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. The proposed method scales friendly when the number of particles increases and provides a simple alternative to other more complicated approaches.

The BCS and/or HFB theories are extended by treating the effect of four quasi-particle 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 non-perturbative approaches breaking 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 + projection is almost perfect.

The importance of particle number restoration is finally recalled. It is then explained how to take advantage of both perturbative approaches and BCS/HFB theory. Theories breaking explicitly the particle number, like 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 it is the case in mesoscopic systems like in 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.

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 [3, 4] and/or using the secular equation originally proposed by Richardson [5, 6]. Accurate description of the ground state energy of superfluid systems with larger particle number can be obtained using either Quantum Monte-Carlo technique (see for instance [9, 10]) or extending quasi-particle theories using Variation After Projection approaches [11, 12] (for recent applications see [13, 14]). 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 theory. The importance of particle number restoration is finally highlighted.

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I. INTRODUCTION

Theories breaking explicitly the particle number, like 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 it is the case in mesoscopic systems like in 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.

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 [3, 4] and/or using the secular equation originally proposed by Richardson [5, 6]. Accurate description of the ground state energy of superfluid systems with larger particle number can be obtained using either Quantum Monte-Carlo technique (see for instance [9, 10]) or extending quasi-particle theories using Variation After Projection approaches [11, 12] (for recent applications see [13, 14]). 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 theory. 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. [4, 10]. We assume a two-body pairing hamiltonian given by:

$$ H = \sum_{i=1}^{\Omega} \varepsilon_i (a_i^\dagger a_i) + \sum_{i \neq j}^{\Omega} v_{ij} a_i^\dagger a_i^\dagger a_j a_j $$

$$ \equiv H_0 + V. $$

Here, \((i, \bar{i})\) denotes time-reversed pair. Such an hamiltonian can be for instance constructed starting from a realistic self-consistent mean-field calculation providing single-particle energies and two-body matrix elements [9].

Here \(\Omega\) 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 times ago [17] and recently re-discussed [10, 18], 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 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:

$$ E_0 = E_0 + E_0^{(2)} $$

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

$$ E_0^{(2)} = \sum_{n \neq 0} \frac{|\langle \Phi_0 | V | \Phi_n \rangle|^2}{E_0 - E_n} $$
In the specific case considered here, i.e. Eq. (1), only 2p-2h states contribute to the second order correction. More precisely, the states \( \Omega \) 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 \( i \)): \( |\Phi_{i,j}\rangle = a_j^\dagger a_i^\dagger a_i a_j |\Phi_0\rangle \) and are eigenstates of \( H_0 \) with energy \( E_{ij} = \tilde{E}_0 + 2(\varepsilon_j - \varepsilon_i) \). This leads to

\[
E^{(2)}_0 = -\frac{1}{2} \sum_{i=1,N_{\text{pair}}} \sum_{j=N_{\text{pair}}+1,N_{\text{max}}} |v_{ij}|^2 \varepsilon_j - \varepsilon_i
\]

with \( N_{\text{pair}} = N/2 \) and \( N_{\text{max}} = \Omega/2 \). This expression has been obtained in ref. [18] using a different approach based on the Richardson-Gaudin equation. It is known [16, 17] that standard perturbation theory provides an appropriate description in the weak coupling regime.

In figure 1, an example of standard perturbation theory (SPT) is presented 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), Eq. (3) and QPST theory with second order correction Eq. (4) (blue filled circles), are displayed.

![Graph showing correlation energy vs g/\Delta\varepsilon for N=8, \Omega=8](image)

**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), Eq. (3) and QPST theory with second order correction Eq. (4) (blue filled circles), are displayed.

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 \( E_0 \) obtained with STP are compared to the exact solution and BCS result. In the latter case, pairing correlation is non-zero only above the threshold value \( g/\Delta\varepsilon \approx 0.3 \). 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 even in the strong interaction case by breaking the U(1) symmetry associated to particle number conservation.

