General pairing interactions and pair truncation approximations for fermions in a single-j shell

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We investigate Hamiltonians with attractive interactions between pairs of fermions coupled to angular momentum J. We show that pairs with spin J are reasonable building blocks for the low-lying states. For systems with only a $J=J_{max}$ pairing interaction, eigenvalues are found to be approximately integers for a large array of states, in particular, for those with total angular momenta $I \leqslant 2j$. For $I=0$ eigenstates of four fermions in a single-j shell we show that there is only one nonzero eigenvalue. We address these observations using the nucleon pair approximation of the shell model and relate our results with a number of currently interesting problems.

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I. INTRODUCTION

Since pairing has proven to be important in atomic, nuclear, and condensed matter physics, pair truncation approximations to many body wave functions have been extensively studied. The first example is the seniority scheme, introduced by Racah [1,2], for the classification of states in atomic spectra and later applied extensively in nuclear physics, where S pairs with angular momentum zero are related with a strong and attractive monopole pairing interaction. The second example is the interacting boson model (IBM) introduced by Arima and Iachello [3], where the low-lying excitations of complex even-even nuclei are described successfully by s bosons which correspond to correlated S nucleon pairs with angular momentum zero and d bosons which correspond to D nucleon pairs with angular momentum two. Again, the success of the IBM in nuclear physics partly comes from the validity of the pairing plus quadrupole-quadrupole force for effective interactions between valence nucleons. Monopole and quadrupole pairing are important as well in low- and high-temperature superconductiviy in materials [4,5].

In this paper we investigate the general pair truncation approximation for fermions in a single-j shell. The examples explored may provide a clue as how to classify the states which come from the diagonalization of an attractive pairing interaction for which two fermions are coupled to an angular momentum J,

$$H_J = -\sum_{M=-J}^{J} A_M^{J\dagger} A_M^J,$$

$$A_M^{J\dagger} = \frac{1}{\sqrt{2}}[a_j^\dagger \times a_j^\dagger]^J, \quad A_M^J = -(-1)^M \frac{1}{\sqrt{2}}[\tilde{a}_j \times \tilde{a}_j]^J_{-M}, \quad (1)$$

where $[]^J_M$ means coupled to angular momentum J and projection M. Most of the examples pursued in this paper have $n=4$, where n is the nucleon number.

We first point out in this paper that the low-lying eigenstates of Eq. (1) can be approximated by wave functions with pairs with angular momentum J only. We shall next show that a large array of eigenvalues of four nucleons in a single-j shell are asymptotic integers when $J \sim J_{max}=2j-1$ and the total angular momentum I is not very close to $I_{max}=4j-6$, and that this phenomenon originates from the validity of the pair truncation scheme and special features of coupling coefficients. We shall finally prove that the pair Hamiltonian (1) has exactly *one and only one* nonzero eigenvalue for four fermion eigenstates with total angular momentum zero, $I=0$. This sheds light on the problem of angular momentum zero ground state dominance in many-body systems interacting by random interactions [6].

II. COMPARISON OF THE PAIR APPROXIMATION TO THE SHELL MODEL

Figure 1 compares the exact ground state angular momentum I for four nucleons in a single-j shell interacting by the attractive pair Hamiltonian H_J with the angular momentum I of the ground state in the truncated space of pairs coupled to angular momentum J only. We have examined all the cases up to $J=20$ and $j \leqslant 31/2$ but here we show only two typical examples with $J=6$ and 14. In the case of $J=0$, the seniority scheme (S-pair approximation) produces the exact ground state. In case of $J=2$ and $n=4$, a D-pair approximation is found to be always very good. When $J>2$, the J-pair approximation of low-lying states is not perfect but always very reasonable. In Fig. 1, most of ground state angular momenta are correctly reproduced by the J-pair truncation. In Fig. 1(b), there are two exceptions in which the ground state is not correctly given by two $J=14$ pairs: $2j=19$ and 25.

