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A particle-number-conserving solution to the generalized pairing problem

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Abstract

An exact, number-conserving solution to the generalized, orbit-dependent pairing problem is derived by introducing an infinite-dimensional algebra. A method for obtaining eigenvalues and eigenvectors of the corresponding Hamiltonian is also given. The relevance of the orbit-dependent pairing solution is demonstrated by comparing predictions of the model with shell-model calculations.

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Pairing has long been considered an important interaction in physics. The concept can be traced back to the seniority scheme introduced by Racah in atomic physics [1]. Its physical significance was first realized in the study of superconductivity [2]. Following the suggestions of Bohr, Mottelson, and Pines [3], the first detailed application of pairing in nuclei was made by Belyaev [4]. The concept has since been applied to other phenomena: high T_c superconductivity [5,6], applications using the Hubbard model [7], and pairing phenomena in liquids [8] and metal clusters [9].

BCS methods have yielded major successes in studies of superconductivity. When applied to nuclei, however, one must remember that the number of spectroscopically active nucleons is typically too small ($n \sim 10$) to support underlying assumptions of the theory, namely $\delta n/n$ is not negligible, and as a consequence particle-number nonconservation effects can enter and give rise to spurious states, nonorthogonal solutions, etc. Although this challenge can be partially remedied by making use of particle-number projection techniques [10], the elegance and simplicity of the BCS method are then compromised. Secondly, an essential feature of pairing correlations are even-odd differences, which are driven mainly by Pauli blocking. It is difficult to treat these differences in the BCS formalism because different quasi-particle bases must be introduced for different blocked levels. After an investigation into the accuracy of the BCS approximation, Kerman and Lawson suggested that an exact diagonalization of the pairing Hamiltonian is necessary [10]. Based on these observations, a particle-number-conserving method for treating the pairing problem in well-deformed nuclei was put forward [11]. The method uses a configuration-energy truncation scheme and takes the strength of the pairing interaction to be the same for all orbitals. Unfortunately, because of the deformation, each orbital can only accommodate a single pair of particles and this limits the applicability of the theory. Complementary mean-field techniques with approximate Lipkin-Nogami number projection and non-trivial pairing interactions [12,13] have also been found to be a useful means for handling pairing correlations in such systems [14–16]. However, exact shell-model solutions, when feasible, even if only approximate, are the best way to probe the true nature of many-body correlation effects.

The purpose of this contribution is to give an exact, particle-number-conserving solution to the generalized, orbit-dependent pairing problem. The method can be applied to any number of pairs in any model space, even to cases where exact diagonalization is computationally prohibitive.

The generalized pairing Hamiltonian for spherical nuclei can be written as

$$\hat{H} = \sum_{jm} \epsilon_j a_{jm}^\dagger a_{jm} - |G| \sum_{jj'} c_{jj'} S^+(j) S^-(j'), \quad (1)$$

where the ϵ_j are single-particle energies and $S^\pm(j)$ and $S^0(j)$ are the pairing operators for a single- j shell defined by

$$\begin{aligned} S^+(j) &= \sum_{m>0} (-)^{j-m} a_{jm}^\dagger a_{j-m}^\dagger, \\ S^-(j) &= \sum_{m>0} (-)^{j-m} a_{j-m} a_{jm}, \\ S^0(j) &= \frac{1}{2} \sum_{m>0} (a_{jm}^\dagger a_{jm} + a_{j-m}^\dagger a_{j-m} - 1) = \frac{1}{2} (\hat{N}_j - \Omega_j), \end{aligned} \quad (2)$$

where $\Omega_j \equiv j + 1/2$ is the maximum number of pairs in the j -th shell, \hat{N}_j is the j -th shell particle number operator, and the $c_{jj'}$ measure the orbit-orbit pairing strength. Note that Hamiltonians with degenerate single-particle energies ($\epsilon_j = \epsilon$ for all j -orbitals) and separable pairing strengths ($c_{jj'} = c_j^* c_{j'}$) are special cases of the general theory.

In general, for N pairs, Eq. (1) can be diagonalized with bases states that are products of the single- j shell pairing wave functions:

$$|N\rangle = \sum_{k_i} B_{k_1 k_2 \dots k_p} S_{j_1}^{+ k_1} S_{j_2}^{+ k_2} S_{j_3}^{+ k_3} \dots S_{j_p}^{+ k_p} |0\rangle, \quad (3)$$

where the summation is restricted so that

$$\sum_{i=1}^p k_i = N, \quad (4)$$

and the $B_{k_1 k_2 \dots k_p}$ are expansion coefficients to be determined. Here, $|0\rangle$ is the pairing vacuum state that satisfying the condition

$$S_j^- |0\rangle = 0 \quad \text{for all } j. \quad (5)$$

The dimensionality of the Hamiltonian matrix in this basis increases rapidly with increasing N and the number of shells p . Due to the Pauli Principle, it is less than or equal to the dimension of the irreducible representation (irrep) $[N\hat{0}]$ of the unitary group $U(p)$,

$$\dim \leq \frac{(p+N-1)!}{N!(p-1)!}. \quad (6)$$

The equal sign in Eq. (6) holds when all the single- j shell pairing wave functions in the summation of Eq. (3) are Pauli allowed. From Eq. (6), it is clear that the problem quickly becomes intractable because there are no analytical expressions or recursion relations for determining the $B_{k_1 k_2 \dots k_p}$ coefficients.

