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A NEW SENIORITY SCHEME FOR NON-DEGENERATE SINGLE PARTICLE ORBITS

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A new method is proposed in the treatment of the seniority scheme. The method enables us to evaluate analytically the contribution from $J=0$ Cooper pairs in non-degenerate single-particle orbits to many-body matrix elements. It includes the SU(2) quasi-spin and the BCS approximation as two extreme limits. The effect of particle number conservation is properly taken into account.

Various methods have been reported in the treatment of the seniority scheme to include many j-orbits [1–4]. In this letter we propose a new method which has the advantage of both the SU(2) quasi-spin and the BCS. First we briefly review these approaches in order to introduce the concepts and notations used in this letter. Generalized seniority (or Cooper pair) operators are usually written as

$$S_+ = \sum \alpha_j S_{j+} , \quad S_- = (S_+)^\dagger , \tag{1,2}$$

where α_j is an amplitude for an orbit with spin j and

$$S_{j+} = \sum_{m>0} (-)^m a^\dagger_{j,m} a^\dagger_{j,-m} . \tag{3}$$

Let us first consider the simplest generalization by assuming that all orbits are degenerate [1]. In this case $|\alpha_j|$ is equal to unity and the SU(2) quasi-spin can be defined as the same as for a single j-orbit. The following commutation relation also holds exactly:

$$[S_+, S_-] = \hat{N} - \Omega , \tag{4}$$

where $\hat{N}$ is the number operator, $\Omega = \Sigma\Omega_j$ and $\Omega_j = j + 1/2$. It follows that essentially the same reduction formulas can be obtained in this case as those for a single j-orbit [2]. Here with reduction formula we mean the expressions in which matrix elements of an operator between two n-particle states with seniority v and v' are written in terms of matrix elements of states with max (v, v') particles.

As is well known, degeneracy is badly broken in actual nuclei. This situation can be remedied by treating the α_j's as free parameters different from unity and then by constructing an n-body state [3,4]:

$$|j^n, v = 0, 0^+\rangle = \mathcal{N}^{-1}_{n,v=0} (S_+)^{n/2} |0\rangle , \tag{5}$$

where $\mathcal{N}_{n,v}$ is a normalization constant and $|0\rangle$ is a vacuum (i.e. closed shell). Here we have introduced the concept

of seniority v. The operator S_+ creates the $v=0$ pair; thus the state in eq. (5) has $v=0$. Note that the exact reduction formula cannot be obtained since the $|\alpha_j|$'s are no longer equal to unity. In the following we report analytic reduction formulas which are approximate, but simple and useful in the description of nuclei.

A commutation relation between the operators (1) and (2) is generally written as

$$[S_+, S_-] = \sum \alpha_j^2 \hat{N}_j - \sum \alpha_j^2 \Omega_j , \tag{6}$$

where $\hat{N}_j$ is the number operator for a particular j-orbit. If $\Sigma \alpha_j^2 \hat{N}_j$ in eq. (6) is approximated by $\hat{N}$, eq. (6) is essentially the same as eq. (4) and the normalization constant $\mathcal{N}_{n,v}$ of an n-body state with seniority v can be written as

$$\mathcal{N}_{n,v} = \sqrt{\tfrac{1}{2}(n-v)\,\Gamma(\Omega_e - v + 1)/\Gamma(\Omega_e - \tfrac{1}{2}(n+v) + 1)} , \tag{7}$$

where $\Omega_e = \Sigma \alpha_j^2 \Omega_j$. The seniority v should be zero for the state in eq. (5) and the states with non-vanishing seniority will be discussed later. We emphasize that the only approximate made here is the equality

$$\hat{N} = \sum \alpha_j^2 \hat{N}_j , \tag{8}$$

in a relevant subspace. The approximation will be called hereafter the number operator approximation.

In order that this approximation is good, we have to choose a proper overall normalization of the α_j's. For this purpose we impose the condition

$$\langle \tilde{j}^k, v=0 | \sum \alpha_j^2 N_j | \tilde{j}^k, v=0 \rangle = k , \tag{9}$$

for the following reason. In the evaluation of n-body matrix elements we use the approximations

$$\sum \alpha_j^2 \hat{N}_j (S_+)^m |0\rangle = 2m (S_+)^m |0\rangle \quad \text{for} \quad m = \tfrac{1}{2}n - 1, \ldots, 1 .$$

The best value of k in eq. (9), therefore, should be some average of these m-values. Since Ω_e was found to be insensitive to k, we take $k = 4$ for simplicity in this paper.

