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Algebraic Solutions of an Extended Pairing Model for Well-Deformed Nuclei

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A Nilsson mean-field plus extended pairing interaction Hamiltonian with many-pair interaction terms is proposed. Eigenvalues of the extended pairing model are easy to obtain. Our investigation shows that one- and two-body interactions continue to dominate the dynamics for relatively small values of the pairing strength. As the strength of the pairing interaction grows, however, the three- and higher many-body interaction terms grow in importance. A numerical study of even-odd mass differences in the $^{154-171}$Yb isotopes shows that the extended pairing model is applicable to well-deformed nuclei.

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Pairing is an important residual interaction that is used in nuclear physics as well as in other fields such as the study of metallic clusters. The Bardeen-Cooper-Schrieffer (BCS) [1] and Hartree-Fock-Bogolyubov (HFB) [2] methods for finding approximate solutions are well known. The limitations of these methods when applied in nuclear physics are also well understood. First of all, not only is the number of nucleons in a nucleus typically small, the number of valence particles ($n \sim 10$) which dominate the behavior of low-lying states is too few to support the underlying assumptions of the approximations, that is, particle number fluctuations are non-negligible. As a result, particle number-nonconservation effects can lead to serious problems such as spurious states, nonorthogonal solutions, etc. Furthermore, an essential feature of pairing correlations are differences between neighboring even and odd mass nuclei, which are driven mainly by Pauli blocking effects, and it is difficult to treat even-odd differences with either the BCS or HFB theories because different quasi-particle bases must be introduced for different blocked levels. Another problem with approximate treatments of the pairing Hamiltonian is related to the fact that both the BCS and the HFB approximations break down for an important class of physical situations. A remedy that uses particle number projection techniques complicates the algorithms considerably and does not help to achieve a better description of the higher-excited part of the spectrum of the pairing Hamiltonian. Similar conclusions were found to hold within the context of the energy spectra of nano-scale metallic grains [3,4].

Driven by the importance of having exact solutions of the pairing Hamiltonian, much attention and progress, building on Richardson's early work [5–7] and extensions to it based on the Bethe ansatz, has been made in the past few years [8–14]. For all these algebraic Bethe ansatz approaches, the solutions are provided by a set of highly non-linear Bethe Ansatz Equations (BAEs). Though these applications demonstrate that the pairing problem is exactly solvable, solutions of these BAEs are not easy and normally require extensive numerical work, especially when the number of levels and valence pairs are large. This limits the applicability of the methodology to relatively small systems; it cannot be applied to large systems such as well-deformed nuclei.

The standard pairing Hamiltonian for well-deformed nuclei is given by

$$\hat{H} = \sum_{j=1}^{p} \epsilon_j n_j - G \sum_{i,j=1}^{p} a_i^+ a_j, \tag{1}$$

where p is the total number of Nilsson levels considered, $G > 0$ is the overall pairing strength, ϵ_j is single-particle energies taken from the Nilsson model, $n_j = c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow}$ is the fermion number operator for the j-th Nilsson level, and $a_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$ ($a_i = (a_i^+)^\dagger = c_{i\downarrow} c_{i\uparrow}$) are pair creation (annihilation) operators. The up and down arrows in these expressions refer to time-reversed states. Since each Nilsson level can only be occupied by one pair due to the Pauli Principle, the Hamiltonian (1) is also equivalent to a finite site hard-core Bose-Hubbard model with infinite range one-pair hopping and infinite on-site repulsion. Specifically, the operators a_i^+, a_i, and $n_i^a = n_i/2$ satisfy the following hard-core boson algebra:

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$$(a_i^+)^2 = 0, \quad [a_i, a_j^+] = \delta_{ij}(1 - 2n_i^a), \quad [a_i^+, a_j^+] = [a_i, a_j] = 0. \tag{2}$$

