eigenstates of the particle number operator.

The most direct way to remove spurious contributions due to the mixing of different particle numbers is to introduce the operator P^N

$$P^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \; e^{i\varphi(\hat{N}-N)}. \quad (18)$$

that projects onto particle number N.

The most straightforward way to combine projection with quasiparticle perturbation theory is to directly take the expectation value

$$\mathbf{E}_0 = \frac{\left\langle \Psi_0^N \middle| H \middle| \Psi_0^N \right\rangle}{\left\langle \Psi_0^N \middle| \Psi_0^N \right\rangle} \quad (19)$$

with $|\Psi_0^N\rangle = P^N|\Psi_0\rangle$ and where $|\Psi_0\rangle$ is truncated at a given order in perturbation. This approach will be referred to as the projected quasiparticle perturbation theory (QP^{3}T) in the following. When only the zero order in perturbation is retained in Eq. (16), the QP^{3}T identifies with the projection after variation (PAV) that is commonly used, especially in the nuclear energy density functional (EDF) approach [35]. Formulas useful to compute the expectation values of one- and two-body operators with projection are given in Appendix. The projection is performed numerically using these expressions and the Fomenko discretization procedure of the gauge-space integrals [36,37]. Here, 199 discretization points have been used. Note that the number of points can be reduced down to five without changing the result. The correlation energies obtained for $N = 2$, $N = 8$, and $N = 12$ (each time with $\Omega = N$) using the second-order QP^{3}T are shown in Figs. 2–4 respectively. In each case, the original BCS, the PAV, and the exact solution are also shown. The result of QP^{3}T almost superimposed with the exact solution. Only a slight difference can be seen around the BCS threshold.

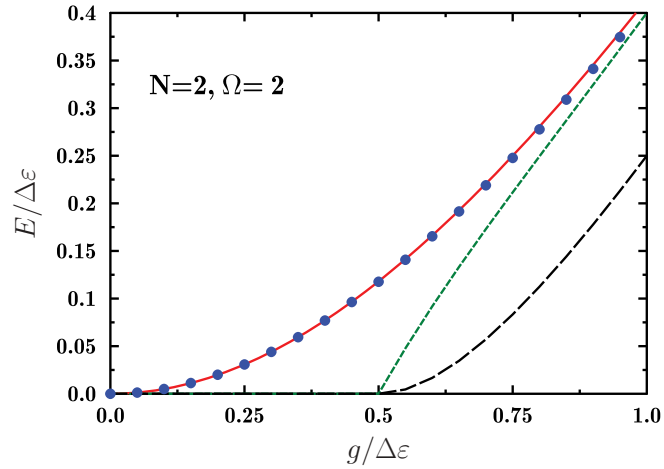

FIG. 2. (Color online) Illustration of the correlation energy as a function of the coupling strength for the case of $N = 2$ particles and $\Omega = 2$. The exact result solution (red solid line), PAV result (green short-dashed line), and the QP^{3}T theory (blue filled circles) are shown. The original BCS (black long dashed line) is also shown as a reference.

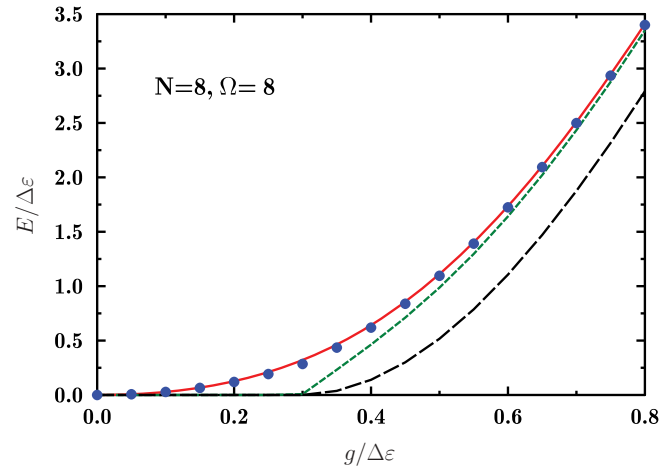

FIG. 3. (Color online) Same as Fig. 2 for the $N = \Omega = 8$ case.