Even in those cases where the ground state angular momenta are not correctly predicted by the J-pair truncation, the low-lying state energies are reasonably reproduced (including the binding energies). As a "bad" example in which the ground state angular momentum is not reproduced, we show

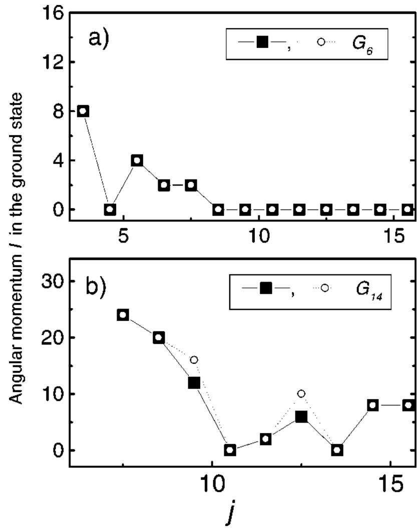

FIG. 1. Ground state angular momenta I for four fermions in a single-j shell for the pair Hamiltonian H_J for J=6 in (a) and 14 in (b) as a function of j. The solid squares are ground state angular momenta obtained by truncating the space of states to those with two pairs with angular momentum J only, and the open circles are ground state angular momenta calculated by diagonalizing the pair Hamiltonian in the full shell model space.

in Fig. 2 the case of four nucleons in a j=25/2 shell with J=14. The calculated levels using two J=14 pairs are shown in the first column. The next two columns are the shell model states obtained by diagonalizing the Hamiltonian in the full space. The states in the second column are the shell model states corresponding to the pair truncation states in the first column. All the levels below 0^+ are included. One sees that the lowest four states 2_1^+, 6_1^+, 12_1^+, and 10_1^+ are well approximated by two J=14 pairs, although the ground state angular momentum is not correctly given by this J=14 pair approximation. The 0_1^+ state is always precisely reproduced (as we shall see, there is only one nonzero eigenvalue for I=0 states and that eigenstate is constructed by J pairs). The states with odd I are always outside the pair truncation space but their energies are quite high in all cases that we have checked. In Fig. 2, the 9_1^+ is the lowest state with odd value of I. Below the 9_1^+ there are ten states with even values of I and most of them are reasonably described by the J=14 pair approximation. The angular momenta of those states for which excited energies are not well reproduced by two J pairs are labeled by italic font in Fig. 2.

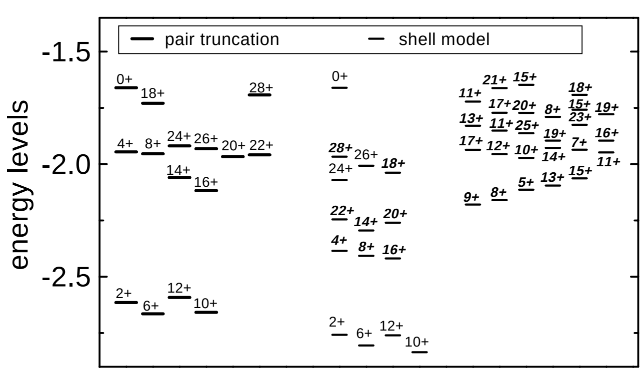

FIG. 2. A comparison of low-lying spectra calculated with wave functions with two pairs with angular momentum J=14 (the column on the left hand side) and by a diagonalization of the full space (the column in the middle and the column on the right hand side) for the case of four nucleons in a single-j (j=25/2) shell. The middle column plots the lowest shell model states with even spin and the right column plots the other shell model states. All the levels below 0_1^+ in the full shell model space are included. One sees that the low-lying states with I=2_1^+, 6_1^+, 12_1^+, and 10_1^+ are well reproduced. It is noted that the 0_1^+ coupled by two J=14 pairs is equivalent to that obtained by a full shell model diagonalization; refer to the text.

For J=J_{max}=2j−1, the I=I_{max}=4j−6 or I=I_{max}−2 states are always the lowest. These two states may be constructed by pairs with angular momentum either J_{max} or J_{max}−2. However, pairs with angular momentum J_{max}−2 do not present a good classification for other I states while those with angular momentum J_{max} do.

For n=3, the J-pair truncation describes the low-lying states precisely. We note without details that bosons with spin l exhibit a similar situation. It would be interesting to know the situation in more complicated systems.

III. INTEGER EIGENVALUES

We next report a very interesting regularity in the spectrum of Hamiltonian (1) with J=J_{max}=2j−1. The eigenvalues of most states with $I \leqslant 2j-3$ are found to be very close to integers corresponding to the number of pairs with angular momentum J_{max} except for a very few eigenvalues. Taking four nucleons in a j=31/2 shell as an example, the diagonalization of H_J (J=30) gives "integer" eigenvalues for low I states—all eigenvalues are 0, −1, and −2 to within a precision of 0.01 for all states with $I<22$. For states with $22 \leqslant I \leqslant 52$, these three "integer" eigenvalues continue to be valid except that seven eigenvalues which are not close to 0, −1, or −2 come in. These "noninteger" eigenvalues are very stable in magnitude for states with $22 \leqslant I \leqslant 52$. The states with $I \geqslant 53$ are one dimensional, so the corresponding eigenvalues (which saturate quickly with j) may be analytically derived [7]. These "integer" eigenvalues are best seen in case of J=J_{max} and becomes less dominant for smaller J and the same single-j.

