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Nuclear pairing correlations within and beyond HFB-BCS models

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Abstract. Pairing correlations in nuclear systems play a crucial role in several aspects, i.e. binding energies and odd-even effects, superfluid phenomena and pair transfer mechanisms, just to quote few of them. On the theoretical side, the standard description of these features is done by using BCS or HFB models which allow to describe in a simple way pairing effects. However, due to the explicit breaking of the particle number, these theories present some limitations which can be cured by using particle number projection techniques. In this paper, we will show the merits of these techniques and their accuracy in treating pairing correlations. First, a beyond BCS-HFB method is introduced where the effect of four quasi-particle states is included perturbatively and subsequently the particle number is restored. We will then show the need of restoring the good particle number also for excited states that are essential in the pair transfer process between superfluid systems. Applications to the Richardson model are shown and discussed.

1. Introduction

The mean-field description of pairing correlations in superconducting systems is typically described within the Bardeen-Cooper-Schrieffer (BCS) or Hartree-Fock-Bogoliubov (HFB) approximations, eventually augmented by Quasi-particle Random Phase Approximation (QRPA) for the description of excited states. Both levels of approximation violate the particle number symmetry. These methods suffer thus from particle number fluctuations that have to be cured in the case of finite systems, (for a recent review see refs [1]). This goal can be accomplished by using projection techniques, usually performed in the projection after variation (PAV) scheme, where unphysical components are “a posteriori” projected out. Only few calculations have been done at the variation after projection scheme, which allows a fully self-consistent treatment of the symmetries but is numerically highly demanding. In the last decades, several approaches have been used to overcome these difficulties. When the number of particle is small enough, the exact solution of the pairing problem is accessible by direct diagonalization of the Hamiltonian [2, 3, 4], Quantum Monte-Carlo technique (see for instance [5, 6]) or extending quasi-particle theories using Variation After Projection approaches [7, 8] (for recent applications see [9, 10, 11]), or the generalized seniority scheme [12]. All of these methods are however rather involved and



demanding in terms of computational power. In this paper we discuss two accurate methods where the particle number symmetry is restored by using projection techniques in a PAV like spirit. In Section 2 the treatment of the ground state correlation are discussed [13] while in Section 3 a method for the description of excited states is proposed [14]. Applications are done in the Richardson model [15].

2. Quasi-particle perturbative approach for g.s. correlations

Let's consider 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 time-reversed pair and Ω denotes the number of levels. 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 $N = \Omega$.

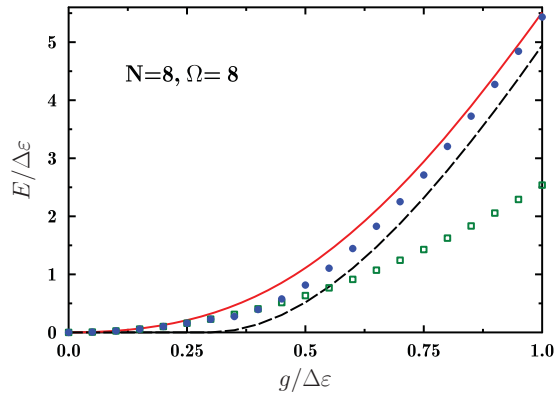


Figure 1. (color online) Illustration of the correlation energy as a function of the coupling strength for the case of $N=8$ particles and $\Omega = 8$. The exact result solution (red solid curve), BCS (black dashed line), standard perturbation theory (green open squares), QP²T theory with second order correction equation (6) (blue filled circles), are displayed.

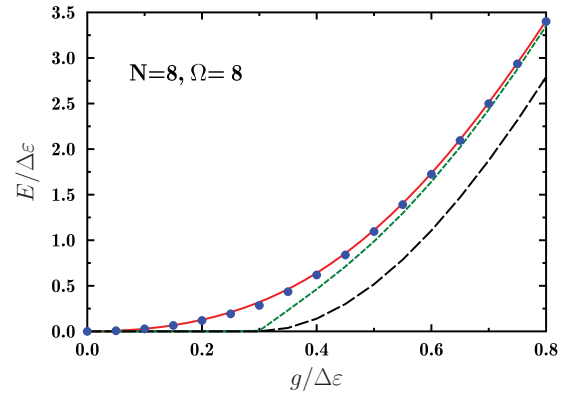


Figure 2. (color online) Illustration of the correlation energy as a function of the coupling strength for the case of $N=8$ particles and $\Omega = 8$. The exact result solution (red solid line), PAV result (green short-dashed line) and the combination of projection and perturbation theories (blue filled circles) are shown. The original BCS (black long dashed line) is also shown as a reference.