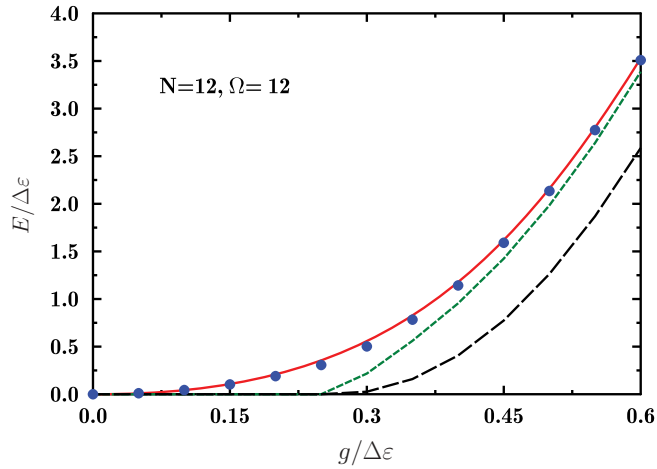

FIG. 4. (Color online) Same as Fig. 2 for the $N = \Omega = 12$ case.

Besides the energy, other observables can also be estimated. As an example, the quantity $n_i(1 - n_i)$ is shown in Fig. 5 as a function of single-particle energies, where n_i are the occupation numbers of single-particle states. This quantity is a measure of the deviation from the independent particle picture where it is strictly zero for all states. The use of perturbation and projection considerably improves the description of one-body observables especially at intermediate coupling where the original BCS deviates significantly from the exact solution. In addition, even if the PAV differs significantly from the exact

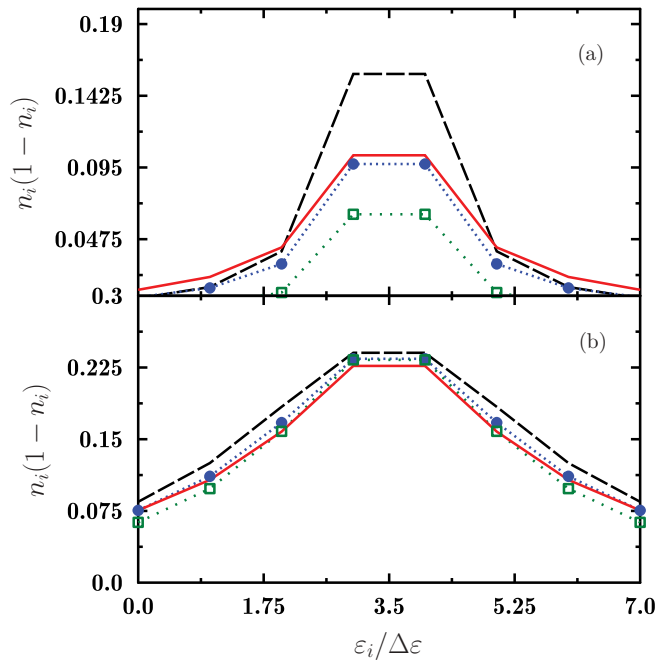

FIG. 5. (Color online) Example of evolution of the quantity $n_i(1 - n_i)$ obtained with QP^{3}T (filled blue circles) as a function of single-particle energy for the $N = \Omega = 8$ case with $g/\Delta\varepsilon = 0.4$ (a) and 0.8 (b). In both cases, the exact result (red solid line), the BCS result (black dashed line), and the PAV result (green open squares) are shown.

case as it was noted in Ref. [22], the extra mixing with the 4QP states compensates this drawback of PAV.

In view of this agreement, it seems that the QP^{3}T does automatically select important many-body states, namely projected ground state and projected 4QP states, on which the true eigenstate decomposes. These states are highly nontrivial multiparticle multihole mixings that can also be described by direct diagonalization of the Hamiltonian but that are much more demanding numerically. Indeed, the size of the 4QP Hilbert space is $\Omega(\Omega - 1)/2$ while the size of the matrix to diagonalize the hamiltonian is $(\Omega!/[N_{\text{pair}}!(\Omega - N_{\text{pair}})!])$. It is important to recall that here no diagonalization is required since the mixing coefficients are directly given by the quasiparticle perturbation theory [Eq. (17)]. These features make the approach rather simple to implement on existing BCS-HFB codes to provide a much better approximation than the PAV that is often currently used. In addition, by contrast to the variation after projection that is rather involved [23,25], no extra minimization is required.