To understand the validity of the pair approximation and the occurrence of these "integer" eigenvalues we consider the pair basis of four nucleons,

$$|j^4[J_1J_2]I, M\rangle = \frac{1}{\sqrt{N^{(I)}_{J_1J_2;J_1J_2}}}(A^{J_1\dagger}\times A^{J_2\dagger})^{(I)}_M|0\rangle, \qquad (2)$$

where $N^{(I)}_{J_1J_2;J_1J_2}$ is the diagonal matrix element of the normalization matrix

$$N^{(I)}_{J_1'J_2';J_1J_2} = \langle 0|(A^{J_1'}\times A^{J_2'})^{(I)}_M(A^{J_1\dagger}\times A^{J_2\dagger})^{(I)}_M|0\rangle$$
$$= \delta_{J_1,J_1'}\delta_{J_2,J_2'} + (-)^I\delta_{J_1,J_2'}\delta_{J_2,J_1'} - 4\hat{J}_1\hat{J}_2\hat{J}_1'\hat{J}_2'\begin{Bmatrix} j & j & J_1 \\ j & j & J_2 \\ J_1' & J_2' & I. \end{Bmatrix}. \qquad (3)$$

In general, this basis is overcomplete and the normalization matrix may have zero eigenvalues for a given I.

The matrix elements of H_J are [8]

$$\langle j^4[J_1'J_2']I,M|H_J|j^4[J_1J_2]I,M\rangle = -\frac{1}{\sqrt{N^{(I)}_{J_1J_2;J_1J_2}N^{(I)}_{J_1'J_2';J_1'J_2'}}}\sum_{J'=\text{even}} N^{(I)}_{J_1J_2;JJ'}N^{(I)}_{J_1'J_2';JJ'}, \quad (4)$$

where $\hat{J}_1$ is a shorthand notation of $\sqrt{2J_1+1}$. There are two terms in $N^{(I)}_{J_1J_2;JJ'}$: the second term is a nine-j coefficient which is usually much less than unity in magnitude, in particular, when J is large and I not large (refer to Appendix A). Neglecting this nine-j symbol, the allowed states are $|j^4[J_1J_2]I,M\rangle \approx (A^{J_1\dagger}\times A^{J_2\dagger})^{(I)}_M|0\rangle$ for $J_2 < J_1$, and $|j^4[J_1J_1]I,M\rangle \approx 1/\sqrt{2}(A^{J_1\dagger}\times A^{J_1\dagger})^{(I)}_M|0\rangle$, I even only, and the Hamiltonian matrix becomes

$$\langle j^4[J_1'J_2']I,M|H_J|j^4[J_1J_2]I,M\rangle \approx -\frac{[\delta_{J_1,J_1'}\delta_{J_2,J_2'}+(-1)^I\delta_{J_1,J_2'}\delta_{J_2,J_1'}]}{\sqrt{1+(-1)^I\delta_{J_1,J_2}}\sqrt{1+(-1)^I\delta_{J_1',J_2'}}}(\delta_{J_1,J}+\delta_{J_2,J}). \quad (5)$$

First of all we see that the matrix is diagonal, which validates the pair approximation. Second the eigenvalues are either 0, −1, or −2 with their corresponding wave functions having 0, 1, or 2 pairs with angular momentum J, respectively. Therefore, the integer eigenvalues of many I states originate from both the special properties of these nine-j symbols and the validity of J-pair truncation.

From the J-pair coupling scheme, the number of $|j^4[J_1J_2]I,M\rangle$ with $J_1=J_2=2j-1$ is $1+(-)^I/2$, and the number of $|j^4[J_1J_2]I,M\rangle$ with $J_1=2j-1$, $J_2<J_1$, and $I<2j-1$ is $[I/2]$ (the largest integer not exceeding $I/2$). According to the above discussion, the number of states with eigenvalues $\simeq -2$ is $1+(-)^I/2$ and the number of states with eigenvalues $\simeq -1$ is $[\frac{I}{2}]$. This is confirmed in *all* cases with $I<2j-8$. Eigenvalues not close to integers arise in states with $2j-8 \leqslant I \leqslant 4j-12$. These "noninteger" eigenvalues are found to be almost the same for the $2j-8\leqslant I\leqslant 4j-12$ states; an understanding of this regularity is in progress.