In figure 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 within the SPT are compared to the exact solution and BCS result. In the latter case, pairing correlation is non-zero 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 non-perturbative nature of the pairing quantum phase-transition. On the opposite, one of the advantage a theory like BCS is the possibility to incorporate non-perturbative physics.

In order to obtain a better description we can combine theories based on quasi-particles and perturbative approaches. Let's consider then the BCS/HFB state

$$|\Phi_0\rangle = \prod_{i>0} (U_i + V_i a_i^\dagger) |-\rangle, \quad (2)$$

and the effective mean field BCS/HFB Hamiltonian

$$H_0 = E_0 + \sum_i E_i (\beta_i^\dagger \beta_i + \beta_i^\dagger \beta_i) \quad (3)$$

where E_0 is the BCS/HFB ground state energy, while E_i corresponds to the quasi-particle energy given by. It is easy to see that

$$H|\Phi_0\rangle = \left(H_0 - \sum_{i \neq j} v_{ij} U_i^2 V_j^2 \beta_i^\dagger \beta_i^\dagger \beta_j^\dagger \beta_j^\dagger \right) |\Phi_0\rangle, \quad (4)$$

showing that that the main effect of the neglected residual interaction is due to the coupling of Φ_0 with the 4QP states. We consider thus the perturbation V :

$$V = - \sum_{i \neq j} v_{ij} U_i^2 V_j^2 \beta_i^\dagger \beta_i^\dagger \beta_j^\dagger \beta_j^\dagger. \quad (5)$$

coupling the ground state with the 4QP states. The present approach, that is a direct extension of standard perturbation theory, is called hereafter quasi-particle perturbation theory (QP²T). The second order correction to the ground state energy is equal to:

$$E_0^{(2)} = -\frac{1}{2} \sum_{i>j} v_{ij}^2 \frac{(U_i^2 V_j^2 + U_j^2 V_i^2)^2}{E_i + E_j}. \quad (6)$$

The result obtained with the QP²T approach at second order in perturbation (6) are displayed in figure 1 with filled circles. Similarly to the original quasi-particle theory, the energy deduced from the QP²T contains spurious contribution coming from the fact that the perturbed state does not preserves particle number. The most direct way to remove spurious contributions due to the mixing of different particle number is to introduce the operator P^N

$$P^N = \frac{1}{2\pi} \int_0^{2\pi} d\varphi e^{i\varphi(\hat{N}-N)}. \quad (7)$$

that projects onto particle number N . The most straightforward way to combine projection with quasi-particle perturbation theory is to directly take the expectation value

$$\mathbf{E}_0 = \frac{\langle \Psi_0^N | H | \Psi_0^N \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle} \quad (8)$$

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 as the projected quasi-particle perturbation theory (QP³T) in the following. The correlation energies obtained for $N = \Omega = 8$ using the second order QP³T are shown in figure 2. In each case, the original BCS, the PAV and the exact solution are also shown. The result of QP³T almost superimposed with the exact solution.

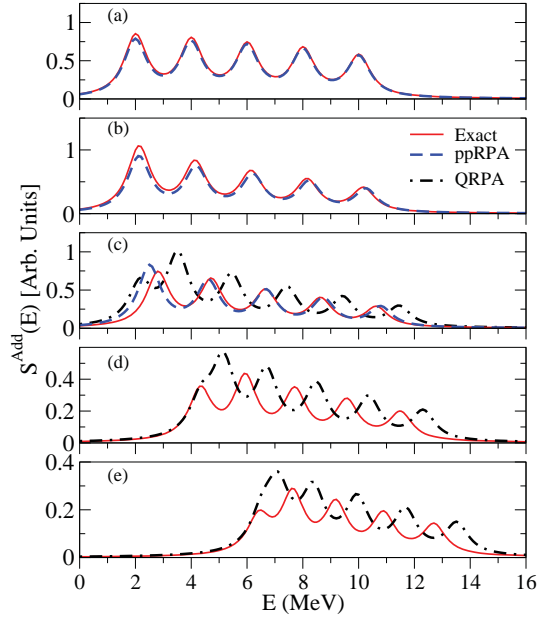


Figure 3. Addition strength function as a function of the excitation energy E for different pairing strength g obtained for a system of $N = 8$ particles to $N = 10$ in the case of $\Omega = 10$ equally spaced levels. From top to bottom: (a) $g/\Delta\varepsilon = 0.1$, (b) 0.3, (c) 0.5, (d) 0.7 and (e) 0.9 are shown. The results of the ppRPA (blue dashed line) and QRPA (black dot-dashed line) are presented and compared with the exact results (red solid line).

