

# Improvement to the Projected BCS Approximation

S. Pittel<sup>1</sup>, J. Dukelsky<sup>2</sup>, and C. Esebbag<sup>3</sup>

<sup>1</sup>Bartol Research Institute and Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 USA

<sup>2</sup>Instituto de Estructura de la Materia, CSIC, Serrano 123, 28006 Madrid, Spain

<sup>3</sup>Departamento de Matemáticas, Universidad de Alcalá, 28871 Alcalá de Henares, Spain

E-mail: [pittel@bartol.udel.edu](mailto:pittel@bartol.udel.edu)

**Abstract.** We consider the structure of the number projected BCS wave function in the particle-hole basis, and use it to study several approximate treatments of pairing. The analysis is carried out for the exactly solvable Richardson model involving a pure pairing hamiltonian acting in a space of equally spaced doubly degenerate levels at half filling.

## 1. Introduction

Pairing correlations are ubiquitous in strongly-correlated systems, ranging from condensed matter to quantum optics to cold atomic gases to atomic nuclei. A traditional starting point for the description of these correlations is through the use of the Bardeen Cooper Schrieffer (BCS) approximation [1], whereby the correlations are described by means of a coherent state of collective pairs that breaks the conservation of particle number. This method is especially useful in the description of systems with a very large number of interacting particles where the fluctuations in the particle number is negligible. For systems with a fairly small number of particles, e.g. atomic nuclei or superconducting grains, it is important to restore particle number, through the use of the number projected BCS (PHBCS) approximation [2].

Pairing correlations can be treated exactly using the Richardson method when the hamiltonian is of a pure BCS form [3]. Likewise, more general pairing Hamiltonians are exactly solvable if they can be expressed as a linear combination of the set of integrals that define the Richardson-Gaudin models [4]. This exact solvability has enabled the test of approximate methods of treating pairing for a wide variety of systems, like small superconducting grains [5, 6] or realistic atomic nuclei [7, 8, 9, 10, 11]. Such tests have illustrated that for a large enough number of active orbits over which the pairing acts, even the PBCS approximation misses important pairing correlations, making its use in large scale energy density functional treatments of finite nuclei suspect. This has led to a multitude of efforts to develop improved approximate treatments of pairing correlations. This includes, *e.g.*, the use of RPA methods [8] and the use of coupled cluster methods [11].

In this work we study the accuracy of the PBCS approximations and propose an alternative method based on a generalization of the PBCS wave function for an improved approximate treatment of pairing correlations. The method starts with the PBCS approximation, which is then expanded in terms of particle-hole excitations around the Hartree-Fock Fermi surface. In the PBCS approximation, each term in the series expansion is defined by the expansion coefficients of a single collective pair and furthermore the contribution of each term is prescribed.



In our improved method, we diagonalize the Hamiltonian in the space of collective particle-hole pair excitations, thereby permitting the contribution of each term in the full series to be modified and indeed optimized. We gradually increase the number of terms included in the series expansion until convergence is achieved. We refer to this new approximation, for the sake of terminology, as the Particle-Hole BCS (PHBCS) approximation [6].

The structure of the paper is as follows. In section II, we describe the PHBCS approximation and detail its differences relative to the other approximations against which we will compare it. In Section III, we describe the model that we use to carry out comparative tests of the various approximations and then in Section IV we describe the results of this comparison and draw some conclusions. In Section V we summarize the main results of the work and outline some issues for future consideration.

## 2. The Particle-Hole BCS approximation

Consider a set of  $N$  particle pairs moving in a space of  $\Omega$  doubly-degenerate single-particle states  $i, \bar{i}$  and denote the single-particle creation and annihilation operators associated with these states as  $c_i^\dagger, c_i^\dagger$  and  $c_i, c_{\bar{i}}$ , respectively. Furthermore, denote the operators that create and annihilate a pair of particles in doubly-degenerate time-reversed states as

$$P_i^\dagger = c_i^\dagger c_{\bar{i}}^\dagger, \quad (1)$$

$$P_i = [P_i^\dagger]^\dagger = c_{\bar{i}} c_i, \quad (2)$$

which satisfy the commutation

$$[P_i, P_j^\dagger] = \delta_{ij} (1 - N_i) \quad [N_i, P_j^\dagger] = 2\delta_{ij} P_j^\dagger \quad (3)$$

where  $N_i = c_i^\dagger c_i + c_{\bar{i}}^\dagger c_{\bar{i}}$ .

