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EXACT SOLUTION OF THE NUCLEAR PAIRING PROBLEM

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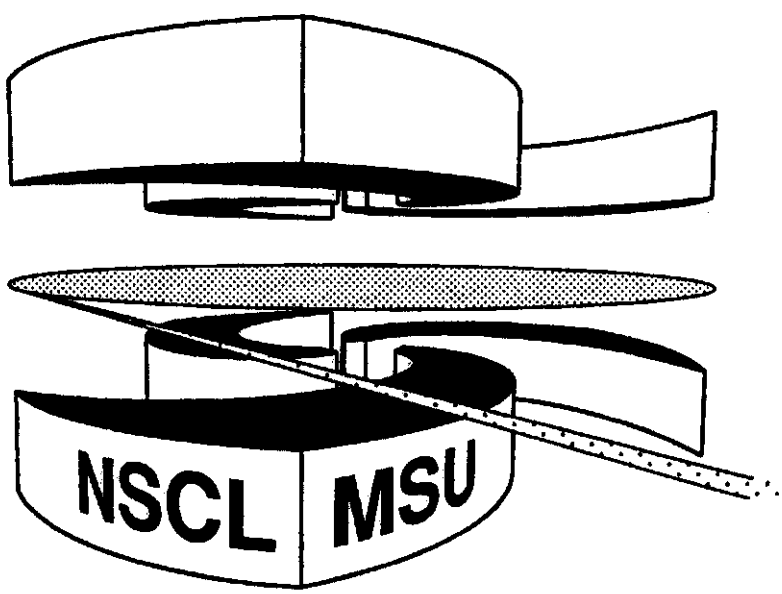

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Exact solution of the nuclear pairing problem

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A method is developed for exact treatment of the general pairing problem in a finite Fermi-system. The method is based on SU(2) quasispin algebras that are present in the problem. We show examples of practical applications of the method and its comparison with approximate treatments.

Pairing correlations play an essential role in nuclear structure properties including binding energies, odd-even effects, single-particle occupancies, excitation spectrum, electromagnetic and beta-decay probabilities, transfer reaction amplitudes, low-lying collective modes, level densities, and moments of inertia [1–3]. The revival of interest in pairing correlations is related to studies of nuclei far from stability and predictions of exotic pairing modes [4,5]. Metallic clusters, organic molecules and Fullerenes are other examples of finite Fermi systems with possibilities for pairing correlations of the superconducting type [6].

The conventional description of pairing in small systems usually employs the classical BCS approach [7] used in theory of superconductivity. This approximate solution has a very good accuracy for large systems and becomes exact in the asymptotic limit [8]. The major drawback of the BCS is violation of particle number conservation, which gives rise to deviations from the exact solutions for small systems. Various ideas have been suggested to correct this deficiency, such as the particle projection technique [20], number projection mean-field methods [10–12], stochastic number projection [13], statistical descriptions [14], treatments of residual parts of the Hamiltonian in the random phase approximation [15,16], and recurrence relation methods [17]. These methods have found only a limited number of practical applications; for some approaches the obtained results did not manifest the desired accuracy whereas other methods are limited by practical complications. BCS-like approximate theories have a number of other deficiencies when applied to small systems.

In particular, in the region of weak pairing the BCS has a sharp phase transition from the paired condensate to the normal state with no pairing (so-called trivial or zero gap solution), whereas exact solutions exhibit the existence of exponentially decreasing pairing correlations all the way down to the zero pairing strength [18]. This difficulty makes the BCS method unreliable for applications to weakly bound nuclei and calls for improvements and extensions such as BCS+RPA [19].