A state of the highest seniority, $|\tilde{j}^n, v=n, \gamma\rangle$, where γ stands for all other quantum numbers is constructed so as to satisfy a condition

$$S_- |\tilde{j}^n, v=n, \gamma\rangle = 0 . \tag{10}$$

This equation guarantees that the state does not contain an S-pair (or spurious component). The highest seniority state thus constructed is orthogonal to a subspace spanned by lower seniority states:

$$|\tilde{j}^n, v', \gamma'\rangle = \mathcal{N}_{n,v'}^{-1} (S_+)^{(n-v')/2} |\tilde{j}^{v'}, v', \gamma'\rangle , \tag{11}$$

where $n > v'$ and $\mathcal{N}_{n,v'}$ is given by eq. (7) in the number operator approximation. The states defined by eq. (11) are orthogonal to each other in this approximation.

In order to illustrate the procedure for obtaining the approximated reduction formulas, let us consider an example. We take a seniority conserving matrix element of a one-body operator $[a_i^\dagger \tilde{a}_k]^{(L)}$:

$$\begin{aligned} \langle \tilde{j}^n, v, \gamma | [a_i^\dagger \tilde{a}_k]^{(L)} | \tilde{j}^n, v, \gamma' \rangle &= \mathcal{N}_{n,v}^{-2} \langle \tilde{j}^v, v, \gamma | (S_-)^{(n-v)/2} [a_i^\dagger \tilde{a}_k]^{(L)} (S_+)^{(n-v)/2} | \tilde{j}^v, v, \gamma' \rangle \\ &= \langle \tilde{j}^v, v, \gamma | [a_i^\dagger \tilde{a}_k]^{(L)} | \tilde{j}^v, v, \gamma' \rangle + \frac{n-v}{2(\Omega_e - v)} \alpha_i \langle \tilde{j}^v, v, \gamma | [\tilde{a}_i \tilde{a}_k]^{(L)} S_+ | \tilde{j}^v, v, \gamma' \rangle . \end{aligned} \tag{12}$$

In the last step we exchanged all S_-'s and the one-body operator. Eqs. (7), (8) and (10) are then used to eliminate the S_+'s and S_-'s in the first term and all but one S_+ in the second. One S_+ survives in the second term due to a

contraction of S_- with the one-body operator. Alternatively we can exchange the S_+'s in eq. (12) to the left in a similar way. These two procedures produce the same result for a diagonal matrix element of a hermitian operator. The accuracy of the number operator approximation (8) depends on the quantum number γ of the nuclear states so that in general different results are obtained in the two procedures. The difference is, however, small when the approximation is a good one. Expecting that this is the case, we average the two quantities obtained by the two procedures. The result is the following expression for the matrix element (12):

$$\langle \tilde{j}^{\upsilon}, \upsilon, \gamma | \left\{ \left(1 - \frac{n-\upsilon}{\Omega_e - \upsilon} \tfrac{1}{4}(\alpha_i^2 + \alpha_k^2) \right) [a_i^+ \tilde{a}_k]^{(L)} - \frac{n-\upsilon}{2(\Omega_e - \upsilon)} \alpha_i \alpha_k s_{i,k}^{(L)} [a_k^+ \tilde{a}_i]^{(L)} \right.$$

$$\left. - \frac{n-\upsilon}{2(\Omega_e - \upsilon)} \alpha_i^2 \delta_{i,k} \delta_{L,0} \sqrt{2\Omega_i} \right\} | \tilde{j}^{\upsilon}, \upsilon, \gamma' \rangle , \tag{13}$$

where $s_{i,k}^{(L)} = (-)^{j_i - j_k + L}$. It should be noticed that only eqs. (8) and (10) play an essential role in deriving eq. (13).

We next discuss a seniority non-diagonal matrix element

$$\langle \tilde{j}^n, \upsilon, \gamma | [a_i^+ \tilde{a}_k]^{(L)} | \tilde{j}^n, \upsilon - 2, \gamma' \rangle = \mathcal{N}_{n,\upsilon}^{-1} \mathcal{N}_{n,\upsilon-2}^{-1} \langle \tilde{j}^{\upsilon}, \upsilon, \gamma | (S_-)^{(n-\upsilon)/2} [a_i^\dagger \tilde{a}_k]^{(L)} (S_+)^{(n-\upsilon)/2+1} | \tilde{j}^{\upsilon-2}, \upsilon - 2, \gamma' \rangle . \tag{14}$$