3. Pair transfer and excited states

Due to the absence of residual coupling between quasi-particle excitations, it is known that HFB alone cannot properly describe excited states. Then, linear response theory including possible particle-particle (pp), hole-hole (hh), or particle-hole (ph) excitations is applied to describe excited states, and then transfer probabilities, within the QRPA approach. In QRPA, the excited states, denoted by $|\nu\rangle$, are obtained by considering coherent superposition of 2 quasi-particle (2QP) excitations through the operators

$$Q_\nu^\dagger = \sum_i (X_j^\nu \alpha_i^\dagger \alpha_i^\dagger - Y_j^\nu \alpha_i \alpha_i). \quad (9)$$

In QRPA, the addition transition probability is given by

$$P_\nu^{\text{Add}} = |\langle 0 | \hat{T}^{\text{Add}} | \nu \rangle|^2 = \left| \sum_i (V_i^2 X_i^{(\nu)} - U_i^2 Y_i^{(\nu)}) \right|^2. \quad (10)$$

where $\hat{T}^{\text{Add}} = \sum_i T_{i\bar{i}} a_i^\dagger a_{\bar{i}}^\dagger$ is non-Hermitian addition transition operator.

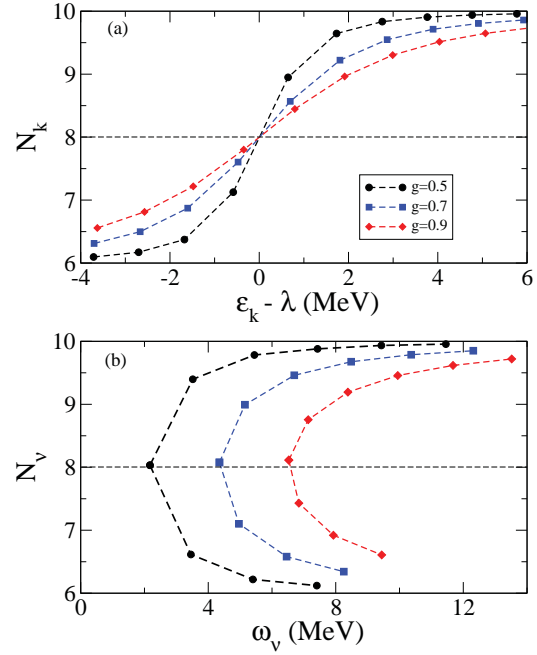


Figure 4. (color online) Bottom: mean number of particles N_ν of the QRPA states as a function of their excitation energy $\hbar\omega_\nu$. Top: mean number of particles N_k of 2QP states as a function of $(\epsilon_k - \lambda)$, where λ is the Fermi energy.

In the weak coupling limit, below a certain threshold value of g denoted by g_{cr} , the minimization of the energy in HFB identifies to the Hartree-Fock approach with no pairing and the excited states are described by using the particle-particle RPA (ppRPA) where the phonon creation operators and the corresponding addition probability simply write as

$$Q_{\nu}^{\dagger} = \sum_p X_p^{\nu} a_p^{\dagger} a_{\bar{p}}^{\dagger} + \sum_h Y_h^{\nu} a_h^{\dagger} a_{\bar{h}}^{\dagger}, \quad P_{\nu}^{\text{Add}} = \left| \sum_p X_p^{\nu} - \sum_h Y_h^{\nu} \right|^2. \quad (11)$$

Contrary to the QRPA, the $U(1)$ symmetry associated to particle number conservation is not broken in ppRPA.

In Fig 3 the ppRPA (dashed line) and QRPA (dot-dashed line) are compared to the exact results. Above a given threshold g_{cr}^{RPA} , ppRPA collapses and leads to imaginary energies making not possible a direct comparison with the exact and QRPA results. However, in Fig. 3 we show in the panel (c) corresponding to a pairing strength $g = 0.5 \text{ MeV}$ the ppRPA results obtained at the collapse point, i.e. $g_{cr}^{RPA} = 0.48$, in order to show that its description is still reasonable even in the superfluid phase. From these comparisons we can also see that although the QRPA provides a global reproduction of the exact results, in general QRPA leads to peaks in the strength that are at slightly higher energies compared to the exact solution while probabilities are slightly overestimated. These discrepancies can be, at least partially, traced back to the violation of the number of particle in QRPA.