The exact pairing (EP) method presented in this work allows one to solve exactly the general pairing Hamiltonian

$$H = \sum_{j\,m} \epsilon_j a^\dagger_{j\,m} a_{j\,m} + \frac{1}{4} \sum_{j,j'} G_{j\,j'} \sum_{m,m'} a^\dagger_{j\,m} \tilde{a}^\dagger_{j\,m} \tilde{a}_{j'\,m'} a_{j'\,m'}\,, \quad \tilde{a}_{j\,m} \equiv (-1)^{j-m} a_{j\,-m}\,, \qquad (1)$$

where $\{\epsilon_j\}$ is the set of single-particle energies, diagonal $G_{j\,j}$ are pairing energies, and $G_{j\,j'} = G_{j'\,j}$ for $j \neq j'$ are pair transfer matrix elements, $(j' \leftrightarrow j)$. The practical usefulness of the EP algorithm comes from the facts that it is exact, fast and allows a straightforward extension for an approximate treatment of other components of residual interactions. Some realistic examples are presented in this work to emphasize these points. As a result, it becomes inappropriate to use complex approximate methods, such as BCS and all those associated with it, when exact results that are free of all problems discussed above can be obtained with an almost equal or even smaller effort compared to BCS.

The ideas that provide the conceptual basis for the EP are not new, see for example [20]. The existence of quasispin symmetry in paired systems has been known from the 1940's when it was introduced by Racah [21] as a very convenient mathematical tool. The EP solution gains its simplicity from the use of quasispin algebra for each subset of degenerate single-particle levels. The fact that Racah's degenerate model is analytically solvable comes purely from this algebraic feature. The spherical shell model with its m-degeneracies is a perfect arena for applying this method and therefore we will use notations associated with the case of spherical symmetry and j-j coupling. This certainly does not limit the generality of approach.

The Hamiltonian Eq. (1) can be rewritten as

$$H = \sum_j \epsilon_j \Omega_j + 2 \sum_j \epsilon_j L_j^z + \sum_{jj'} G_{jj'} L_j^+ L_{j'}^- , \tag{2}$$

by introducing the partial quasispin operators L_j^+, L_j^- and L_j^z for each j-level as follows

$$L_j^- = \frac{1}{2} \sum_m \tilde{a}_{jm} a_{jm} , \quad L_j^+ = \left(L_j^-\right)^\dagger = \frac{1}{2} \sum_m a_{jm}^\dagger \tilde{a}_{jm}^\dagger , \tag{3}$$

$$L_j^z = \frac{1}{2} \sum_m \left(a_{jm}^\dagger a_{jm} - \frac{1}{2} \right) = \frac{1}{2}(N_j - \Omega_j) , \tag{4}$$

where N_j is the particle number operator and $\Omega_j = (2j+1)/2$ is the pair degeneracy of a given single-particle level j. It can be shown directly from the definitions of L_J^+, L_j^- and L_j^z that they form an SU(2) algebra of angular momentum,

$$\left[L_j^+, L_{j'}^-\right] = 2\delta_{jj'} L_j^z , \ \left[L_j^z, L_{j'}^+\right] = \delta_{jj'} L_j^+ , \ \left[L_j^z, L_{j'}^-\right] = -\delta_{jj'} L_j^- . \tag{5}$$

Expressed in terms of quasispins, the Hamiltonian in (2) makes the pairing problem equivalent to the problem of interacting spins in a magnetic field, a generalized form of the Zeeman effect [22]. It is clear that every square of the partial quasispin $\mathbf{L}_j^2 = L_j^+ L_j^- - L_j^z + (L_j^z)^2$ commutes with the Hamiltonian making L_j, corresponding to the eigenvalue $L_j(L_j+1)$ of $\mathbf{L}_j^2$, a good quantum number in the pairing problem. This brings in the major simplification of the problem. The maximum value that L_j can take is $\Omega_j/2$, which happens for a fully paired subshell, such as, for example, the completely occupied subshell case where $N_j = 2\Omega_j$, $L_j^z = L_j = \Omega_j/2$. Lower values of the quasispin quantum number correspond to the Pauli blocking of a part of the pair space Ω_j by s_j unpaired particles. This reduces the allowed space to $\Omega_j - s_j$. The number s_j can be called the seniority of a given j-shell. Being related to the quasispin, s_j are conserved by the pairing interaction (2). Introducing the partial seniority s_j and partial occupancy N_j by means of

$$L_j = \frac{1}{2}(\Omega_j - s_j) \quad L_j^z = \frac{1}{2}(N_j - \Omega) , \tag{6}$$

we will use $|s_j, N_j\rangle$ instead of the SU(2) notation $|L_j, L_j^z\rangle$.