### III. QUASI-PARTICLE PERTURBATION THEORY

To provide a proper description of both the weak and strong pairing strength regime, it seems quite natural to try to combine theories based on quasi-particles and perturbative approaches. This possibility has been explored long time ago in Refs. [23, 24] mainly to discuss the removal of "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 [28] based on Gorkov-Green function formalism [27]. In the following, it is assumed that the BCS/HFB approach has been applied in a preliminary study and that the hamiltonian \( \hat{H}_0 \) is written in the canonical basis of the quasi-particle ground state. Then, the ground state takes the form

\[
|\Phi_0\rangle = \prod_{i>0} \left( U_i + V_i a_i^\dagger a_i^\dagger \right) |\rangle,
\]

and is the vacuum of the quasi-particle creation operators defined through:

\[
\beta_i^\dagger = U_i a_i^\dagger - V_i a_i^\dagger, \quad \beta_i^\dagger = U_i a_i^\dagger + V_i a_i^\dagger.
\]

In the HFB/BCS theory, the original hamiltonian is replaced by an effective Hamiltonian that is conveniently written as \(^1\):

\[
H_0 = E_0 + \sum_i E_i \left( \beta_i^\dagger \beta_i + \beta_i^\dagger \beta_i^\dagger \right)
\]

where \( E_0 \) is the BCS/HFB ground state energy, while \( E_i \) corresponds to the quasi-particle energy given by:

\[
E_i = \sqrt{\left( \varepsilon_i - \lambda \right)^2 + \Delta^2}
\]

where \( \lambda \) is the Lagrange multiplier used to impose the average particle number while \( \Delta \) is the pairing gap (for a detailed discussion see [19]).

For even systems, excited states of \( H_0 \) are 2 quasi-particle (2QP), 4 quasi-particle (4QP), ... excitations with respect to the ground state. The original hamiltonian \( H \) contains many terms that are neglected in \( H_0 \) and that are responsible from the deviation between the quasi-particle and the exact solution. However, noting that:

\[
H|\Phi_0\rangle = \left( H_0 - \sum_{i \neq j} v_{ij} U_i^2 U_j^2 \beta_i^\dagger \beta_j^\dagger \beta_i \beta_j \right) |\Phi_0\rangle,
\]

it can be anticipated that the main source of discrepancy is due to the coupling of \( \Phi_0 \) with the 4QP states. Some

\(^1\) Note that here, it is implicitly assumed that \( H \) is replaced by \( H - \lambda N \).
arguments showing that 4QP states should improved the description of pairing especially in the weak coupling regime have been given in ref. 29.

Below, perturbation theory is applied assuming that $H_0$ (Eq. 3) is the unperturbed Hamiltonian while the perturbation $V$ is given by:

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

(11)

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

$$|\Phi_{i,j}⟩ = \beta_i^\dagger \beta_j^\dagger \beta_i \beta_j|Φ_0⟩$$

(12)

and associated to the unperturbed energy

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

(13)

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

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

(14)

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

$$E_i + E_j \to |ε_i - λ| + |ε_j - λ| = ε_i - ε_j,$$

(15)

and the standard perturbation theory case is recovered.

The result obtained with the QP2T approach at second order in perturbation (14) are displayed in figure 2 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 quasi-particle 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 quasi-particle theory, the energy deduced from the QP2T contains spurious contributions coming from the fact that the perturbed state does not preserves particle number. Indeed, using standard formulas, to second order in perturbation, the ground state expresses as:

$$|Ψ_0⟩ = |Ψ_0^{(0)}⟩ + |Ψ_0^{(1)}⟩ + |Ψ_0^{(2)}⟩ + \cdots$$

$$= |Φ_0⟩ + \sum_{i > j} c_{ij} |Φ_{i,j}⟩ + \cdots$$

(16)

where $|Ψ_i⟩$, $i = 0, 1, ...$ denotes the contribution to the state at $i$th order in perturbation and where

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

(17)

Above the BCS threshold, neither $|Φ_0⟩$ nor $|Φ_{i,j}⟩$ are eigenstates of the particle number operator.

The most direct way to remove spurious contributions due to the mixing of different particle number is to introduce the operator $P_N$:

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

(18)

that projects onto particle number $N$.