It should be noted that the way we apply the perturbation theory is rather unusual. Indeed, here we directly take the coefficients obtained from a perturbative approach based on quasiparticle states and use them to express the ground state in terms of the projected states. Doing so, we clearly break the self-consistency as in PAV. A more consistent approach would be to develop a perturbative approach directly with the projected states. The difficulty in the latter case is that, while the separation into an unperturbed Hamiltonian and residual interaction parts was straightforward in the quasiparticle case, such a separation is not easy for projected states

Contrary to the exact diagonalization, the QP^{2}T and QP^{3}T can be performed even for large particle number. As an illustration, in Fig. 6, a systematic study of the correlation energy evolution obtained with some of the approaches presented above as the number of particle increases up to $N = 100$ for the case $g/\Delta\varepsilon = 0.8$. With standard diagonalization techniques, the exact solution can hardly be obtained for $N > 14$. Other approaches based on quasiparticle theories can be applied without difficulties. Note however, that the QP^{3}T requires to perform more and more gauge angles integrations (see

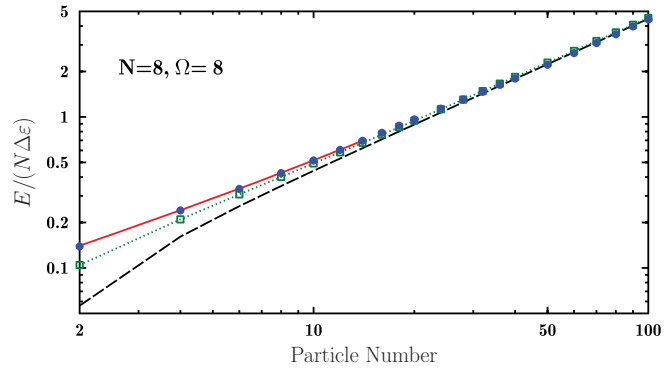

FIG. 6. (Color online) Evolution of the correlation energy per particle as a function of the number of particles for $g/\Delta\varepsilon = 0.8$ for the BCS (black dashed line), QP^{2}T (green open squares), and QP^{3}T (blue filled circles). The exact case (solid red line) is also shown up to $N = 14$ particles.

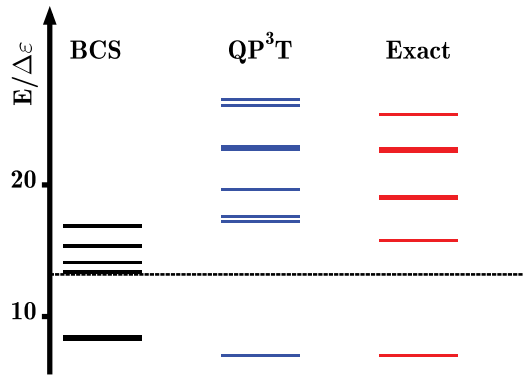

FIG. 7. (Color online) Example of energies of 2QP excited states obtained with BCS (left), QP^{3}T built on 2QP states (middle), and exact (right) using $N = \Omega = 8$ and $g = 0.8$. The ground state is also shown. The horizontal dashed line corresponds to the HF energy. Note that to avoid specific aspects related to degeneracy, the fourth single-particle level has been shifted to $2.9\Delta\varepsilon$ (instead of $3\Delta\varepsilon$).

Appendix) as N increases making the calculations more time consuming with respect to the nonprojected theories such as BCS or QP^{2}T.

From Fig. 6, we also note that differences between theories are seen only for rather small particle number $N < 30$, while above BCS and QP^{3}T cannot be distinguished. However, as it has been discussed previously, for $N < 30$, the QP^{3}T is the only theory that can provide an excellent reproduction of the exact result when available.

A. Discussion

Perturbation theory can also be applied to get excited states. Starting from 2QP, 4QP, ... one can get a correction to the energies of excited states with or without projection. An illustration of energies obtained starting from 2QP states is given in Fig. 7. We see in this figure that both original 2QP states and the energies obtained with QP^{3}T are still quite far from the exact results.

Since the present study underlines the relevance of projected states based on quasiparticle excitation, one possible way to improve the description of the excited state would be to directly diagonalize the Hamiltonian in a truncated space of these projected states.

