Optimum Pair Basis in the Nuclear Shell Model

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An unusual optimum pair basis exists in the nuclear shell-model wave function for an even system of like particles. This prompts the proposal of a generalized pair mean-field method, in which the desired goal of avoiding the dimensional difficulty in the traditional shell-model approaches may be possible.

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A central effort in nuclear structure physics in the past two decades was the utilization of collective pairs as building blocks to construct many-body wave functions. To this end, low-spin pairs were always used. Basically there were two approaches in this regard. One was to construct a model space from the collective S and D pairs and at the same time introduce effective interactions. Archetypical examples of this approach are the successful interacting boson model [1] and the fermion dynamical symmetry model [2]. The other approach began with interactions which supposedly were appropriate for the full major shell and then tried to "improve" the wave functions by adding pairs other than S and D (G, say) [3,4]. A salient feature of such a low-spin pair basis, albeit S and D, or S, D, and G, is that the many-body wave functions usually manifest strong pair configuration mixing, especially in the deformed system. Therefore, it is natural to inquire whether the utilization of a traditional low-spin pair basis constitutes a unique choice in studying such physics. Could a basis *without significant configuration mixing* (i.e., *pairs* moving in a *pair mean field*) exist in which the many-body wave functions appear as direct products of these pairs? This paper intends to reveal this possibility, and the resultant pairs are called *optimum pairs*.

We shall first illustrate this idea via a simple solvable model: like particles moving in a single-j shell. This example is chosen because it is solvable and contains generic features for fermion pairs [5]. We begin by performing a pair-component analysis of the shell-model wave functions in order to demonstrate the existence of the optimum pairs. This is followed by the introduction of a generalized pair mean-field method (GPFM), from which we will show how a pair mean field can be generated from a given Hamiltonian, and how the optimum pairs can be chosen. Finally, a comparison between the GPFM results and the exact shell-model solutions are given. The general case of protons and neutrons in multi-j shells will be published elsewhere.

The most general Hamiltonian for like particles in a single-j shell is

$$H=\varepsilon_j\sqrt{2j+1}(a_j^\dagger\times\tilde{a}_j)^0+\frac{1}{2}\sum_j\sqrt{2J+1}C_J(A_J^\dagger\times\tilde{A}_J)^0, \tag{1}$$

where $A_J^\dagger=(a_j^\dagger\times a_j^\dagger)^J$, $C_J=\langle jjJ|V|jjJ\rangle$, and $a_j^\dagger$ ($\tilde{a}_j$) the creation (annihilation) operator with angular momentum j and energy ε_j. Throughout this Letter, ε_j is set equal to zero. In this paper, we shall consider a four-particle system. To facilitate the pair-component analyses, we have chosen a *nonorthogonal, unnormalized, and overcomplete* two-pair basis for the shell-model calculations. They are $|J_1J_2J\rangle=(A_{J_1}^\dagger\times A_{J_2}^\dagger)^J|0\rangle$. In this basis, the components are correlated through the following relation:

$$|J_1J_2J\rangle=-\sum_{J_1'J_2'}\hat{J}_1\hat{J}_2\hat{J}_1'\hat{J}_2'X(jjJ_1;jjJ_2;J_1'J_2'J)|J_1'J_2'J\rangle, \tag{2}$$

where the symbol $\hat{J}_i$ stands for $(2J_i+1)^{1/2}$, and X the 9-j symbol. Equation (2) reveals a profound difference between a fermion pair and a boson. It shows that for a fermionic many-body wave function, a complicated mixing of different pair configurations can result in a pure pair configuration, and vice versa. This opens the possibility of a optimum pair description for a many-body system which we will now discuss.

The four-particle basis of Eq. (2) is used to construct the H matrix. It is well known that an overcomplete basis will result in nonunique independent sets. For instance, in the $j=\frac{21}{2}$ and $J=2$ case, although there are thirty different pair configurations, only six can be independent. One may choose $|0,2;2\rangle$, $|2,2;2\rangle$, $|2,4;2\rangle$, $|4,4;2\rangle$, $|4,6;2\rangle$, and $|6,6;2\rangle$ (referred to as low-spin pair basis), or $|20,20;2\rangle$, $|18,20;2\rangle$, $|18,18;2\rangle$, $|16,18;2\rangle$, $|16,16;2\rangle$, and $|14,16;2\rangle$ (the highest-spin pair basis), or any other combinations. Of course different bases must all lead to the same physics. Hence, using low-spin pairs as the building blocks does not necessarily imply the loss of high-spin correlations, and vice versa.

