Stochastic number projection method in the pairing-force problem

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A new stochastic number projection method is proposed. The component of the BCS wave function corresponding to the right number of particles is obtained by means of a Metropolis algorithm in which the weight functions are constructed from the single-particle occupation probability. Either standard BCS or Lipkin-Nogami probability distributions can be used, thus the method is applicable for any pairing strength. The accuracy of the method is tested in the computation of pairing energies of model and real systems.
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The microscopic model of superconductivity introduced in 1957 by Bardeen, Cooper, and Schrieffer (BCS) [1] has had astonishing success in correlating and explaining the properties of simple superconductors in terms of a few experimental parameters. For its conceptual and computational simplicity, the BCS method has been widely used as the first step in nuclear structure calculations involving pairing forces [2]. The theory is quite satisfactory when the number of valence nucleons is large and the pairing interaction is strong (as compared with the level spacing). But in a nucleus with a relatively small number of valence nucleons, or with a large spacing between levels, the BCS method fails. As is well known, the method has two inherent drawbacks.

(1) The BCS wave function is not an eigenstate of the number operator. The energy obtained from this wave function is, therefore, biased with an inaccuracy caused by the number fluctuation.

(2) In some cases, there may be a critical value of the pairing force below which the BCS equations have no nontrivial solution. Exact calculations show that this behavior is spurious [3].

Attempts have been made at improving the method. Kerman *et al.* [4] showed that the wave function obtained by projecting out the BCS function to the sector with the right number of particles is a very good approximation to the exact wave function. Many works have been devoted to particle-number conserving approaches, including projection before and after variation [5–11], and many others, see for example Ref. [12]. However, it is well known that these approximate methods can lead, in some cases, to significant errors.

The exact solution of this problem is only available for some very simple systems, such as a single-level or a two-level model [3,12,13], or the case of equispaced doubly degenerate single-particle levels [14]. Richardson and Sherman [15] have also developed a general method for determining the exact eigenvalues and eigenstates of the pairing force Hamiltonian when the pairing strength is constant.

In a recent paper, Cerf [16] has proposed the application of a diffusion Monte Carlo (DMC) technique to the treatment of the pairing force in nuclei. By making use of DMC, it is possible to compute exactly the ground-state energy of the system with a general, state-dependent, pairing interaction, at least in principle. However, the DMC method can only deal with pairing Hamiltonians in which the interaction matrix elements are strictly positive. This is always the case for the nuclear pairing Hamiltonian, but other types of pairing problems, involving Coulomb interacting particles for example, cannot be solved in this way. Monte Carlo techniques have been widely applied to solve the nuclear shell model [17–22], where pairing plays also an important role.

In this paper, we present a novel stochastic algorithm, based on the Metropolis method [23], for projecting out the component of the BCS wave function with the correct number of particles. The method does not depend on the type of interaction involved, as long as we can assume that the particular BCS functional form holds for our ground-state wave function. Moreover, number projection can be done starting either from the BCS or Lipkin-Nogami [7,8] calculated occupation probability distribution. Therefore, it can be applied for any strength of the pairing interaction. In what follows, we first introduce the model Hamiltonian, then discuss our Monte Carlo projection method. Next, we apply the method to simple systems, and compare the results with those obtained from other approaches.

We consider the problem of a many-body system described by the Hamiltonian

$$H=\sum_{j>0}^{\Omega}\epsilon_j(a_j^{\dagger}a_j+a_{\bar{j}}^{\dagger}a_{\bar{j}})-\sum_{j,,j'>0}^{\Omega}\langle j'\bar{j'}|V_{\text{pair}}|j\bar{j}\rangle a_{j'}^{\dagger}a_{\bar{j'}}^{\dagger}a_{\bar{j}}a_j\,. \tag{1}$$

$a_j^{\dagger}$ and $a_{\bar{j}}^{\dagger}$ create particles in time-reversed conjugate single-particle states $|j\rangle$ and $|\bar{j}\rangle$ with energies ϵ_j. The interaction V_{pair} scatters only time-reversed pairs of particles from the occupied levels $|j,\bar{j}\rangle$ to the empty ones $|j',\bar{j'}\rangle$. The indices

