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Pair truncation for rotational nuclei: $j=\frac{17}{2}$ model

P. Halse, L. Jaqua, and B. R. Barrett
Department of Physics, University of Arizona, Tucson, Arizona 85721
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The suitability of the pair condensate approach for rotational states is studied in a single $j=\frac{17}{2}$ shell of identical nucleons interacting through a quadrupole-quadrupole Hamiltonian. The ground band and a $K=2$ excited band are both studied in detail. A direct comparison of the exact states with those constituting the *SD* and *SDG* subspaces is used to identify the important degrees of freedom for these levels. The range of pairs necessary for a good description is found to be highly state dependent; *S* and *D* pairs are the major constituents of the low-spin ground-band levels, while *G* pairs are needed for those in the γ band. Energy spectra are obtained for each truncated subspace. *SDG* pairs allow accurate reproduction of the binding energy and $K=2$ excitation energy, but still give a moment of inertia which is about 30% too small even for the lowest levels.

I. INTRODUCTION

An unresolved problem in nuclear structure is that of finding a shell-model truncation scheme which includes the states capable of describing nuclear collective motion in a basis of manageable size. This is motivated in part by interest in the microscopic description of macroscopic nuclear phenomena such as rotations and vibrations. However, the ability to perform realistic calculations for heavy nuclei would also further the investigation of such fundamental physical problems as double-β decay and the nonconservation of symmetries.

The phenomenological success of the interacting boson model (IBM), which describes nuclei with $2n$ valence nucleons as systems of n scalar (s) and quadrupole (d) bosons,[1] suggests that these degrees of freedom could represent those of importance in nuclear structure. A possible interpretation is the correspondence of Otsuka, Arima, Iachello, and Talmi, in which the bosons represent scalar (S) and quadrupole (D) nucleon pairs.[2] This approach, known as OAI, need not be regarded merely as a prescription for obtaining parameters to be used in IBM calculations, but as a shell-model truncation scheme, inspired by the IBM. However, the extent to which low-energy nuclear states can indeed be constructed using only these pairs has yet to be conclusively determined. The present work concerns rotational motion, for which intrinsic states are already known to give a natural description; the rationale for investigating a pair description is the goal of finding a unified description of both vibrational and rotational states.

Many different conclusions have been drawn from previous work, ranging from apparently successful applications of the *SD* scheme to claims that $J=4$ (G)-pair content is high in even the lowest levels: The former typically consist of comparing with data the results of an IBM calculation using parameters obtained by evaluating matrix elements of a shell-model Hamiltonian in the low-seniority part of the *SD* subspace.[3-5] On the other hand, the early opinion[2] that the scheme would not be useful in systems where seniority is not conserved has been reinforced by studies of pair structure in intrinsic states optimized for realistic Hamiltonians,[6,7] where pairs of higher spin, in particular $J=4$, play an important role.

However, with regard to the applications of the OAI mapping, it is not known whether the data would be correctly reproduced in a full shell-model calculation for which the Hamiltonian used is supposed to be appropriate. While this is precisely the type of application for which the scheme is intended, at this stage the results are not conclusive in that: (i) Errors may be due to either the *SD* truncation or to the shell-model interaction, and indeed an apparently correct result could be due to some fortuitous cancellation of errors. (ii) States outside the *SD* subspace are not investigated; this is critical in that if such states would occur in an energy region lower than that of any experimental candidates, then the shell-model Hamiltonian used, and so the whole study, would be invalidated. Such uncertainties concerning the physical relevance of the *SD* subspace can be eliminated in studies of model systems for which exact calculations may be performed, with of course the corresponding disadvantage that one may not have all the critical elements of a realistic system. We argue that calculations for realistic nuclei, and for exactly solvable model systems, are both necessary to determine the extent of validity of the OAI correspondence.

With regard to the intrinsic state calculations, these states contain levels with angular momenta beyond the range of the IBM that cannot be constructed with S and D pairs, their presence lowering the *SD* content and hence underestimating this for the low-J levels. Again, such uncertainty may be resolved by constructing states with good angular momentum.

Even for exactly solvable systems, an ambiguity surrounds calculations where only observables, such as energies, are evaluated; a difference between values for a model state and the level to which it is assigned could be due to the effects of small admixtures from outside the chosen subspace, or to the model state in fact describing a totally different level. Renormalization would be appropriate in the first case, but not in the second. Thus it is important to ascertain the degrees of freedom of primary importance for each eigenstate.

It is commonly believed that the *SD* subspace has comparable relevance to all low-energy levels, including those in both the ground and excited bands.[3-5,8] However, some studies for ^{20}Ne (Ref. 9) and ^{156}Gd (Ref. 10) have shown that this may not always be the case, with an excited band not being accurately reproduced using the pairs optimized for the ground state. We believe that it is important to determine whether this result represents a general feature. With regard to the ^{156}Gd calculations, we note that, as already remarked, conclusions based on comparisons of spectra give ambiguous information on the nature of the states, and that direct investigations of calculated eigenstates should be used where possible, as in this paper.

Many applications of boson-fermion mapping procedures have been made to systems consisting of a single j shell.[11-13] Such model spaces do not afford a realistic description of actual collective nuclei; of particular relevance to the investigation of the OAI scheme is a possible greater emphasis on the role of higher-spin pairs, in the sense that there is only a single pair for each angular momentum while in more realistic multi-j spaces there are relatively more with low spin. Nevertheless, some of the effects believed to be important in rotational motion, such as mixing of seniority, can certainly be induced by the imposition of a suitable Hamiltonian. Indeed, Hamiltonians of the quadrupole-quadrupole type produce spectra which can be readily interpreted in terms of rotational bands. In addition to single j-shell tests of mapping procedures via comparisons of spectra, an eigenstate study of the type to be described here has previously been performed for a $j=\frac{13}{2}$ shell,[14,15] with the conclusion that the ground-state band levels that fall within the range of the IBM ($J\le 2n$) do lie almost entirely within the *SD* subspace. However, in that system there are no low-spin excited bands for which to investigate the structure of such bands, previously discussed. In contrast, the system to be discussed here, $j=\frac{17}{2}$, possesses a well-defined $K=2$ band, and is also sufficiently large that it is meaningful to investigate the role of G pairs.