In Table I, the shell-model results are presented. The $Q\cdot Q$ interaction is chosen to simulate a strongly deformed system. One sees that the eigenvalues for both sets are equal, as expected, but with significantly different pair structures. A striking feature is that while there is strong mixing for the low-spin basis, there is very little mixing for the highest-spin basis. Indeed, this feature persists for all J states up to spin 10 in the g, β, and γ bands. For higher bands, the remnant of this feature still survives. Physically, this means that one can sum up the pair components of the low-spin basis to form a nearly

TABLE I. Pair component analysis of $J=2$ shell-model wave functions ($j=\frac{21}{2}$, $H=-Q\cdot Q$, energies are in arbitrary units).

	Highest-spin pair basis					
E	14-16	16-16	16-18	18-18	18-20	20-20
−1.45	0.00	0.00	0.00	0.04	0.01	1.41
−0.86	−0.01	0.00	−0.13	−0.01	−1.99	0.01
−0.35	0.06	0.20	0.08	1.38	−0.02	−0.04
−0.08	0.63	0.16	1.79	−0.13	−0.13	0.00
0.24	0.84	0.98	−0.77	−0.17	0.03	0.00
0.47	−1.49	1.10	0.41	−0.06	−0.01	0.00
	Low-spin pair basis					
E	0-2	2-2	2-4	4-4	4-6	6-6
−1.45	0.23	0.33	0.37	−0.04	0.39	−0.07
−0.86	0.95	0.08	0.97	−0.05	0.72	−0.53
−0.35	0.62	0.30	0.93	0.21	−0.55	1.02
−0.08	−0.86	−0.08	0.93	0.89	1.41	0.70
0.24	−0.42	−0.48	−1.51	0.29	0.93	−0.05
0.47	−0.23	0.36	1.57	−0.83	0.12	0.23

single highest-spin pair component [see Eq. (2)]. Hence this analysis suggests that for this example, the g-band can in fact be labeled purely as (20-20) (predominantly coming from the state $|20,20;J\rangle$). Similarly, (18-18) for β band and (18-20) for γ band, etc. The entire spectrum for an exact shell-model calculation is shown in part a of Fig. 1. One sees clearly for the $Q\cdot Q$ interaction the existence of highest-spin optimum pairs.

This example prompted us to ask whether the optimum pair concept can persist more generally and if so, what is the underlying dynamics? To answer these questions, a generalized pair mean-field method is introduced which we will now discuss. We begin by considering an auxiliary Hamiltonian with a multiplier ω,

$$H'=H-\omega\sum_{i\neq j}I_{ij}\,, \tag{3}$$

where $\sum_{i\neq j}I_{ij}$ stands for the identity interaction and is chosen for its simplicity. Obviously, H' and H must have the same wave functions, while the energies can differ by a constant. We will again consider the four-particle system as an example to illustrate the basic idea. By applying H' to the basis $|J_1J_2J\rangle$, we get

$$H'|J_1J_2J\rangle=(C_{J_1}+C_{J_2}-2\omega+k_{12})|J_1J_2J\rangle+\Delta\,, \tag{4}$$

where

$$k_{12}=-\frac{4}{1+\delta_{J_1J_2}}(C_{J_1}+C_{J_2}-2\omega)(2J_1+1)(2J_2+1)\times X(jjJ_1;jjJ_2;J_1J_2J) \tag{5}$$