Similarly to eq. (12), we exchange all S_-'s and the one-body operator. Using eqs. (7), (8) and (10), we obtain the following reduction formula of eq. (14):

$$\left[\frac{(n-\upsilon+2)(\Omega_e - \upsilon + 1)}{2\Omega_e - n - \upsilon + 2} \right]^{1/2} \langle \tilde{j}^{\upsilon}, \upsilon, \gamma | \left\{ [a_i^+ a_k]^{(L)} \right.$$

$$\left. - \frac{n-\upsilon}{4(\Omega_e - \upsilon + 1)} \alpha_i (\alpha_i [a_i^+ \tilde{a}_k]^{(L)} + \alpha_k [\tilde{a}_i a_k^+]^{(L)}) \right\} | \tilde{j}^{\upsilon}, \upsilon - 2, \gamma' \rangle . \tag{15}$$

The factor $\sqrt{n - \upsilon + 2}$ is independent of the α_j's and can be considered to express essentially the presence of $J = 0$ pairs created by the S_+ operator [‡1]. When the α_j's are replaced by unity in eq. (15) (i.e. going from non-degenerate j-orbits to degenerate ones), the factor $\sqrt{n - \upsilon + 2}$ is unchanged, and other factors which are functions of n, υ, Ω_e, and α_j become functions of n, υ, and Ω. The expression thus obtained from eq. (15) is the *exact* reduction formula given by the SU(2) quasi-spin. The same conclusion can be obtained for eq. (13) in the same way.

Our procedure discussed so far is general; it can be applied to other operators which yield their approximated reduction formulas [6]. The formulas can be then shown to become identical to the *exact* ones given by the SU(2) quasi-spin when the α_j's are replaced by unity. Note that the hole operators can be treated exactly in the same way.

Next we consider the expectation value of a hamiltonian in a state with n identical nucleons and $\upsilon = 0$. Following the procedure described above, we obtain:

$$\langle H \rangle_{\upsilon=0} = \frac{n}{\Omega_e} \sum \Omega_j \epsilon_j \alpha_j^2 + \frac{n}{\Omega_e} \sum_{i \leqslant j} V_{ii,jj}^{(0)} \alpha_i \alpha_j \frac{1}{1 + \delta_{i,j}} \sqrt{\Omega_i \Omega_j} \left(1 - \tfrac{1}{4}(\alpha_i^2 + \alpha_j^2) \frac{n-2}{\Omega_e - 1} \right)$$

$$+ \frac{n(n-2)}{\Omega_e(\Omega_e - 1)} \sum_{i \leqslant j} \left\{ \sum_k (2k+1) V_{ij,ij}^{(k)} \right\} \tfrac{1}{4} \alpha_i^2 \alpha_j^2 , \tag{16}$$

where the ϵ_j's are single-particle energies and $V_{ij,kl}^{(L)}$ is an antisymmetrized matrix element of a two-body interaction. The first term of the r.h.s. of eq. (16) is obtained as a simple application of eq. (13). It is empirically established that $V_{ii,jj}^{(0)}$ is strongly attractive, while $\Sigma_K (2K+1) V_{ij,ij}^{(K)}$ is mostly repulsive and sometimes weakly attractive [7]. Actual the α_j's do not vary so much in a small region of the periodic table. A part proportional to n in eq. (16) is therefore attractive and the rest, which is proportional to $n(n-2)$, is repulsive. Since the ground state of semi-

[‡1] Utilizing this fact, we can generalize a correspondence [5] between the $J = 0$ pair and the s-boson in the interacting boson model to be applicable in non-degenerate cases [6].

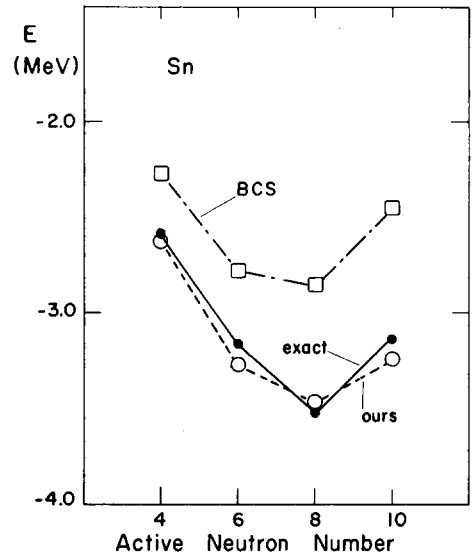

Fig. 1. Comparison of results of the exact diagonalization, the BCS approximation and our method. The hamiltonian consists of a pairing force plus single-particle energies and the parameters are the same as those used in ref. [1].

magic nuclei seems to be described as a seniority zero state in eq. (5) [3], this observation is consistent with the empirical formula of the binding energy [8].