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j and j' run from 1 to Ω, where Ω is the total number of conjugate orbit pairs. Our purpose is to compute the exact N-particle ground-state energy of H. We construct the ground state of H by projecting BCS-type wave functions onto the N-particle sector. Let us define the number of pairs $N_p = N/2$. The following projected function is obtained:

$$|\Psi_0^N\rangle = C_N \sum_{j_1,\cdots,j_{N_p}} \left[\prod_{k=j_1}^{j_{N_p}} \frac{v_k}{u_k} a_k^\dagger a_{\bar{k}}^\dagger \right] |\mathrm{vac}\rangle, \tag{2}$$

where

$$C_N = \left(\sum_{j_1,\ldots,j_{N_p}} \frac{v_{j_1}^2 \ldots v_{j_{N_p}}^2}{u_{j_1}^2 \ldots u_{j_{N_p}}^2} \right)^{-1/2}$$

are the normalization coefficients, $|\mathrm{vac}\rangle$ is the vacuum state, v_j is the amplitude for finding a pair of particles in time-reversed levels $|j,\bar{j}\rangle$, and u_j is the amplitude for the levels being empty. These amplitudes are obtained either by BCS [1] or Lipkin-Nogami (LN) [7,8] methods. Using the Hamiltonian given by Eq. (1) and the wave function (2), we arrive to the following expression for the projected ground-state energy:

$$E_{\mathrm{BCS}}^N = \sum_{j_1,\cdots,j_{N_p}} W(j_1,\ldots,j_{N_p}) \varepsilon(j_1,\ldots,j_{N_p}), \tag{3}$$

where the sum runs over all possible combinations of N_p occupied single-particle double degenerated states $\{j_1,\ldots,j_{N_p}\}$, from a maximum of Ω states allowed in the Monte Carlo evaluation. The ''weights'' W and ''energies'' $\varepsilon(j_1,\ldots,j_{N_p})$ are defined as

$$W(j_1,\ldots,j_{N_p}) = \frac{v_{j_1}^2 \cdots v_{j_{N_p}}^2}{u_{j_1}^2 \cdots u_{j_{N_p}}^2} \left(\sum_{j_1',\ldots,j_{N_p}'} \frac{v_{j_1'}^2 \ldots v_{j_{N_p}'}^2}{u_{j_1'}^2 \ldots u_{j_{N_p}'}^2} \right)^{-1}, \tag{4}$$

$$\varepsilon(j_1,\ldots,j_{N_p}) = \sum_{j \in \{j_1,\ldots,j_{N_p}\}} (2\epsilon_j - \langle j\bar{j}|V_{\mathrm{pair}}|j\bar{j}\rangle) - \sum_{j \in \{j_1,\ldots,j_{N_p}\}} \sum_{j' \notin \{j_1,\ldots,j_{Np}\}} \times \langle j'\bar{j}'|V_{\mathrm{pair}}|j\bar{j}\rangle \frac{u_j v_{j'}}{u_{j'} v_j}. \tag{5}$$

This summation is impracticable as it involves a huge number of terms $\binom{\Omega}{N_p}$ for usual model spaces. Fortunately, the expression (3) for the projected energy allows a simple Monte Carlo evaluation, where the ensembles $\{j_1,\ldots,j_{N_p}\}$ are generated with probability $W(j_1,\ldots,j_{N_p})$ by means of a Metropolis algorithm [23]. Other equivalent forms of Eq. (3), see for example Ref. [24], are not suited for the Monte Carlo evaluation.

TABLE I. Pairing energies for selected values of the interaction strength in the two-level model with $\Omega = 10$ double degenerate levels and $N = 4,10$ particles.

G	Exact	BCS	LNM	DMC	$\mathrm{MCP_{BCS}}$	$\mathrm{MCP_{LNM}}$
			$\Omega = 10, N = 4$			
0.024	0.202	0.161	0.205	0.205(3)	0.203(3)	0.205(3)
0.138	1.495	1.269	1.507	1.498(3)	1.500(5)	1.500(5)
1.105	18.05	16.276	18.05	18.05(9)	18.05(2)	18.05(2)
			$\Omega = 10, N = 10$			
0.024	0.147		0.122	0.146(2)		0.145(5)
0.060	0.36		0.311	0.373(9)		0.353(9)
0.100	0.711		0.603	0.717(5)		0.696(7)
0.500	10.56	9.300	10.56	10.56(5)	10.56(5)	10.56(5)
1.105	28.40	25.64	28.40	28.40(7)	28.40(2)	28.40(2)