Besides the description of excitations, such a diagonalization could also be anticipated as a possible way to treat the effect of other degrees of freedom like deformation. Currently, the generator coordinate method (GCM) [1] is widely used to account for quantum fluctuations associated to collective degrees of freedom [35]. Most often, only the lowest-energy BCS or HFB state is included in the mixing of configurations. The natural extension would be to include excited states based on projected QP excitations. This idea has been, for instance, followed in Ref. [38] where the effect of 2QP states is investigated. Here we clearly point out that the inclusion of 4QP states is desirable. It should however be kept in mind that this will further increase the complexity of the calculation.

V. SUMMARY

In this work an extension of the standard many-body theory to treat the pairing problem is introduced. Including the effect of 4QP perturbatively to extend usual BCS-HFB removes the problem of sharp transition from normal to superfluid phase and significantly improves the description of pairing. Last, when restoration of particle number is performed within the perturbative approach, a perfect agreement with the exact results is found. This finding provides a direct proof of the importance of 4QP state to extend mean-field theories. In addition, it is shown that the quasiparticle perturbation theory can be implemented even for a large particle number without special difficulties, making the technique rather attractive and much simpler than other approaches, like full diagonalization, variation after projection or quantum Monte Carlo techniques. Last, it is worth mentioning that the present technique can be directly and rather easily implemented on existing BCS-HFB codes [39,40] to improve the description of pairing correlations.

Recently, the use of Gorkov-Green function theory has been proposed [31] as a possible tool to perform *ab initio* calculation for nuclei. This theory provides a general formalism based on quasiparticle states. The result obtained in the present study are rather encouraging to pursue in that direction and that projection might be needed.

ACKNOWLEDGMENTS

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APPENDIX: EXPRESSION OF PROJECTED QUANTITIES

Starting from the standard expression of the quasiparticle ground state [Eq. (5)], the 4QP states are given by

$$|\Phi_{i,j}\rangle = (-V_i + U_i a_i^\dagger a_{\bar{i}}^\dagger)(-V_j + U_j a_j^\dagger a_{\bar{j}}^\dagger) \times \prod_{k>0, k\neq(i,j)} (U_k + V_k a_k^\dagger a_{\bar{k}}^\dagger)|-\rangle. \quad \text{(A1)}$$

For compactness, this expression is written as

$$|\Phi_m\rangle = \prod_{k>0} \left(U_k^m + V_k^m a_k^\dagger a_{\bar{k}}^\dagger\right)|-\rangle. \quad \text{(A2)}$$

This notation includes the ground-state case ($m = 0$). The state obtained in QP^{3}T can be generically written as $|\Psi_0^N\rangle = \sum_m c_m P_N |\Phi_m\rangle$, and for any operator O that conserves the particle number, we have

$$\left\langle \Psi_0^N \middle| O \middle| \Psi_0^N \right\rangle = \sum_{m,n} c_n^* c_m \langle \Phi_n | O P^N | \Phi_m \rangle, \quad \text{(A3)}$$

where

$$\langle \Phi_n | O P^N | \Phi_m \rangle = \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi} \langle \Phi_n | O | \Phi_m(\varphi) \rangle, \quad \text{(A4)}$$

and

$$|\Phi_m(\varphi)\rangle = \prod_{k>0} \left(U_k^m + V_k^m e^{2i\varphi} a_k^\dagger a_{\bar{k}}^\dagger\right)|-\rangle. \tag{A5}$$

Starting from this expression it could be deduced that

$$\begin{aligned}
\langle\Phi_n|P^N|\Phi_m\rangle &= \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\varphi N} \prod_{k>0}\left(U_k^n U_k^m + V_k^n V_k^m e^{2i\varphi}\right),\\
\langle\Phi_n|a_i^\dagger a_i P^N|\Phi_m\rangle &= \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\varphi N} V_i^n V_i^m e^{2i\varphi} \prod_{k>0,k\neq i}\left(U_k^n U_k^m + V_k^n V_k^m e^{2i\varphi}\right),\\
\langle\Phi_n|a_i^\dagger a_{\bar{i}}^\dagger a_{\bar{j}} a_j P^N|\Phi_m\rangle &= \frac{1}{2\pi}\int_0^{2\pi} d\varphi e^{-i\varphi N} V_i^n U_i^m U_j^n V_j^m e^{2i\varphi} \prod_{k>0,k\neq(i,j)}\left(U_k^n U_k^m + V_k^n V_k^m e^{2i\varphi}\right),
\end{aligned} \tag{A6}$$

where the latter expression is valid for $i \neq j$.

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