The quasispin projections L_j^z, or the partial occupancies N_j, are not conserved because of the pair transfer term $G_{jj'}$ (pair vibration). The usual constraints on angular momentum

$0 \leq |L_j^z| \leq L_j$ lead to $s_j \leq N_j \leq 2\Omega_j - s_j$ and $s_j \leq \Omega_j$ that have obvious interpretations. Furthermore, since both L_j and L_j^z must be simultaneously either integers or half-integers, s_j is of the same parity as N_j, confirming that particles are transfered only in pairs. Finally, there is a given total number of particles in the system $N = \sum_j N_j$, and one can introduce the total seniority $s = \sum_j s_j$. Both quantities are conserved by the Hamiltonian and must be of the same parity.

For each representation given by the set of quantum numbers $\{s_j\}$, one can construct basis states $|\{s_j\}, \{N_j\}\rangle$ going through all permutations of N fermions allowed by above constraints. Finally, a Hamiltonian matrix can be constructed in this basis using standard properties of the momentum operators

$$L^{\pm}|L, L_z\rangle = \sqrt{(L \mp L_z)(L \pm L_z + 1)}\,|L, L \pm 1\rangle\,. \tag{7}$$

Diagonal elements become

$$\langle\{s_j\}, \{N_j\}|H|\{s_j\}, \{N_j\}\rangle = \sum_j \left(\epsilon_j N_j + \frac{G_{jj}}{4}(N_j - s_j)(2\Omega_j - s_j - N_j + 2)\right)\,, \tag{8}$$

and off-diagonal elements that transfer pairs are

$$\begin{aligned}&\langle\{s_j\}, \ldots N_j + 2, \ldots N_{j'} - 2, \ldots|H|\{s_j\}, \ldots N_j, \cdots N_{j'}, \ldots\rangle \\ &= \frac{G_{jj'}}{4}\sqrt{(N_{j'} - s_{j'})(2\Omega_{j'} - s_{j'} - N_{j'} + 2)(2\Omega_j - s_j - N_j)(N_j - s_j + 2)}\,.\end{aligned} \tag{9}$$

Diagonalization of this matrix for each representation, a given set of partial seniorities $\{s_j\}$, is the final step in the solution. The largest Hamiltonian matrix in partial seniority basis, which corresponds to the lowest allowed total seniority, has a dimension extremely smaller than the total fermionic many-body space. Even for the set of valence orbits encountered in heavy nuclei it does not exceed several thousands. As seen from the above discussion the Hamiltonian matrix is very sparse.

Each state of a non-zero seniority is degenerate since s_j unpaired particles are untouched by the Hamiltonian and are free to move within a given j-shell, provided that they all remain unpaired. The number of these fermionic degrees of freedom for each j is

$C(2\Omega_j, s_j) - C(2\Omega_j, s_j - 2)$ where $C(m,n) = m!/(n!(m-n)!)$ is a binomial coefficient. The total degeneracy of each state in the $\{s_j\}$ seniority class is

$$\prod_j \left[C(2\Omega_j, s_j) - C(2\Omega_j, s_j - 2)\right] . \tag{10}$$

The resulting degenerate states that carry seniority quantum numbers can be further classified according to other symmetry groups of the Hamiltonian such as angular momentum. All total seniority zero states have spin zero. For non-zero seniorities, one first has to determine all possible angular momenta for a given subshell j with s_j unpaired particles and then make all possible couplings of subshells to a total spin.

To illustrate the practical application of this algorithm, we show below examples involving chains of Ca and Sn isotopes. The Ca isotopes occupy the *fp* shell with the model space consisting of four levels $f_{7/2}$, $p_{3/2}$, $f_{5/2}$, and $p_{1/2}$. This amounts to a total neutron capacity of 20. The pair transfer matrix elements are taken from the FPD6 interaction [23]. The results in Fig. 1(b) are obtained with single-particle energies appropriate for the above mentioned j-levels in ^{48}Ca: -9.9, -5.1, -1.6, and -3.1 MeV, respectively. Fig. 1(b) shows the correlation energies in the Ca isotopes, defined as

$$E_{\rm corr} = E - \sum_j \epsilon_j \bar{N}_j - \frac{1}{4}\sum_j \frac{G_{jj}}{\Omega_j - 1}\bar{N}_j(\bar{N}_j - 1)\,, \tag{11}$$