In the Metropolis evaluation, we start from the unperturbed ground state and perform 10^5 thermalization steps. We define a trial Metropolis move as a random transition of one pair from the occupied levels $|j,\bar{j}\rangle$ to the empty ones $|j',\bar{j}'\rangle$. The trial move is accepted or rejected according to the Metropolis rule $W(j_1',\ldots,j_{N_p}')/W(j_1,\ldots,j_{N_p}) > \gamma$, where γ is a random number uniformed distributed between 0 and 1. An acceptance ratio R is obtained from the thermalization loop. Using this ratio a total number of Metropolis steps, $N_{\mathrm{Metropolis}} = 300\, N_{\mathrm{decorrelation}}$ is used to estimate average values of ground-state energies. The number of decorrelation steps were taken as $N_{\mathrm{decorrelation}} = 50/R$.

In the following, we will compare results for several soluble models with those obtained by BCS, LN [7,8], and DMC [16] methods. We are interested in the two-body pairing energy E_{pair}, which we define as $E_{\mathrm{pair}} = E_{(V_{\mathrm{pair}}=0)} - E_{(V_{\mathrm{pair}}\neq 0)}$, where $E_{(V_{\mathrm{pair}}=0)}$ and $E_{(V_{\mathrm{pair}}\neq 0)}$ are, respectively, the ground-state energies of the system without and with pairing interaction.

The symmetric two-level model. Here, we study an exactly solvable, symmetric, two-level model, with number of particles N and level degeneracy Ω. The pairing interaction is taken constant and equal to G. This model was first examined by Hogaasen [25], and its exact solution was studied in detail by Rho and Rassmussen [3] in the case $N = \Omega$. More recently, the general case $N \neq \Omega$ was discussed in Ref. [10]. The exact pairing energy E_{pair} is obtained by introducing two sets of quasispin operators, so that the problem finally reduces to the diagonalization of a tridiagonal matrix [3,10]. The results of the BCS approximation, the LN prescription, and the DMC and Metropolis projection methods (MCP) using v_j and u_j either from BCS ($\mathrm{MCP_{BCS}}$) or LN ($\mathrm{MCP_{LNM}}$) calculations are compared against exact results in Table I for $\Omega = 10$ and $N = 4,10$ for several values of the interaction strength G. It is shown that Metropolis projection methods give very good agreement with the exact results (the same quality of agreement as the DMC method). Recall that for $N \neq \Omega$ the BCS ansatz always have a nontrivial minimum [26]. For $N = \Omega$, a nontrivial solution is found only for G greater than $1/(N-1)$.

We make in Fig. 1 a more detailed comparison among

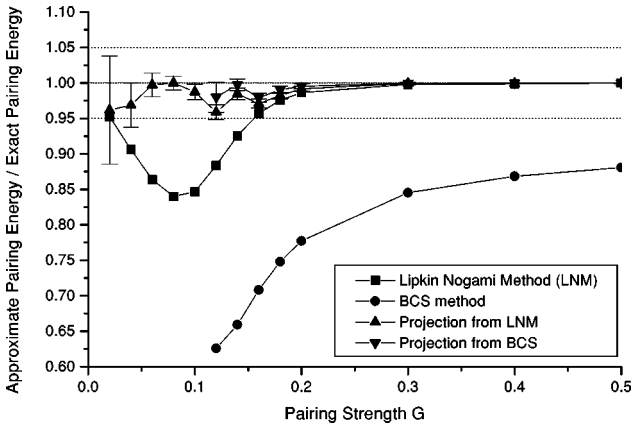

FIG. 1. Pairing energies in the symmetric two-level model.

BCS, LNM, and MCP for $N=\Omega=10$. Attention has been specially paid to the region $G\approx 0.1$, where the BCS solution dissapears and the LNM shows a relative error approximately equal to 15%. The results are presented as a ratio of the given pairing energy to the exact one. The projected solution is consistent with the exact solution (within statistical errors) in the whole range of pairing strength values. Note that, for small G, i.e., at the low density limit or weak pairing, the Monte Carlo estimation of the pairing energy becomes inaccurate because it is dominated by the statistical noise (in this case the acceptance probability of the Metropolis chain is almost equal to zero). However, this situation has no practical importance since the pairing energy becomes very small compared to the one-body energy. Notice also that perturbation methods work very well in this low-pairing regime.