From a more general expression of Eq. (4), say, Eq. (5.8) of Ref. [9], we expect that the "integer" eigenvalues appear not only in even systems, but also in odd-A systems. According to our numerical results, the pattern of "integer" eigenvalues also appears in the states with small I for $j\geqslant 11/2$ and $n=3$, and for $j\geqslant 23/2$ and $n=5$, etc. For cases with $n=3$, a similar proof is readily obtained in terms of six-j symbols. An explicit proof for more nucleons will be quite complicated.

IV. EXACT RESULTS FOR ANGULAR MOMENTUM ZERO STATES

We now come to the last point of this paper by pointing out that there is only one nonzero eigenvalue for $I=0$ and $n=4$. We define a new basis for the $I=0$ states for the pair Hamiltonian H_J,

$$|j^4J_1\rangle = |j^4[J_1J_1]I=M=0\rangle - \frac{N^{(0)}_{J_1J_1;JJ}}{\sqrt{N^{(0)}_{JJ;JJ}N^{(0)}_{J_1J_1;J_1J_1}}}|j^4[JJ]I=M=0\rangle (J_1\neq J), \quad (6)$$

$$|j^4J\rangle = |j^4[JJ]I=M=0\rangle. \quad (7)$$

The unnormalized states $|j^4J_1\rangle$, $J_1\neq J$, are orthogonal with respect to *only* $|j^4[JJ]I=M=0\rangle$. From Eq. (4) one has

$$\langle j^4[J_1'J_1']0,0|H_J|j^4[J_1J_1]0,0\rangle = -\frac{N^{(0)}_{J_1J_1;JJ}N^{(0)}_{J_1J_1;JJ}}{\sqrt{N^{(0)}_{J_1'J_1';JJ}N^{(0)}_{J_1J_1;JJ}}}, \quad (8)$$

where $J_1', J_1=0,2,\ldots,2j-1$. Using this formula, one easily confirms that all matrix elements of the Hamiltonian in basis (6), $\langle j^4J_1'|H_J|j^4J_1\rangle$, $J_1'\neq J$, are zero. Therefore all the eigenvalues for $n=4$ and $I=0$ are zero except for the single state with both pairs having angular momentum J and its eigenvalue is $E_0^{J(j)}=-N^{(0)}_{JJ;JJ}$.

Since H_J is a negative definite operator, its eigenvalues will be negative or zero. From above we see that, for $I=0$, there is only one state with a nonzero eigenvalue, $E_0^{J(j)}$. Therefore one expects this eigenvalue to be the lowest in the spectrum because the eigenvalues of $I\neq 0$ states are more or less scattered in many states, generally speaking. Thus the probability that the $I=0^+$ is the lowest state of four fermions in a single-j shell in the presence of random two-body interactions is expected to be larger than the probability for all other angular momentum I, according to the empirical rule of Ref. [7]. For $j\leqslant 31/2$ there are only two exceptions, $j=7/2$ and 13/2.

The sum rule of diagonal matrix elements [10] gives $\sum_J E_0^{J(j)} = -\frac{1}{2}n(n-1)D_0^{(j)} = -6D_0(j)$, where $D_0^{(j)}$ is the number of $I=0$ states and here $n=4$. For $n=4$ the number of states is $D_0^{(j)}=[(2j+3)/6]$ [11], which gives 1, 1, 1, 2, 2, 2, 3, 3, 3, … for $2j=3,5,7,9,11,13,15,\ldots$, etc., regularly. Thus the staggering in the number of states is expected to be reflected in the staggering of the energy which was pointed out in Refs. [7,12] but without an explanation.

V. SUMMARY

In this paper we have shown that an attractive Jth pairing interaction favors pairs with angular momentum J in low-lying states of fermions in a single-j shell. Therefore, one may use pairs with angular momentum J as building blocks of wave functions of low-lying states. This is in contrast to repulsive pair interactions, used, for example, in the fractional quantum Hall effect [13–15], for which the pair truncation approximation is not valid.

In addition, we discovered that the eigenvalues of states with low angular momentum I for pair Hamiltonians with J larger than j are approximately integers. We explain the origin of this fact for four nucleons in a single-j shell from the validity of pair truncation and special properties of nine-j symbols. We point out without details that the same holds for $n=3$ and $j\geqslant 11/2$ and for $n=5$ ($j\leqslant 23/2$).