The traditional PBCS state can be expressed as a condensate of  $M = \frac{N}{2}$  collective pairs, viz.

$$|PBCS\rangle = \frac{1}{\sqrt{Z_{1,\Omega,M}}} [\Gamma^\dagger(x)]^M |0\rangle, \quad \Gamma^\dagger(x) = \sum_{i=1}^{\Omega} x_i P_i^\dagger, \quad (4)$$

where the normalization coefficients  $Z_{1,\Omega,M}$ , which depend on the pair structure amplitudes  $x_i$ , can be obtained straightforwardly from the commutation relations of (3) using recursive techniques [6].

In the PBCS approximation, the  $\Omega$  structure coefficients  $x_i$  of the condensed pair are considered as variational parameters chosen to minimize the expectation value of the hamiltonian. This approach is completely equivalent to the usual formulation of PBCS approximation [2].

We now separate the collective pair operator  $\Gamma^\dagger$  into its particle and hole components

$$\Gamma^\dagger(x) = \Gamma_P^\dagger(x) + \Gamma_H^\dagger(x)$$

where

$$\Gamma_P^\dagger(x) = \sum_{p=M+1}^{\Omega} x_p P_p^\dagger, \quad \Gamma_H^\dagger(x) = \sum_{h=1}^M x_h P_h^\dagger \quad (5)$$

The PBCS state can then be rewritten as

$$\begin{aligned} |PBCS\rangle &= \frac{1}{\sqrt{Z_{1,\Omega,M}}} \left[ \Gamma_P^\dagger(x) + \Gamma_H^\dagger(x) \right]^M |0\rangle = \\ &= \frac{1}{\sqrt{Z_{1,\Omega,M}}} \sum_{l=0}^M \binom{M}{l} \left[ \Gamma_P^\dagger(x) \right]^l \left[ \Gamma_H^\dagger(x) \right]^{M-l} |0\rangle \end{aligned} \quad (6)$$

Taking into account that the Hartree-Fock state can be written in this notation as

$$|HF\rangle = \frac{1}{\sqrt{Z_{1,M,M}}} \left[ \Gamma_H^\dagger(x) \right]^M |0\rangle, \quad (7)$$

after some straightforward algebra, the PBCS wave function in the particle-hole basis reduces to

$$|PBCS\rangle = \sqrt{\frac{Z_{1,M,M}(x)}{Z_{1,\Omega,M}(x)}} \sum_{l=0}^M \frac{1}{l!^2} \left[ \Gamma_P^\dagger(x) \Gamma_H(1/x) \right]^l |HF\rangle. \quad (8)$$

This expression for the PBCS wave function is one of the most important results of this work. Notice that the expansion in terms of particle and hole pairs on top of the HF reference state goes with the inverse of the factorial square, and the amplitudes of the hole destruction pair are the inverse of the amplitudes of the coherent PBCS pair. By inserting the definition (5) for the particle and hole collective pairs, we obtain a more transparent form of the PBCS wave function

$$|PBCS\rangle = \sqrt{\frac{Z_{1,M,M}(x)}{Z_{1,\Omega,M}(x)}} \sum_{l=0}^M \frac{1}{l!^2} \left[ \sum_{p,h} \frac{x_p}{x_h} P_p^\dagger P_h \right]^l |HF\rangle. \quad (9)$$

Here the expansion coefficients with the factorial square are the fingerprints of the PBCS wave function. Replacing these coefficients by a simple factorial allows us to define an Exponential form of the wave function,

$$|EA\rangle \propto \sum_{l=0}^M \frac{1}{l!} \left[ \sum_{p,h} \frac{x_p}{x_h} P_p^\dagger P_h \right]^l |HF\rangle, \quad (10)$$

which we will explore as an alternative to the PBCS approximation. Though the norm of this state cannot be expressed in closed form, it is not needed for the analysis to follow.