As an extension of (1), we construct the following new (extended) pairing Hamiltonian:

$$\hat{H} = \sum_{j=1}^{p} \epsilon_j n_j - G \sum_{i,j=1}^{p} a_i^+ a_j - G \left(\sum_{\mu=2}^{\infty} \frac{1}{(\mu!)^2} \sum_{i_1 \neq i_2 \neq \cdots \neq i_{2\mu}} a_{i_1}^+ a_{i_2}^+ \cdots a_{i_\mu}^+ a_{i_{\mu+1}} a_{i_{\mu+2}} \cdots a_{i_{2\mu}} \right). \tag{3}$$

Besides the usual Nilsson mean-field and the standard pairing interaction (1), this form includes many-pair hopping terms that allow nucleon pairs to simultaneously scatter (hop) between and among different Nilsson levels. With this extension in place, we will show that the model is exactly solvable.

Because of the infinite on-site repulsion, the infinite sum in (3) truncates for $\mu \leq p$. It is also easy to see that each term of the form $a_i^+ \cdots a_j^+$ that forms eigenstates of (3) should enter with different indices $i \neq \cdots \neq j$. Let $|j_1, \cdots, j_m\rangle$ be the pairing vacuum state that satisfies

$$a_i |j_1, \cdots, j_m\rangle = 0 \tag{4}$$

for $1 \leq i \leq p$, where $j_1, j_2, \cdots, j_m$ indicates those m levels that are occupied by single nucleons. Any singly-occupied state is blocked by the Pauli principle.

Following the algebraic ansatz used in [15], one can write k-pair eigenstates of (3) as

$$|k; \zeta; j_1, \cdots, j_m\rangle = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq p} C^{(\zeta)}_{i_1 i_2 \cdots i_k} a_{i_1}^+ a_{i_2}^+ \cdots a_{i_k}^+ |j_1, \cdots, j_m\rangle, \tag{5}$$

where $C^{(\zeta)}_{i_1 i_2 \cdots i_k}$ is an expansion coefficient that needs to be determined, and the strict ordering to the indices $i_1, i_2, \cdots, i_k$ reminds us that double occupation is not allowed. It is always assumed that the level indices $j_1,\ j_2, \cdots, j_m$ should be excluded from the summation in (5). Since the formalism for even-odd systems is similar, in the following, we focus on the even-even seniority zero case.

The expansion coefficient $C^{(\zeta)}_{i_1 i_2 \cdots i_k}$ can be expressed very simply as

$$C^{(\zeta)}_{i_1 i_2 \cdots i_k} = \frac{1}{1 - x^{(\zeta)} \sum_{\mu=1}^{k} \epsilon_{i_\mu}}, \tag{6}$$

where, similar to the results given in the Bethe ansatz approach, $x^{(\zeta)}$ is a c-number that is to be determined. To prove that the algebraic ansatz given in (5) and (6) are consistent, one may directly apply Hamiltonian (3) on the k-pair state (5). Using the hard-core boson algebraic relation given by (2) and a procedure that is similar to that used in Ref. [10] for finding exact solution of a Heisenberg algebra Hamiltonian, one can determine rather easily that for the mean-field part of the Hamiltonian (3)

$$\sum_j \epsilon_j n_j |k; \zeta; 0\rangle = \frac{2}{x^{(\zeta)}} \left(|k; \zeta; 0\rangle - \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq p} a_{i_1}^+ a_{i_2}^+ \cdots a_{i_k}^+ |0\rangle \right), \tag{7}$$

and for the extended pairing part of the Hamiltonian (3)

$$\left(\sum_i a_i^+ a_i + \sum_{\mu=1}^{\infty} \frac{1}{(\mu!)^2} \sum_{i_1 \neq i_2 \neq \cdots \neq i_{2\mu}} a_{i_1}^+ a_{i_2}^+ \cdots a_{i_\mu}^+ a_{i_{\mu+1}} a_{i_{\mu+2}} \cdots a_{i_{2\mu}} \right) |k; \zeta; 0\rangle =$$

$$\left(\sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq p} C^{(\zeta)}_{i_1 i_2 \cdots i_k} \right) \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq p} a_{i_1}^+ a_{i_2}^+ \cdots a_{i_k}^+ |0\rangle + (k-1)|k; \zeta; 0\rangle \tag{8}$$