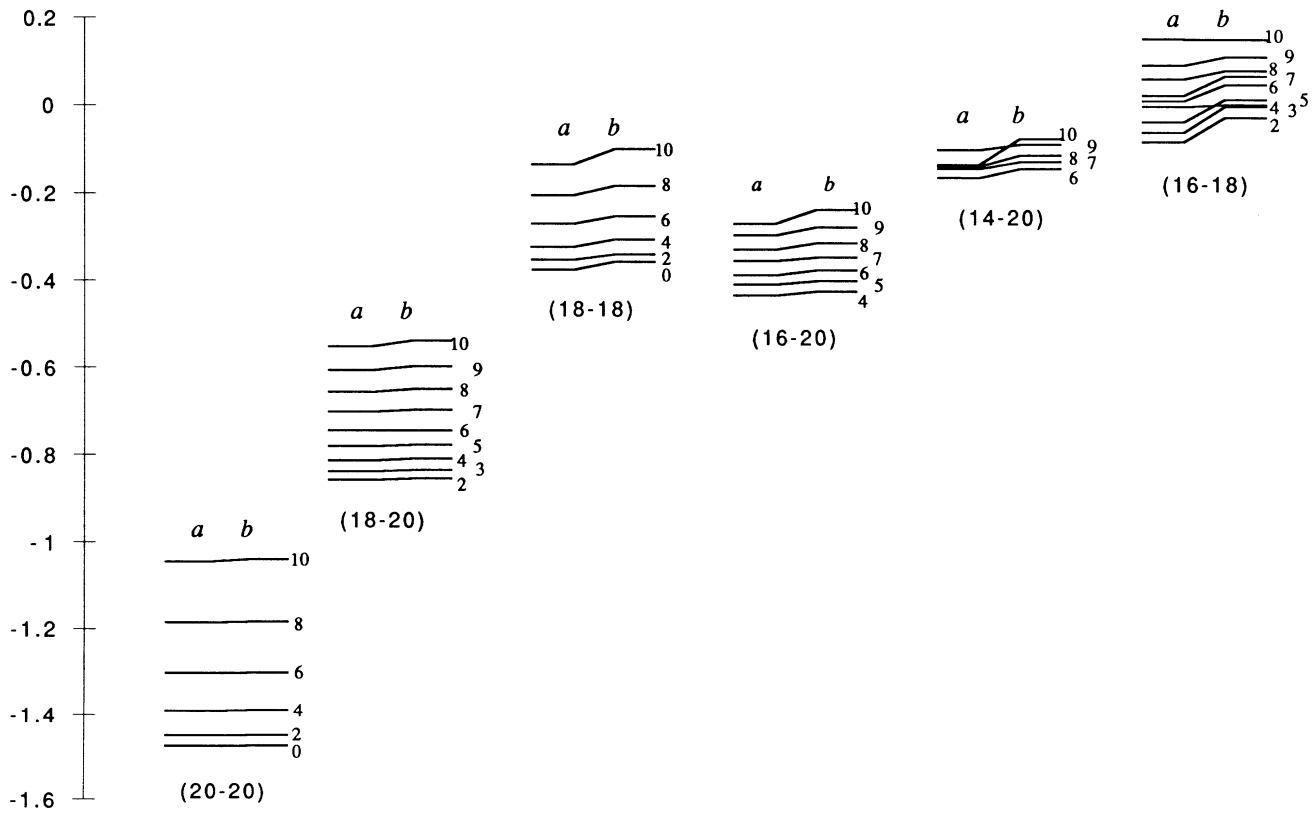

FIG. 1. The spectrum of four particles in a single-j shell ($j=\frac{21}{2}$, $H=-Q\cdot Q$, energies are in arbitrary units). Part a, the shell-model calculation; b, the GPFM calculation.

and

$$\Delta=-\sum_{J_1'J_2'}{}'2(C_{J_1'}+C_{J_2'}-2\omega)\hat{J}_1\hat{J}_2\hat{J}_1'\hat{J}_2' \times X(jjJ_1;jjJ_2;J_1'J_2'J)|J_1'J_2'J\rangle . \quad (6)$$