A third alternative approach, which we call particle-hole BCS (PHBCS), interpolates between PBCS and the Exponential form by using the statistical coefficients as a new set of variational parameters. Effectively, the procedure diagonalizes the Hamiltonian in the basis of particle and hole pairs,

$$H_{l,l'} = \frac{\langle 0 | [\Gamma_P(x)]^l [\Gamma_H(x)]^{M-l} | H | [\Gamma_P^\dagger(x)]^{l'} [\Gamma_H^\dagger(x)]^{M-l'} | 0 \rangle}{\sqrt{Z_{M+1,\Omega,l}(x) Z_{1,M,M-l}(x) Z_{M+1,\Omega,l'}(x) Z_{1,M,M-l'}(x)}}, \quad (11)$$

and then the ground state energy (lowest eigenvalue) is minimized with respect to the amplitudes  $x_i$  selfconsistently. In weak coupling only a limited number of terms survive. A variational analysis for all the approximations discussed above can be carried out straightforwardly using multi-parameter minimization routines.

Coming back to the Exponential approximation (EA) in Eq. (10), we note the similarities of this wave function with the pair Coupled Cluster Doubles (p-CCD) [8, 11] and the particle-particle RPA or self-consistent RPA [12, 13] wave functions in the quasi-boson approximation, both having an exponential form

$$|\Psi\rangle \propto \sum_{l=0}^M \frac{1}{l!} \left[ \sum_{p,h} X_{p,h} P_p^\dagger P_h \right]^l |HF\rangle. \quad (12)$$

where the entries of the structure matrix  $X_{p,h}$  are determined differently in Coupled Cluster and in RPA. Note that here too the statistical factor is the inverse of  $l!$ .

We should realize here a crucial difference between these two classes of approximation. While the approximations related to the PBCS wave function have a restricted separable form of the structure matrix  $X_{p,h} = x_p/x_h$ , Coupled Cluster and RPA preserve the complete freedom of the matrix. As we will see in the numerical study to follow, the matrix  $X$  cannot be factorized as in PBCS in the weak coupling limit dominated by pairing fluctuations.

### 3. Model for testing the approximation methods

As noted in the previous section, we would like to test the PHBCS method relative to the ordinary PBCS method and would also like to compare it with the p-CCD and the associated Exponential Approximation. Furthermore, we would like compare all of these methods with exact results where applicable. Since the Richardson method can be used to obtain exact solutions for a pure BCS hamiltonian, we have chosen to carry out the tests using such a hamiltonian acting in a set of doubly-degenerate single particle orbits with equal spacing, the so-called picket-fence model. We will first describe in a bit more detail the model and then in the next section report results of the comparisons for a specific size of the model space, as a function of the strength of the pairing force relative to the single-particle spacing.

The picket-fence model involves a Hamiltonian

$$H = \sum_{i=1,\Omega} \epsilon_i \hat{N}_i + G \sum_{i,i'} P_i^\dagger P_{i'} \quad (13)$$

with the equally-spaced single-particle energies given by

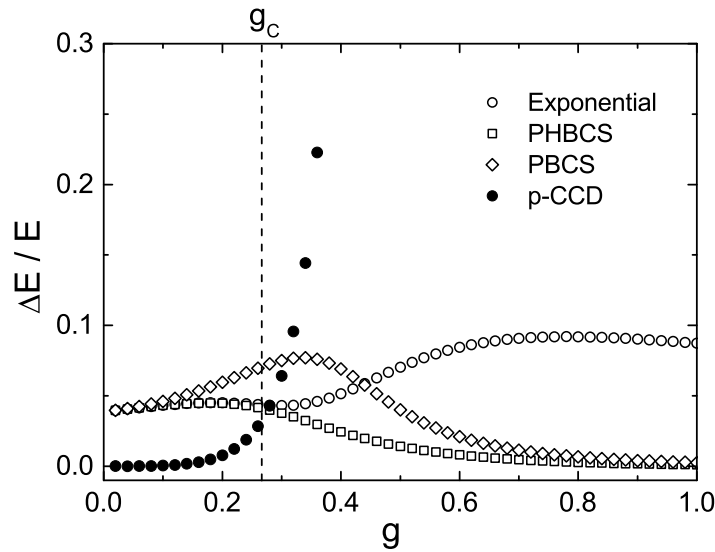
$$\epsilon_i - \epsilon_{i-1} = \epsilon \quad (14)$$

We will consider a system of  $N = \Omega$  particles, namely half filling, and discuss the results as a function of the ratio of the pairing strength to the splitting between levels  $G/\epsilon$ .