where E is the energy of the ground state and $\bar{N}_j$ is the expectation value of the particle number on the j-level, found as a result of EP calculation. It is known [1] that in a system with a discrete single-particle spectrum the nontrivial BCS solution exists only at a sufficiently strong pairing interaction which can overcome the single-particle level spacings. In contrast to that, in macroscopic Fermi-systems the nontrivial Cooper phenomenon exists at any strength of the attractive pairing interaction. Near the ^{48}Ca shell closure there is a 4.8 MeV gap between $f_{7/2}$ and the rest of the single-particle orbitals, and as it can be seen from Fig. 1(b), BCS can no longer support the pairing condensate. It gives instead a normal Fermi-gas solution with zero pairing energy, whereas in reality the EP solution demonstrates significant pairing effects with almost 2 MeV condensation energy.

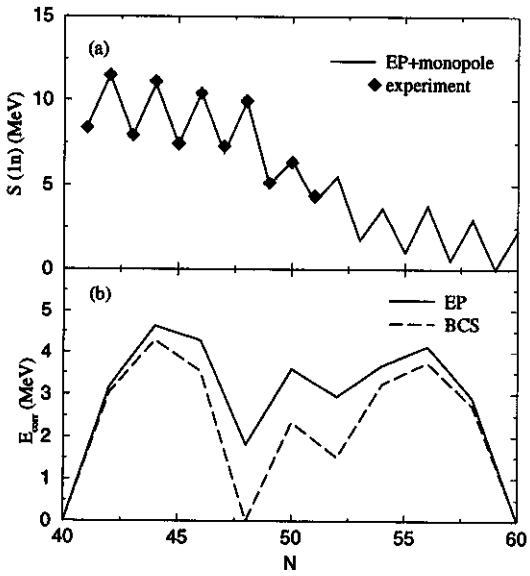

FIG. 1. Panel (a): neutron separation energies in Ca isotopes, EP+monopole treatment of other interactions is compared with experimental points (diamonds); panel (b): pairing correlation energy in even-even Ca isotopes, the exact EP calculation (solid line) is compared with the standard BCS (dashed line).

The results for the pure pairing interaction ($J = 0\,,\ T = 1\,$) can be modified by residual interactions in other channels including the $T = 0$ pairing [24]. For example, we can include the $T = 1$ monopole interaction given by

$$\sum_j \bar{V}_{j\,j} \frac{N_j(N_j - 1)}{2} + \sum_{j \neq j'} \bar{V}_{j\,j'} N_j N_{j'}\,, \tag{12}$$

where

$$\bar{V}_{j\,j'} = \frac{1 + \delta_{j\,j'}}{\Omega_j(\Omega_{j'} - \delta_{j\,j'})} \sum_{J \neq 0} (2J+1) \langle J;\, j\,j' | V | J;\, j\,j' \rangle \tag{13}$$

in the diagonal part of Eq. (8). One-neutron separation energies shown in Fig. 1(a) were calculated with this EP plus monopole method, using the FPD6 interaction and single-particle energies for ^{41}Ca. These results agree very well with experimentally observed separation energies, shown on the figure with diamonds. Ground state energies, obtained with this method for Ca isotopes differ from those from the exact shell model diagonalization results

by less than 0.5 MeV, and certainly the EP plus monopole results are exact for full and empty shells and for one-particle or one-hole cases.