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

FIG. 3: Same as figure 2 for the $N = Ω = 8$ case.
the expectation value
\[
E_0 = \frac{\langle \Psi_0^N | H | \Psi_0^N \rangle}{\langle \Psi_0^N | \Psi_0^N \rangle}
\]  
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 quasi-particle perturbation theory (QP$^3$T) in the following. When only the zero order in perturbation is retained in Eq. (10), the QP$^3$T identifies with the projection after variation (PAV) that is commonly used, especially in the nuclear Energy Density Functional approach (EDF) \[20\]. Formulas useful to compute the expectation values of one- and two-body operators with projection are given in appendix A. The projection is performed numerically using these expressions and the Fomenko discretization procedure of the gauge-space integrals \[21\], \[22\]. Here, 199 discretization points have been used. Note that the number of points can be reduced to 5 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 figures 2, 3 and 4 respectively. In each case, the original BCS, the PAV and the exact solution are also shown. The result of QP$^3$T almost superimposes with the exact solution. Only a slight difference can be seen around the BCS threshold.

Besides the energy, other observables can also be estimated. As an example, the quantity $n_i (1 - n_i)$ is shown in figure 2(a) 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 case as it was noted in ref. \[12\], 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 non-trivial multi-particle multi-hole mixing that can also be described by direct diagonalization of the Hamiltonian but that is 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 $\langle \Omega/|N_{\text{pair}}/(!N_{\text{pair}})] \rangle$. It is important to recall that here no diagonalization is required since the mixing coefficients are directly given by the quasi-particle perturbation theory, Eq. (17). These features make the approach rather simple to implement on existing HFB/BCS 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 \[13\], \[15\], no extra minimization is required.

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 figure 3 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 quasi-particle theories can be applied without

\[\text{FIG. 4: (color online) Same as figure 2 for the } N = \Omega = 12 \text{ case.}\]

\[\text{FIG. 5: (color online) Example of evolution of the quantity } n_i (1 - n_i) \text{ obtained with QP$^3$T (filled blue circles) as a function of single-particle energy for the } N = \Omega = 8 \text{ case with } g/\Delta \varepsilon = 0.4 \text{ (a) and } 0.8 \text{ (b). In both case, the exact result (red solid line) the BCS result (black dashed line) and the PAV result (green open squares) are shown.}\]
difficulties. Note however, that the $\text{QP}^3\text{T}$ requires to perform more and more gauge angles integrations (see appendix A) as $N$ increases making the calculations more time consuming with respect to the non-projected theories like BCS or $\text{QP}^2\text{T}$.

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

Recently, the use of Gorkov-Green function theory has been proposed [28] as a possible tool to perform ab-initio calculation for nuclei. This theory provides a general formalism based on quasi-particle states. The result obtained in the present study are rather encouraging to pursue in that direction and that projection might be needed.

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**Appendix A: Expression of projected quantities**

Starting from the standard expression of the quasi-particle ground state (Eq. (3)), the 4 QP states are given by:

$$|\Phi_{i,j}\rangle = \left(-V_i + U_i a_i^\dagger a_j^\dagger\right)\left(-V_j + U_j a_j^\dagger a_i^\dagger\right) \prod_{k > 0, k \neq (i,j)} \left(U_k + V_k a_k^\dagger a_k^\dagger\right) |\Psi\rangle.$$  \hspace{1cm} (A1)

For compactness, this expression is written as

$$|\Phi_m\rangle = \prod_{k > 0} \left(U_k^m + V_k^m a_k^\dagger a_k^\dagger\right) |\Psi\rangle.$$  \hspace{1cm} (A2)

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

$$\langle \Psi^N | O | \Psi^N \rangle = \sum_{m,n} c_n^* c_m \langle \Phi_n | O P^N | \Phi_m \rangle$$  \hspace{1cm} (A3)

where

$$\langle \Phi_n | O P^N | \Phi_m \rangle = \int_0^{2\pi} d\varphi e^{-i\varphi N} 2\pi \langle \Phi_n | O | \Phi_m (\varphi) \rangle,$$  \hspace{1cm} (A4)

and

$$|\Phi_m (\varphi)\rangle = \prod_{k > 0} \left(U_k^m + V_k^m e^{2i\varphi} a_k^\dagger a_k^\dagger\right) |\Psi\rangle.$$  \hspace{1cm} (A5)
Starting from this expression it could be deduced that:

\[
\langle \Phi_n | P^N | \Phi_m \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\phi N} \prod_{k>0} \left( U_k^m \bar{U}_k^n + V_k^m \bar{V}_k^n e^{2i\phi} \right)
\]

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