### 4. Test results of the PHBCS and other approximate methods

We present here results for a model with 20 levels. We show in figure 1 the relative error with respect to the exact Richardson solution in the ground state correlation energies calculated in PHBCS approximation and in PBCS approximation. We also show the analogous results for the p-CCD and the associated Exponential Approximation. Results are reported for ratios of the pairing strength to the level splitting ranging from weak coupling ( $G/\epsilon \ll 1$ ) to strong coupling ( $G/\epsilon \sim 1$ ).

As can be seen in the figure, none of the approximations based on the PBCS wave function can describe appropriately the weak coupling limit, indicating that the full freedom of the structure matrix  $X$  is needed to reproduce the pairing fluctuations that dominate in this region. Even though the p-CCD procedure is non variational, it is more accurate than the PBCS class of approximations in weak coupling. However, it progressively degrades as the system goes to the



**Figure 1.** Calculated relative error with respect to the exact Richardson solution in the correlation energy calculated in PHBCS approximation and in PBCS approximation. We also show the analogous results for p-CCD and the Exponential Approximation methods. Results are reported for ratios of the pairing strength to the level splitting ranging from very weak coupling ( $G/\epsilon \ll 1$ ) to strong coupling ( $G/\epsilon \sim 1$ ). Also shown is the critical value of the pairing strength  $G_c$  in BCS approximation.

crossover region and fails completely in the superconducting phase. Within the PBCS class of approximations, the Exponential Approximation describes better than PBCS the weak coupling region while PBCS is more efficient in the strong coupling region. As expected, PHBCS, which is not restricted to a prescribed statistical factor, interpolates between the two approximations, giving the optimal description along the complete crossover. As noted earlier, however, it does not become exact in the very weak-coupling regime, due to the separable ansatz assumed for the structure matrix. This is contrary to suggestions made by Sandulescu and Bertsch [14] that the PBCS approximation becomes exact in the weak-coupling limit. As a reminder, these results are to be contrasted with those of the p-CCD which becomes exact in the weak coupling regime, but blows up after the critical pairing strength.

## 5. Summary and concluding remarks

In this work, we have discussed several approximate methods for treating pairing. With atomic nuclei in mind, we have focussed on methods that exactly conserve the particle number. One method we have considered is a variational improvement to the the number-projected BCS approximation, based on a particle-hole expansion of the PBCS wave function about the Fermi surface. The others involve the two-body Coupled Cluster Method and a related Exponential Approximation.

Calculations were reported for a picket-fence model, whereby a pure pairing force acts in a space of doubly-degenerate equally-spaced levels. The calculations were carried out at half-filling for a model space involving 20 doubly-degenerate levels. This model exhibit a phase transition at a critical value of the pairing strength relative to the splitting between levels. In the strong-coupling limit, both the PBCS and the PHBCS variational approximation to it converge

to the exact results, as given by the Richardson solution. In the very weak-coupling limit, the two approximations again agree with one another, but with an error relative to the exact solution. Between the weak- and strong-coupling limit, the PHBCS approximation provides an improvement to the PBCS approximation, often sizable.

The pair Coupled Cluster Doubles approximation and the Self Consistent RPA are able to reproduce the exact results in the weak-coupling limit. This is due to the fact that both approximations exploit the complete freedom of the structure matrix, whereas the PBCS related approximations use a restricted separable form of this matrix. While the PHBCS variational approximation produces an improvement over PBCS around the critical strength, it is actually worse than the p-CCD for strengths below the critical value. Indeed, in the weak-coupling limit it converges to exactly the same solution as both the PBCS and Exponential methods.

Further understanding of the behavior of these various approximate treatments of pairing correlations in the weak-coupling limit is clearly warranted. Variational methods like PBCS, but using an unrestricted structure matrix, seem to be ideally suited to describe both, the fluctuation dominated regime of weak pairing and the superconducting phase of strong pairing.

Additional studies using a larger number of active levels are also called for if we are to make further progress in the search for a reliable approximate treatment of pairing in general scenarios.

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