By combining Eqs. (7) and (8), the k-pair excitation energies of (3) are given by:

$$E_k^{(\zeta)} = \frac{2}{x^{(\zeta)}} - G(k-1), \tag{9}$$

where the undetermined variable $x^{(\zeta)}$ is given by

$$\frac{2}{x^{(\zeta)}} + \sum_{1\le i_1<i_2<\cdots<i_k\le p} \frac{G}{(1 - x^{(\zeta)} \sum_{\mu=1}^{k} \epsilon_{i_\mu})} = 0. \tag{10}$$

The additional quantum number ζ now can be understood as the ζ-th solution of (10). Similar results for even-odd systems can also be derived by using this approach except that the index j of the level occupied by the single nucleon should be excluded from the summation in (5) and the single-particle energy term ϵ_j contributing to the eigenenergy from the first term of (3) should be included. Extensions to many broken-pair cases are straightforward.

Comparing Eqs. (9) and (10) to exact solutions of the Heisenberg algebraic Hamiltonian with a one-body interaction [10], one can regard the operator product $a^+_{i_1} a^+_{i_2} \cdots a^+_{i_k}$ in (5) as a 'grand' boson. The corresponding 'single-particle energy' of the 'grand' boson is $E_{i_1 i_2 \ldots i_k} = \sum_{\mu=1}^{k} 2\epsilon_{i_\mu}$, since (10) and the eigenstates (5) are similar to those for a multi-boson system with a one-body interaction as shown in [10], even though the Hamiltonians are totally different. Although the eigenstates (5) are not normalized, but they can be normalized easily by using a standard procedure. The eigenstates (5) with different roots given by (10) are mutually orthogonal, a result that can be proven as in [10].

Eigenenergies of the standard pairing model are expressed in terms of k variables that satisfy k coupled nonlinear equations that are difficult to solve numerically, especially when the number of pairs k and number of levels p are large. In contrast to BAE solutions to the standard pairing model, there is but a single variable $x^{(\zeta)}$ in the extended model. It should be noted that the solution (10) is only valid when all combinations of the single-particle energies $\sum_{\mu=1}^{k} \epsilon_{i_\mu}$ are different for k-pair excitation cases. Fortunately, this is always the case when single-particle energies are generated from the Nilsson model. In that case, (10) should have $\frac{p!}{(p-k)!p!}$ distinct roots, which could be a very large number for an entire deformed major shell.

If (10) is rewritten in terms of $z^{(\zeta)} = 2/(Gx^{(\zeta)})$ and the dimensionless energy of the 'grand' boson $\tilde{E}_{i_1 i_2 \ldots i_k} = \sum_{\mu=1}^{k} \frac{2\epsilon_{i_\mu}}{G}$, (10) takes the form:

$$1 = \sum_{1\le i_1<i_2<\cdots<i_k\le p} \frac{1}{(\tilde{E}_{i_1 i_2 \ldots i_k} - z^{(\zeta)})}. \tag{11}$$

Since there is only one variable $z^{(\zeta)}$ in (11), the zero points of the function can easily be shown graphically, which is very similar to the one-pair solution appearing in the TDA and RPA approximations with separable potentials [2]. From expression (11), it is clear that any solution $z^{(\zeta)}$ of (11) is located between two nearby values of the dimensionless 'grand' boson energy $\tilde{E}_{i_1 i_2 \ldots i_k} = \sum_{\mu=1}^{k} \frac{2\epsilon_{i_\mu}}{G}$ and the smallest solution $z^{(\zeta)}$ would be smaller than $\min(\{\tilde{E}_{i_1 i_2 \ldots i_k}\})$.