As in the quasi-spin case [17], we consider a slightly simpler Hamiltonian

$$\hat{H} = \epsilon \sum_{jm} a_{jm}^+ a_{jm} - |G| S_0^+ S_0^-, \quad (7)$$

that is, one with degenerate single-particle energies and a separable pairing interaction,

$$S_0^+ = \sum_j c_j^* S^+(j), \quad S_0^- = \sum_j c_j S^-(j) \quad (8)$$

with the coefficients c_i satisfying the condition

$$\sum_i |c_i|^2 = 1. \quad (9)$$

This defines generalized pairing as proposed by Talmi [18]. The separability assumption, though strong, is physically motivated as it links the pair-pair interaction strength to the individual pair formation probability. In the notation of Eq. (1), $c_{jj'} = c_j^* c_{j'}$ with $|c_j|^2$ giving the percentage of single- j shell pairing in the Hamiltonian. In what follows, the c_j are taken to be real. Because the total number of particles is a good quantum number in a number-conserving theory, the single-particle term in Eq. (7) is a constant and can be dropped without loss. Hence, Eq. (7) reduces to

$$\hat{H} = -|G| S_0^+ S_0^-. \quad (10)$$

To diagonalize this Hamiltonian, consider an algebra generated by

$$\begin{aligned}
S_m^0 &= \sum_j c_j^{2m} S^0(j), \\
S_m^\pm &= \sum_j c_j^{2m+1} S^\pm(j).
\end{aligned} \tag{11}$$

It is easy to show that these generators satisfy the following commutation relations:

$$\begin{aligned}
[S_m^+, S_n^-] &= 2S_{m+n+1}^0, \\
[S_m^0, S_n^\pm] &= \pm S_{m+n}^\pm.
\end{aligned} \tag{12}$$

Therefore, the $\{S_m^\mu, \mu = 0, +, -; m = 0, \pm 1, \pm 2, \dots\}$ form an infinite-dimensional algebra, one that differs only slightly from a general Lie-algebra of the affine type without central extension.

The unique lowest-weight state of this algebra is simply the product of the single- j shell pairing vacua with arbitrary seniority quantum numbers. Therefore, it suffices to consider the total seniority zero case. The lowest-weight state satisfies

$$S_m^-|0\rangle = 0; \quad m = 0, \pm 1, \pm 2, \dots, \tag{13}$$

and

$$S_m^0|0\rangle = -\frac{1}{2} \sum_j |c_j|^{2m} \Omega_j |0\rangle = \Lambda_m |0\rangle. \tag{14}$$

Furthermore, it can be proven that the eigenvectors of \hat{H} for any N and non-zero energy eigenvalue can be written as

$$|N\rangle = \mathcal{N} S_0^+ S_{x_1}^+ S_{x_2}^+ \dots S_{x_{N-1}}^+ |0\rangle, \tag{15}$$

where \mathcal{N} is a normalization constant and

$$S_{x_i}^+ = \sum_j \frac{c_j}{1 - c_j^2 x_i} S^+(j). \tag{16}$$

To obtain the variables $\{x_i; i = 1, 2, \dots, N-1\}$, Eq. (15) can be expanded in terms of x_i around $x_i = 0$,

$$|N\rangle = \mathcal{N} \sum_{n_i} x_1^{n_1} x_2^{n_2} \dots x_{N-1}^{n_{N-1}} S_0^+ S_{n_1}^+ S_{n_2}^+ \dots S_{n_{N-1}}^+ |0\rangle, \tag{17}$$

where the $S_{n_i}^+$ are the Fourier-Laurent coefficients in the expansion of $S_{x_i}^+$, namely

$$S_{n_i}^+ = \frac{1}{2\pi i} \oint_0 dx_i x_i^{n_i} S_{x_i}^+. \quad (18)$$

Using Eq. (17) and the commutation relations of Eq. (12), it is easily shown that the x_i , with $i = 1, 2, \dots, N-1$, satisfy the relations

$$-\frac{1}{2} \sum_{j=1}^p \Omega_j c_j^2 \alpha \frac{1}{1 - \alpha y_i c_j^2} = \frac{1}{y_i} + \sum_{k \neq i} \frac{1}{y_i - y_k}, \quad i = 1, 2, \dots, N-1, \quad (19)$$

with

$$\sum_{i=1}^{N-1} \frac{1}{y_i} = 1, \quad (20)$$

where

$$y_i = x_i/\alpha, \quad \alpha = -\frac{2}{h + 2\Lambda_1}, \quad h \equiv E/(-|G|). \quad (21)$$

We note that although these relations were derived for $x_i \approx 0$, they are nonetheless valid in the entire complex plane except at the singularities in Eqs. (19) and (20). Therefore, the coefficients x_i ($i=1, 2, \dots, N-1$) and eigenvalues of the pairing energy $E \neq 0$ are simultaneously determined by the system of equations Eqs. (19) and (20).