For the second example, shown in Fig. 2(b), a model space for the Sn isotopes is considered that consists of five single-particle levels $h_{11/2}$, $d_{3/2}$, $s_{1/2}$, $g_{7/2}$, and $d_{5/2}$. This space can accommodate up to 32 neutrons. The pairing interaction matrix elements were obtained from the G-matrix derived from the recent CD-Bonn [26] nucleon-nucleon interaction with ^{132}Sn as a closed shell, where the $\hat{Q}$-box method includes all non-folded diagrams up to the third order in the interaction and sums up the folded diagrams to infinite order [27]. The most complex case is ^{116}Sn (half-filled shell) with 601,080,390 many-body states of which 272,828 are of spin zero, so that even with the use of the angular momentum projection the problem remains difficult for direct diagonalization. There are only 420 independent seniority sets in the seniority basis. The largest matrix, $s = 0$, has a dimension of 110, the diagonalization of which is a trivial problem. Solution of the pairing problem for ^{116}Sn with the algorithm discussed above is therefore simple and extremely fast. The correlation energies obtained with the above G-matrix and single-hole energies -9.76, -8.98, -7.33, -7.66, and -7.57 MeV, based on the data for the ^{131}Sn isotope [25], are shown in Fig. 2(b). A reduction of pairing also happens between $g_{7/2}$, $d_{5/2}$ and the rest of the single-particle orbitals $h_{11/2}$, $d_{3/2}$, $s_{1/2}$, but here BCS is just weakened by the proximity of the phase transition point which results only in a relatively small deviations in correlation energy.

A related application of EP is shown in Fig. 2(a) where one-neutron separation energies are shown for the Sn isotopes, including those beyond ^{132}Sn. These energies were obtained from the fully self-consistent spherically symmetric solution of Hartree-Fock equations, using the SKX interaction [28], with the EP solution based on the above G-matrix at each Hartree-Fock iteration. The plot exhibits an odd-even staggering that can only be attributed to pairing. The agreement between experiment and theory is excellent given that no parameters have been adjusted for these particular data.

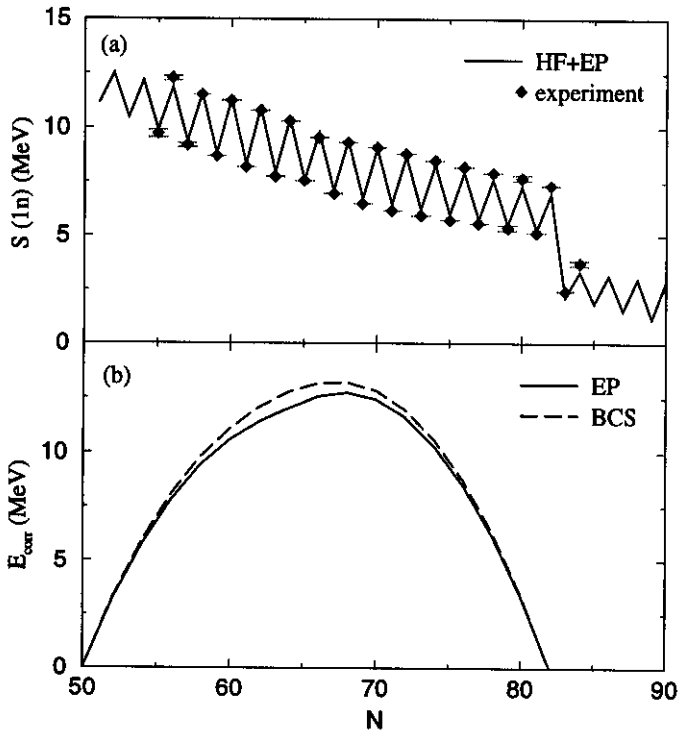

FIG. 2. Panel (a): neutron separation energies calculated for the Sn isotopes using the self-consistent solution of Hartree-Fock plus Exact Pairing. Experimental points are shown for comparison. Panel (b): pairing correlation energy in even-even Sn isotopes, EP (solid line) and BCS (dashed line).

A number of other methods of treating the pairing problem exactly have been previously proposed. The Richardson method, described in the series of papers [29], provides a formally exact way for solving the pairing Hamiltonian. This method reduces the large-scale diagonalization of a many-body Hamiltonian in a truncated Hilbert space to a set of coupled equations with a dimension equal to the number of valence particles. Recently, exact solutions have been approached by introducing sophisticated mathematical tools such as infinite-dimensional algebras [30]. Such formally exact solutions have a certain merit from a mathematical point of view and for developing and understanding approximate calculations. However, due to their complexity they are not very useful in solving practical problems in nuclear physics. The EP algorithm presented here in our view has a good future as a tool

for different calculations related to pairing. It is exact, fast and reliable which makes it perfect for pure shell model calculations with pairing, fast estimates of binding energies and spectroscopic factors, for the use as a basis for treatment of other interactions, iterative Hartree-Fock calculations and many other tasks.

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