As an illustration, the mean number of particles $N_{\nu} = \langle \nu | \hat{N} | \nu \rangle$ is displayed in the bottom panel of Fig. 4 as a function of the excitation energy ω_{ν} . N_{ν} has been estimated using the quasi-boson approximation leading to:

$$N_{\nu} = \sum_i 2(U_i^2 - V_i^2)(X_i^{\nu 2} + Y_i^{\nu 2}) + \langle \hat{N} \rangle, \quad (12)$$

where $\langle \hat{N} \rangle$ is the number of particle in the QP vacuum.

In the same figure, the mean-particle number of the two quasi-particle (2QP) excited states $|k\rangle$ as a function of $(\epsilon_k - \lambda)$ is also shown, where λ is the Fermi energy. The 2QP states and the corresponding mean particle number are given by:

$$|k\rangle = \alpha_k^{\dagger} \alpha_{\bar{k}}^{\dagger} |0, QP\rangle, \quad N_k = \langle k | \hat{N} | k \rangle = \langle \hat{N} \rangle + 2U_k^2 - 2V_k^2. \quad (13)$$

The Figure 4 clearly shows that the 2QP states will be close to a state with $N + 2$ (resp. $N - 2$) particles only if $U_k \rightarrow 1$, i.e. well above the Fermi energy λ (resp. $U_k \rightarrow 0$, i.e. well below the Fermi energy), but will be a bad approximation if the 2QP state involves single-particle state in the vicinity of λ . Consequently, QRPA states will also suffer from the same problems if the state is constructed from 2QP states that are close to the Fermi energy. In order to improve on that, we follow a Tamm-Dancoff approximation spirit, introducing a set of states $|\Phi_k\rangle \hat{P}_{N+2} \alpha_k^{\dagger} \alpha_{\bar{k}}^{\dagger} |0, QP\rangle$. The excited states are then obtained diagonalizing the Hamiltonian in this new space which preserves the particle number symmetry, (for more details see[14]), and the corresponding results are labeled as P-QTDA^(GS).

To illustrate the predictive power of the P-QTDA^(GS) method, some ratios of pair transfer probabilities are shown in Figure 5. In this figure, P_{gs} , P_{ex} and P_{tot} correspond respectively to the probability to transfer to the ground state, the sum of probabilities to transfer to any excited states, while $P_{tot} = P_{gs} + P_{ex}$. Below the pairing threshold, the P-QTDA^(GS) reduces to a ppTDA^(GS), where the diagonalization is made in a reduced space of Slater determinant. In that case, the result are of the same quality as for the ppRPA. This figure clearly confirms that while QRPA is rather far from the exact results in the superfluid phase, especially in the vicinity of the BCS threshold, the projected theory provides a much better reproduction of ground state to excited state pair transfer probabilities. Moreover, theoretical predictions based on the QRPA [16] might significantly overestimate the Giant Pairing Vibration cross section, as suggested also in [17], especially in the vicinity of the normal-superfluid transition.

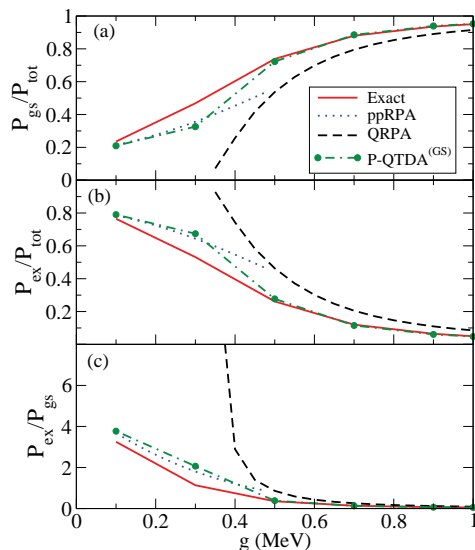


Figure 5. (color online) Ratios of probabilities estimated with different theories for the equidistant level case. The exact (red solid line), QRPA (black dashed line) and P-QTDA (green filled circles) are shown. The ppRPA is also shown (dotted line) up to $g = 0.48$ MeV.

4. Conclusions

In this paper, two methods, preserve the particle number symmetry, for the treatment of pairing correlations in ground state and excited states of finite systems which have been presented. Applications to the Richardson model are shown and discussed. The comparison with exact results allow to show clearly the quality of the presented methods and their improvement with respect to other approaches that do not preserve particle number.

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