Similarly, the eigenvectors for $E = 0$ can be expressed as

$$|N, 0\rangle = \mathcal{N} S_{x_1}^+ S_{x_2}^+ \dots S_{x_N}^+ |0\rangle. \quad (22)$$

Using the same technique as in the $E \neq 0$ case, it can be shown that in this case the x_i with $i = 1, 2, \dots, N$, are determined by the following set of equations

$$\sum_j \Omega_j \frac{c_j^2}{1 - x_1 c_j^2} = 0 \quad \text{for } N = 1, \quad (23)$$

$$\frac{1}{2} \sum_j \Omega_j \frac{c_j^2}{x_i c_j^2 - 1} = \sum_{k \neq i} \frac{1}{x_i - x_k}, \quad i = 1, 2, \dots, N, \quad \text{for } N \geq 2. \quad (24)$$

At this point, we reiterate that our solution is for a separable, orbit-dependent pairing interaction as defined by Eq. (7), and not for the generalized pairing Hamiltonian of Eq. (1). If the separability assumption is valid, the solutions should be good approximations to the

more general theory. The power of the method lies in the fact that it gives the exact, particle-number-conserving solution of the pairing problem for any number of pairs in any model space, even for cases where full matrix diagonalizations cannot be carried out. Next we show, by example, that the separability assumption is consistent with “realistic” shell-model results and hence that theory can be used with confidence to study many-particle correlation phenomena in pair-rich systems.

As a test of the method, comparisons with shell-model calculations for like particles interacting through a “realistic” generalized pairing interaction were carried out. The shell-model calculations were performed within the configuration space defined by the nuclear ds -shell ($0d_{5/2}$, $0d_{3/2}$, and $1s_{1/2}$ orbitals). The generalized pairing Hamiltonian of Eq. (1) was defined using the $J = 0$ two-body matrix elements of the universal ds -shell Hamiltonian of Wildenthal [19]. Since the number of $J = 0$ states for any two-particle system is small (three for the ds -shell), it is reasonable to define the generalized pair in Eq. (8) as the wave function of the shell-model ground state. For our ds -shell example this means the coefficients are: $c_{d_{5/2}} = 0.570243$, $c_{d_{3/2}} = 0.626089$, and $c_{s_{1/2}} = 0.531823$. The strength of the interaction was then adjusted to reproduce the two-particle, ground-state energy, that is, $|G| = 3.12778$. With the Hamiltonian so defined, solutions were obtained for $N = 1, 2$, and 3 pairs of like particles [20]. Shown in Fig. 1 is a comparison between the eigenenergies obtained from the shell model (SM) and the separable, generalized pairing method. For reference, the quasi-spin (QSA) approximation gives -6.389 , -10.684 , and -12.788 , respectively, for the $N = 1, 2$, and 3 pair cases [21]. A further measure of how well the generalized pairing solutions correspond to the shell-model results is illustrated in Table I where the percent overlap between the shell-model and generalized pairing wave functions are given. In all cases, the wave functions obtained with the method presented here have better than a 94% overlap (96% for the ground state) with the shell-model states, which indicates that the assumption of separability is sound.

An exact, particle-number-conserving solution to the generalized, orbit-dependent pairing problem has been derived. A key feature of the derivation is the use of an infinite-

dimensional algebra, which is new in nuclear physics. Because the theory is number-conserving, it goes well-beyond what has been done even for the case of equal pairing strengths which includes to quasi-spin as a special limit. The relevance of the theory was shown by comparing eigenvalues and eigenvectors with “realistic” shell-model results.

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- [20] If a diagonalization of the two-particle system is not feasible, an alternative procedure that work almost as well is to determine the coefficients by the relative weight of the diagonal matrix elements. With this choice, the coefficients would be $c_{d_{5/2}} = 0.766482$, $c_{d_{3/2}} = 0.512492$, and $c_{s_{1/2}} = 0.714841$ with $|G| = 2.28278$.
- [21] Hamiltonian (7) reduces to the quasi-spin approximation when all the parameters c_j are taken to be the same. In this case, the fully paired (seniority zero) solution is well-known: eigenenergy $E = -|G|N(\Omega - N + 1)$ with eigenstate $[\frac{(\Omega-N)!}{N!\Omega!}]^{1/2}(S^+)^N|0\rangle$, where N is the number of pairs, $\Omega = \sum_j \Omega_j$ and $S^+ = \sum_j S^+(j)$.

TABLES

TABLE I. Percent overlap between the eigenstates obtained with the separable, generalized pairing method and the shell model as a function of the number of pairs, N .

eigenstate \ N	1	2	3
1	96.2	99.4	97.8
2	94.7	97.6	97.0
3	99.4	97.2	94.3
4		98.8	95.8
5		99.2	96.8
6			97.0

FIGURES

FIG. 1. Comparison between the spectra obtained from the shell model (SM) and the separable, generalized pairing (SGP) method as a function of the number of pairs, N . The dashed lines indicate the correspondance between the levels in the two models.