It is important to understand the differences between the extended pairing introduced by (3) and the standard pairing given in (1). For this purpose, let us consider a simple example in which there are $p = 10$ levels and the single-particle energies are given by $\epsilon_i = i + \chi_i$ for $i = 1, 2, \cdots, 10$, where χ_i are random numbers within the interval $(0, 1)$ to avoid accidental degeneracy required for exact solvability, and the pairing strength G is allowed to vary from 0.01 to 0.10. Fig. 1 shows the lowest few energies of the standard and extended pairing models. From this graph it is very clear that there are essential differences in the spectral structure of these two models. As shown by Inset (b), the extended pairing model very rapidly develops a paired ground-state configuration which is strongly dependent on the pairing strength G. In this case the transition from mean-field eigenstates to pairing eigenstates is very sharp and fast, while the standard pairing model, Inset (a), exhibits a much slower and smoother transition. The quantitative difference in the two spectra, with the extended pairing case showing a much stronger dependence on G than for standard pairing, is a very clear distinguishing characteristic and can be used to explore cases where the extended pairing concept might be more relevant and appropriate than the standard pairing model.

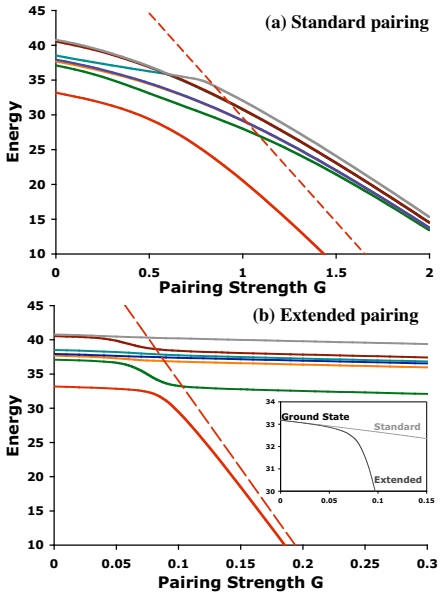

FIG. 1. (a) Spectral structure of the standard pairing interaction given by Eq.(1), and (b) spectral structure of the extended pairing interaction given by Eq.(3), as functions of the pairing interaction strength G for $k = 5$ pairs for a system with $p = 10$ levels and single-particle energies $\epsilon_1 = 1.179$, $\epsilon_2 = 2.65$, $\epsilon_3 = 3.162$, $\epsilon_4 = 4.588$, $\epsilon_5 = 5.006$, $\epsilon_6 = 6.969$, $\epsilon_7 = 7.262$, $\epsilon_8 = 8.687$, $\epsilon_9 = 9.899$, $\epsilon_{10} = 10.201$, where the single-particle energies and G are given in arbitrary units. The straight dash line is the expectation value of the Hamiltonian in the pure pairing ($\epsilon_i = 0$) ground state.

Since there are higher order terms involved in (3), it is important to know whether the dynamics is still dominated by the one- and two-body interactions, and, if not, under what conditions the higher order terms can be treated perturbatively. To explore this, we calculated as a function of G the expectation value of each higher order term $\langle V_\mu \rangle$ defined by:

$$V_1 = \sum_{i,j} a_i^+ a_j, \quad V_\mu = \frac{1}{(\mu!)^2} \sum_{i_1 \neq i_2 \neq \cdots \neq i_{2\mu}} a_{i_1}^+ a_{i_2}^+ \cdots a_{i_\mu}^+ a_{i_{\mu+1}} a_{i_{\mu+2}} \cdots a_{i_{2\mu}} \tag{12}$$