The prime on the sum in Eq. (6) means the exclusion of the values $J_1'J_2'=J_1J_2$ and J_2J_1. The value of ω is chosen so as to minimize χ^2, the square sum of the state amplitude of Eq. (6),

$$\chi^2=\sum_{J_1'J_2'}{}'[(C_{J_1'}+C_{J_2'}-2\omega)\hat{J}_1\hat{J}_2\hat{J}_1'\hat{J}_2'X(jjJ_1;jjJ_2;J_1'J_2'J)]^2, \quad (7)$$

which means that the contribution of Δ is minimized. This is achieved when

$$\omega=\tfrac{1}{2}\langle C_{J_1'}+C_{J_2'}\rangle , \quad (8)$$

where $\langle\cdots\rangle$ stands for the average with the weights $(2J_1'+1)(2J_2'+1)X^2(jjJ_1;jjJ_2;J_1'J_2'J)$ and excluding $J_1'J_2'=J_1J_2$ and J_2J_1 in the sum over J_1' and J_2'. When Δ is negligible,

$$H'|J_1J_2J\rangle\simeq(C_{J_1}+C_{J_2}-2\omega+k_{12})|J_1J_2J\rangle . \quad (9)$$

Equation (9) is an optimum pair approximation where the eigenfunction is a direct product of two individual pairs $|J_1J_2J\rangle$ without mixing, and the eigenvalue is

$$E(J_1J_2J)=E'(J_1J_2J)+6\omega ,$$
$$E'(J_1J_2J)=(C_{J_1}+C_{J_2}-2\omega+k_{12}) . \quad (10)$$

For the $Q\cdot Q$ interaction, $C_J=2(j\|Y_2\|j)^2W(j,j,j,j;2,J)$. By choosing the highest-spin pair basis and inserting C_J, ω [Eq. (8)], and k_{12} [Eq. (5)] into Eq. (10), the exact results are satisfactorily reproduced (see part b in Fig. 1).

The above formulation can be applied to any interaction. The key point is to find the optimum pairs for which Δ is negligible. For the $Q\cdot Q$ interaction, the optimum pairs come from the high-spin pairs; for other interactions, the optimums pairs may differ. In general, they should be determined by minimizing χ^2 which is a measurement of the validity of the optimum pair approximation (i.e., neglecting Δ). For example, if the interaction is monopole pairing, then the optimum pair is found to be the S pair plus other independent pairs which can be chosen arbitrarily. In this case, it is easy to see that choosing $\omega=0$ will lead to $\Delta=0$, and the exact results can be obtained: $E=G_0(N-k)(\Omega-N+1-k)$, where $\Omega=(2j+1)/2$, G_0 the pairing strength, and k the pair number of non-S pairs.

In fact, the GPFM can be formulated generally in terms of a set of coupled dispersion equations via the Richardson method [6]. Following Ref. [6], the pair creation operator is defined as follows:

$$B_{J_i}^\dagger=\frac{C_i^{1/2}}{2e_j-E_i}(a_j^\dagger\times a_j^\dagger)^{J_i} , \quad (11)$$

where the pair amplitude is dependent on E_i and is determined by imposing an optimum pair condition, namely, requiring the eigenfunctions to be a product of individual pairs. For the four-particle system, it is $|\Psi\rangle=(B_{J_1}^\dagger\times B_{J_2}^\dagger)^J|0\rangle$ and

$$H'|\Psi\rangle=(E_1+E_2)|\Psi\rangle+C_{J_2}^{1/2}\left(1+\frac{C_{J_2}-\omega}{2\varepsilon_j-E_2}+\frac{k_{12}}{E_1-E_2}\right)(A_{J_2}^\dagger\times B_{J_1}^\dagger)^J|0\rangle$$
$$+C_{J_1}^{1/2}\left(1+\frac{C_{J_1}-\omega}{2\varepsilon_j-E_1}+\frac{k_{12}}{E_2-E_1}\right)(A_{J_1}^\dagger\times B_{J_2}^\dagger)^J|0\rangle+\Delta , \quad (12)$$

where Δ is similar to Eq. (6),

$$\Delta=-\sum_{J_1'J_2'}{}'2(C_{J_1'}+C_{J_2'}-2\omega)\hat{J}_1\hat{J}_2\hat{J}_1'\hat{J}_2'X(jjJ_1;jjJ_2;J_1'J_2'J)\frac{k_{12}}{E_2-E_1}\{C_{J_1'}^{1/2}(A_{J_1'}^\dagger\times B_{J_2'}^\dagger)^J-C_{J_2'}^{1/2}(B_{J_1'}^\dagger\times A_{J_2'}^\dagger)^J\}|0\rangle \quad (13)$$