Equidistant doubly degenerate levels. In this case, we deal with a system of equispaced doubly degenerate single-particle levels and a constant pairing interaction. This problem has been solved exactly [14,15] for some model spaces with values of the interaction strength reproducing typical nuclear pairing energies. Results obtained from different methods are shown in Table II for $\Omega=N=8$ and three values of G. Again MCP is in good agreement with the exact results.

The ^{100}Zr nucleus. Here we apply our method to compute the ground-state pairing energy of the strongly deformed, neutron-rich nucleus ^{100}Zr. Recently, the pairing problem in this nucleus was studied by the DMC method [27]. The average field was assumed to be an axially deformed Woods-Saxon potential [28] with Cassinian ovals shape parametrization [29]. The universal Woods-Saxon parameters proposed by Dudek *et al*. [30] were used in the single-particle level calculations, except that smaller values ($R_0=1.25$ for both particles) of the central potential radius parameter were employed [31]. The computer code CASSINI [32] using Cassinian ovals parametrization was applied to obtain single-particle level energies. In the pairing calculations, we keep all single-particle levels ($\Omega=20$) obtained in the deformed ground-state potential in a 10 MeV interval around the Fermi level (5 MeV above and 5 MeV below). The single-particle energies relative to Fermi level energy are listed in Table III. The number of pairs in this system is equal to the number of considered single-particle levels below the Fermi energy, i.e., 9 (number of particles $N=18$). The BCS, LN, and MCP results are compared against benchmark DMC calculations in Table IV for interaction strength $G=0.255$. Differences between published [27] and present BCS results arise from the consideration of the self-energy. The accuracy of MCP is, once more, comparable to DMC.

In conclusion, we have proposed a method for projecting out BCS-like wave functions to the N-particle Hilbert space. The method shares with the BCS approach its computational simplicity. The use of LN approximate projection makes it possible to apply the MCP at any pairing strength, even below the BCS critical coupling, if it exists. These properties make the method very suitable for nuclear structure calculations. We stress that, unlike DMC, any pairing interaction can be treated in our approach.

In addition to the nuclear pairing problem, there are other possibilities of application of the MCP method. Recently, we have used it in the computation of the ground-state energy of electron-hole systems in a quantum dot [33]. The electron-hole attractive Coulomb potential is the pairing interaction in this case. MCP is used to improve the BCS estimation. The BCS approach to electron correlations in molecules [34,35] is another example with Coulomb matrix elements. It was shown that this approach fails to reproduce the correlation energy of small molecules, probably because of the need of

TABLE II. Pairing energies for selected values of the interaction strength in the system with $\Omega=8$ double degenerate levels and $N=8$ particles.

G	Exact	BCS	LNM	DMC	MCP_{BCS}	MCP_{LNM}
0.7	5.309	3.89	5.245	5.27(3)	5.28(5)	5.25(6)
0.9	8.018	6.18	7.977	8.06(2)	7.98(5)	7.97(4)
1.1	11.181	8.83	11.05	11.05(4)	11.11(5)	11.09(9)

TABLE III. Single-particle energies of ^{100}Zr in a 10 MeV interval around the Fermi energy. The deformation parameter is $\varepsilon=0.33$.

Levels above Fermi energy	Levels below Fermi energy
4.684	0.0000
4.559	−0.254
4.275	−1.303
3.566	−1.520
3.300	−2.224
2.908	−2.826
2.235	−3.914
1.928	−4.125
1.497	−4.605
1.323	
0.311	

TABLE IV. Ground-state pairing energy for the interaction strength $G=0.255$ in the ^{100}Zr nucleus.

G	DMC	BCS	LNM	MCP_{BCS}	MCP_{LNM}
0.255	5.0	3.87	4.94	5.1(1)	4.98(6)

an exact projection. MCP may be a good alternative. Finally, we shall mention as a possibility of application the recent study of superconductivity in ultrasmall grains [36]. Some of these problems are currently under investigation.

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