Finally, we pointed out that there is only one nonzero eigenvalue for $I=0$ and $n=4$. This result is useful in studying the large probability of angular momentum zero states to be the lowest in energy for $n=4$.

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APPENDIX A: SOME NINE-*j* SYMBOL FORMULAS

These formulas are obtained in the following two steps. First, rewrite the nine-j in terms of six-j symbols, i.e.,

$$\begin{Bmatrix} j & j & r_1 \\ j & j & r_2 \\ s_1 & s_2 & I \end{Bmatrix} = \sum_t (-)^{2t}(2t+1)\begin{Bmatrix} j & j & r_1 \\ r_1 & I & t \end{Bmatrix}\begin{Bmatrix} j & j & r_2 \\ j & t & s_2 \end{Bmatrix} \times \begin{Bmatrix} s_1 & s_2 & I \\ t & j & j \end{Bmatrix},$$

and second, make use of the analytical formulas of six-j. Through these examples (though we are unable to get a universal formulas), one sees that the nine-j symbols in Eq. (3) are much less than unity and may be neglected in Eq. (4) when I is not very large:

$$\begin{Bmatrix} j & j & 2j-1 \\ j & j & 2j-1 \\ 2j-1 & 2j-1 & 0 \end{Bmatrix} = -\frac{j(4j-3)[(2j-1)!]^2}{(4j-1)(4j-1)!},$$

$$\begin{Bmatrix} j & j & 2j-1 \\ j & j & 2j-1 \\ 2j-1 & 2j-1 & 2 \end{Bmatrix} = \frac{j(8j^2-6j-3)[(2j-1)!]^2}{(4j-1)(4j-3)(4j-1)!},$$

$$\begin{Bmatrix} j & j & 2j-1 \\ j & j & 2j-1 \\ 2j-1 & 2j-1 & 4 \end{Bmatrix} = -\frac{3j(2j+1)(4j^2-3j-5)[(2j-1)!]^2}{(4j-1)(4j-3)(4j-5)(4j-1)!},$$

$$\begin{Bmatrix} j & j & 2j-1 \\ j & j & 2j-1 \\ 2j-1 & 2j-1 & 6 \end{Bmatrix} = \frac{5j(j+1)(2j+1)(8j^2-6j-21)[(2j-1)!]^2}{(4j-1)(4j-3)(4j-5)(4j-7)(4j-1)!},$$

$$\begin{Bmatrix} j & j & 2j-1 \\ j & j & 2j-3 \\ 2j-1 & 2j-3 & 2 \end{Bmatrix} = -\frac{j\{36+j(4j-9)[19+2j(-9+4j)]\}[(2j-1)!]^2}{3(4j-3)(4j-5)(4j-1)!},$$

$$\begin{Bmatrix} j & j & 2j-1 \\ j & j & 2j-3 \\ 2j-1 & 2j-3 & 3 \end{Bmatrix} = \frac{j(4j-3)[1+2j(4j-9)][(2j-1)!]^2}{6(4j-5)(4j-1)!}.$$

From the above formulas one sees that these nine-j symbols are proportional to $[(2j-1)!]^2/(4j-1)!$, and are very close to zero when j becomes considerably large. For example, the absolute values of these nine-j symbols are less than $\sim 10^{-15}$ when $j=31/2$.

APPENDIX B: A NEW SUM RULE FOR A SIX-*j* SYMBOL

From Eq. (3) one obtains

$$N^{(0)}_{JJ;JJ} = 2 + 4(2J+1)\begin{Bmatrix} j & j & J \\ j & j & J \end{Bmatrix}.$$

Since $-N^{(0)}_{JJ;JJ}$ is also the unique eigenvalue of the $I=0$ eigenstate of H_J, one has a sum rule that

$$\sum_{\text{even } J} N^{(0)}_{JJ;JJ} = \frac{1}{2}n(n-1)D_0^{(j)},$$

where $n=4$, $D_0^{(j)}=(2j+3)/6$ [11]. One finally obtains that

$$\sum_{\text{even } J} (2J+1)\begin{Bmatrix} j & j & J \\ j & j & J \end{Bmatrix} = \begin{cases} \frac{1}{2} & \text{if } 2j=3k \\ 0 & \text{if } 2j+2=3k \\ -\frac{1}{2} & \text{if } 2j-2=3k. \end{cases} \tag{B1}$$

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