In order to obtain a set of α_j's which gives the lowest value of eq. (16), we minimize eq. (16) with respect to the α_j's under the normalization condition (9).

We now investigate to what extent the minimization procedure provides a good approximation to the exact shell model diagonalization [1]. We take a hamiltonian which consists of a pairing force plus single-particle energies, and choose the tin isotopes as an example. A comparison between the present results and the exact diagonalization results is shown in fig. 1. Since the energy was minimized after the approximation was made, the minimum energy sometimes turns out to be lower than the exact one. Also shown in fig. 1 are results given by the BCS approximation. It appears that the present procedure yields much closer results to the exact values than the BCS. Errors in the former are at most 100 keV, while those in the latter are 300–600 keV. It should be pointed out here that the above minimization technique can be used as easily as that of the BCS, but the particle number is conserved while it is not in the BCS.

The good agreement in the resulting energies suggests that our number operator approximation is a good one. In order to examine its validity in more detail, we consider an example with $n = 10$. First, the α_j's are obtained by the minimization, and the results are shown in table 1. We then evaluate the overlap integrals between the exactly normalized states of $(S_-)^m|\tilde{j}^{10}, v=0\rangle$ and $|\tilde{j}^{10-2m}, v=0\rangle$. They are 0.989, 0.972, 0.964, and 0.971, corresponding to $m = 1, 2, 3$, and 4, respectively. Note that if the approximation is exact these values are identically one. We also computed the exact amplitudes of the vectors produced by the S_+ (S_-) operation on the states $|\tilde{j}^{2m}, v=0\rangle$ and found that within 3% they agree with the results by the number operator approximation, $[(m+1)(\Omega_e - m)]^{1/2}$

Table 1
The quantities α_j, $\tilde{v}_j$ and v_j obtained by minimizing the expectation value of the hamiltonian. Here $\Omega_e = 8.305$ and $n = 10$. The quantities α_j were found to be insensitive to the number of particles n for this hamiltonian.

	$d_{5/2}$	$g_{7/2}$	$s_{1/2}$	$d_{3/2}$	$h_{11/2}$
α_j	1.127	0.969	0.367	0.322	0.258
$\tilde{v}_j$	0.874	0.752	0.285	0.250	0.200
v_j	0.840	0.781	0.291	0.251	0.195

$([m(\Omega_e - m + 1)]^{1/2})$. We comment that the values of the α_j's in table 1 deviate appreciably from unity so that the degenerate j-orbit approximation does not work well in this case.

The quantity $\tilde{v}_j = \sqrt{n/2\Omega_e} \cdot \alpha_j$ and the seniority v correspond to the v_j-factor and the quasi-particle number in the BCS theory, respectively. As shown in table 1, the values of the $\tilde{v}_j$'s and v_j's are close to each other. If we take the limit n and $\Omega_e \to \infty$, and an approximation $\tilde{u}_i^2 + \tilde{u}_k^2 \sim 2\tilde{u}_i\tilde{u}_k$ ($\tilde{u}_i = \sqrt{1 - \tilde{v}_i^2}$), eq. (16) becomes the same as the vacuum expectation value in the quasi-particle formalism. We found that under the same condition eqs. (13) and (15) also become similar to the corresponding expressions in the quasi-particle formalism and that other operators which appear in the nuclear shell model seem to have similar correspondences. The BCS method can thus be regarded as a limiting case of the present method. We emphasize that the v-dependence does not appear in the BCS method, but simply disappears in our reduction formula as a consequence of the limiting procedure.

We have thus shown that our approximated reduction formulas include two extreme limits: one described by the exact quasi-spin formalism and the other by the BCS. A state which has occupation probabilities of single-particle orbits similar to those in S_+ will be included in the subspace where the number operator approximation works well [6]. In some cases of odd-A nuclei, however, the last odd particle has to be treated separately from the others as in the blocked BCS. A similar situation occurs in some states with $v \neq 0$, if particles carrying non-vanishing seniority occupy definite orbits.

In summary, we state two major advantages of the present scheme over the BCS approximation: (i) the number of nucleons is conserved, and (ii) the seniority dependences in matrix elements are properly taken into account. We conclude that the present method supersedes the BCS approximation.

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