and can be neglected if Eq. (8) is used to determine ω and the basis is constructed by the optimum pairs which will minimize the χ^2. By demanding that E_1 and E_2 should satisfy the following coupled dispersion equations,

$$1+\frac{C_{J_1}-\omega}{2\varepsilon_j-E_1}+\frac{k_{12}}{E_2-E_1}=0 ,$$
$$1+\frac{C_{J_2}-\omega}{2\varepsilon_j-E_2}+\frac{k_{12}}{E_1-E_2}=0 , \quad (14)$$

Eq. (12) becomes

$$H'|\Psi\rangle=(E_1+E_2)|\Psi\rangle . \quad (15)$$

Thus, we obtained a pair mean-field solution for H': The eigenfunction is the direct product of individual optimum pairs $(B_{J_1}^\dagger\times B_{J_2}^\dagger)^J|0\rangle$; and the eigenenergy is the sum of individual pair energies, which are individually ascertained from the coupled dispersion equations [Eq. (14)]. For the four-particle example, Eq. (14) can easily be solved:

$$E'(J_1J_2J)=E_1+E_2$$
$$=4\varepsilon_j+(C_{J_1}+C_{J_2}-2\omega+k_{12}) . \quad (16)$$

This is exactly the result given by Eq. (10) with $\varepsilon_j=0$.

In this paper we have only shown the existence of optimum pairs for the simplest systems. For multi-j case, the GPFM in the form of coupled dispersion equations can be easily extended. The traditional shell-model eigenvalue problem is now replaced by solving N coupled dispersion equations (where N is the pair number), which appears to be numerically tractable even for heavy systems. The detail discussions about the extension to the multi-j case is beyond the scope of this paper and will be reported elsewhere. However, there are still many important questions requiring further studies. For instance, when both pairing and $Q\cdot Q$ interactions are present, in particular, when there is an n-p $Q\cdot Q$ interaction, the existence of an optimum pair basis remains to be explored. Such work is now in progress. Nevertheless, what particularly intrigues us is that although the chosen simple system was well investigated in the past, it was not expected that such an interesting and nonintuitive physics, that a strongly deformed system can be represented by a pure pair configuration, could emerge from it.

Emphasis must be made that although the present optimum pair picture is akin to an independent pair picture in many aspects, they are not the same. Unlike the concept of a static common potential well, the pair mean field here is sensitively *particle number and state dependent*. For instance, the pair energy E_1 for spin J_1 in the state $|J_1J_2J\rangle$ is not the same as a "free" pair, nor is it the same if J_2 or J changes. The reason is because there are exchange effects in ω and k_{12}, which are state and number dependent. Only by neglecting ω and k_{12} will a common potential emerge which is equivalent to the boson energies in the Tamm-Dancoff approximation. In addition, the choice of optimum pairs (for an n-p system, one may have to include n-p pairs) and their structure will also vary from state to state. Thus, the determination of pair mean field in the GPFM is highly nontrivial. For each state the energies and structures of the optimum pairs must be self-consistently determined from the coupled dispersion equations. Furthermore, one should note that there is actually a free choice of the auxiliary Hamiltonian and Eq. (3) is merely the simplest one. In fact any scalar, if it is known to be (or approximately) diagonal in the optimum pair basis and has parameters to minimize χ^2 making Δ negligible, will be a good choice to replace $\omega\sum I_{ij}$. With a multitude of rich structures, it is certainly not inconceivable that the GPFM could very well describe a realistic nuclear many-body system and reveal new physics which have so far escaped notice. Work along this direction is now in progress.

In summary, a novel optimum pair basis is proposed to construct the many-body shell-model wave functions. This is followed by the introduction of a generalized pair mean-field method to solve the many-body problem. We have shown that for the single-j case, the GPFM is an excellent approximation to the exact solutions for both the vibrational and rotational limits. This method avoids the formidable, and probably impossible, task of a matrix diagonalization, thus avoiding the dimensional difficulty in the traditional shell-model approaches for heavy nuclei and restricts one to compute only states of interest.

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