with $\mu = 2, 3, \cdots$, for k-pair ground states. Then, we calculate the ratio $R_\mu = \langle V_\mu \rangle / \langle V_{\text{total}} \rangle$, where $\langle V_{\text{total}} \rangle$ is the sum of all terms given in (12). The results up to the half-filled case are shown in Fig. 2. It can be seen that the two-body pairing interaction (V_1) dominates the dynamics of the system as long as the interaction strength G is small. With increasing interaction strength, the system is driven mainly by V_2, less by V_3 (but it may be comparable with V_2), and much less by the higher order terms. As one would expect, increasing the number of pairs k drives the critical point where V_2 becomes dominant towards smaller G values. The situation and the graphs beyond the half-filled case are qualitatively similar because of the particle-hole symmetry. The critical point where V_2 becomes dominant is actually at higher G values for $p - k$ pairs than for the $k < p/2$ pairs. Even though, higher order terms appear beyond the half-filled case, these terms are always less important than V_1 for small G and V_2 for big values of G. It is important to note that for large values of G when the dynamics is dominated by the pairing interaction, and thus independent of G, the V_2 term dominates followed in importance by the V_3 term.

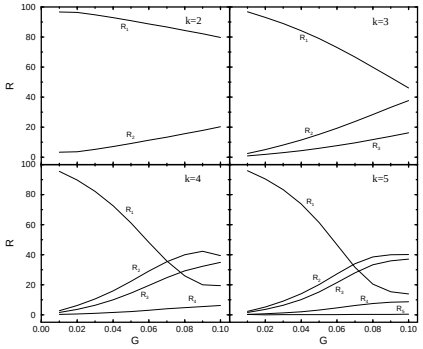

FIG. 2. Ratios $R_\mu(\%)$ with $\mu = 1, 2, \cdots, 5$ as function of the pairing interaction strength G for $k = 2, \cdots, 5$ for a system with $p = 10$ levels. The parameters that were used are the same as those shown in Fig. 1.

As an example of an application of the theory to well-deformed nuclei, we fit even-odd mass differences of the $^{154-171}$Yb isotopes. The single-particle energies of each nucleus were calculated using the Nilsson deformed shell model with experimentally evaluated deformation parameters [16]. Fig. 3 shows the fitted results in comparison with the corresponding experimental values [17]. Except for small deviations for $^{157-161}$Yb, the results are well reproduced.

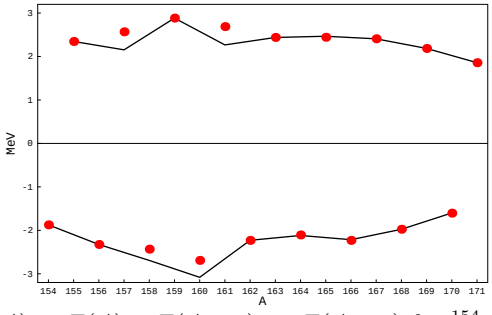

FIG. 3. Even-odd mass difference $P(A) = E(A) + E(A-2) - 2E(A-1)$ for $^{154-171}$Yb, where $E(A)$ is the total binding energy, and the dots correspond to the experimental quantities. The theoretical values for even-odd mass P(A) are connected by the lines.

The corresponding G values are given in Table I, from which one can see that the pairing interaction strength decreases with increasing number of pairs k from 245keV for 1 pair to 0.0948keV for 9 pairs, while the single-particle energy gaps are always about a few hundreds keV. This situation is characteristic of the extended pairing model. Overall, the results suggest that the model may be applicable to well-deformed nuclei. The model may also be useful in studying pairing phenomena in metallic clusters of nano-scale size.

TABLE I. Pairing interaction strength $|G|$ (keV) used in Fig. 3 for the $^{154-171}$Yb isotopes.

	^{154}Yb	^{156}Yb	^{158}Yb	^{160}Yb	^{162}Yb	^{164}Yb	^{166}Yb	^{168}Yb	^{170}Yb
k	1	2	3	4	5	6	7	8	9
G	245	41.1	6.5	3.02	1.11145	0.4675	0.2337	0.1376	0.094816
	^{155}Yb	^{157}Yb	^{159}Yb	^{161}Yb	^{163}Yb	^{165}Yb	^{167}Yb	^{169}Yb	^{171}Yb
k	1	2	3	4	5	6	7	8	9
G	270.7	42.0	10.9	1.0	1.471	0.649	0.3477	0.2185	0.16113

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