The OAI correspondence between bosons and fermion pairs is summarized in Sec. II. In Sec. III, the validity of the *SD* and *SDG* descriptions for low-lying bands is examined for a $j=\frac{17}{2}$ shell by direct comparison with the eigenstates of a quadrupole-quadrupole Hamiltonian; the corresponding energy spectra are also presented.

II. PAIR-BASED TRUNCATION SCHEMES

A. The interacting boson model

The IBM treats nuclei with $2n$ valence nucleons as systems of n bosons with angular momenta 0 (s) and 2 (d), giving a U(6) algebra whose subgroup chains can each be associated with a particular regime of collective motion:[1]

$$\mathrm{U}(6)\supset\mathrm{U}(5)\supset\mathrm{SO}(5)\supset\mathrm{SO}(3)\quad(\text{vibrational})\,, \tag{1a}$$

$$\mathrm{U}(6)\supset\mathrm{SO}(6)\supset\mathrm{SO}(5)\supset\mathrm{SO}(3)\quad(\gamma\text{ soft})\,, \tag{1b}$$

$$\mathrm{U}(6)\supset\mathrm{SU}(3)\supset\mathrm{SO}(3)\quad(\text{axially symmetric rotor})\,. \tag{1c}$$

Extending the model space to include in addition bosons with angular momentum 4 (g) gives a U(15) algebra whose subgroups include[16]

$$\mathrm{U}(15)\supset\mathrm{U}(1)\times[\mathrm{U}(5)\supset\mathrm{SO}(5)\supset\mathrm{SO}(3)]\times[\mathrm{U}(9)\supset\mathrm{SO}(9)\supset\mathrm{SO}(3)]\supset\mathrm{SO}(3)\,, \tag{2a}$$

$$\mathrm{U}(15)\supset\mathrm{SU}(3)\supset\mathrm{SO}(3)\,, \tag{2b}$$

where Eq. (2a) describes a basis where states are classified according to the numbers of s, d, and g bosons, and Eq. (2b) describes a rotational band classification which differs qualitatively from that in Eq. (1c) by the appearance of low-lying bands with $K=1$ and 3, and also by the extension of corresponding bands.

B. Boson-shell model state correspondence

For a single j-shell of identical nucleons, the only classification scheme which conserves angular momentum is[17]

$$\mathrm{U}(2j+1)\supset Sp(2j+1)\supset\mathrm{SU}(2)\,. \tag{3}$$

A possible interpretation of the s, d, (and g) bosons is that they represent $J=0$, 2 (S, D), [and $J=4$ (G)] nucleon pairs[2]

$$s^\dagger\to S^\dagger=A^{\dagger(0)}\,, \tag{4a}$$

$$\mathbf{d}^\dagger\to\mathbf{D}^\dagger=P\,\mathbf{A}^{\dagger(2)}\,, \tag{4b}$$

$$\mathbf{g}^\dagger\to\mathbf{G}^\dagger=P\,\mathbf{A}^{\dagger(4)}\,, \tag{4c}$$

where, for a single j shell,

$$A_M^{\dagger(J)}=\sqrt{1/2}[\mathbf{a}^{\dagger(j)}\mathbf{a}^{\dagger(j)}]_M^{(J)}\,, \tag{5}$$

and P is a projection operator onto states of highest seniority, eliminating the need for explicit orthogonalization for many states. Thus

$$|s^{n-n_d-n_g},d^{n_d}(\gamma_d J_d),g^{n_g}(\gamma_g J_g);J\rangle\to|j^{2n},v=2(n_d+n_g)(D^{n_d}\text{“}\gamma_d\text{”}J_d,G^{n_g}\text{“}\gamma_g\text{”}J_g),J\rangle \tag{6}$$

where γ represents all additional labels needed to completely specify a state, and explicit orthogonalization and normalization has been performed when required.

The classification scheme appropriate to the boson states in Eq. (6) is that of Eq. (2a), with a restriction to the U(5) chain of the standard *sd* boson model [Eq. (1a)] corresponding to setting $n_g=0$. However, shell-model analogues of any combinations of boson states, say those classified according to SU(3) [Eqs. 1(c) and 2(b)], may be obtained using the boson SU(3) to U(5) or SU(3) to $\mathrm{U}(5)\times\mathrm{U}(9)$ transformation coefficients as appropriate on both sides of the correspondence [Eq. (6)].

III. APPLICATION TO A $j=\frac{17}{2}$ SHELL WITH $H=-Q\cdot Q$

A. The full shell-model calculation

A model system of identical nucleons in a single $j=\frac{17}{2}$ shell allows an exact calculation, but is capable of providing rotational-like spectra. Rotational motion is generally associated with a quadrupole-quadrupole interaction,[18] inducing the effect of a nuclear quadrupole deformation; we choose

$$H=-Q\cdot Q \tag{7}$$

where

$$Q=-[\mathbf{a}^{\dagger(j)}\mathbf{a}^{(j)}]^{(2)} . \tag{8}$$

The resulting spectra, obtained using the Oxford-Buenos Aires shell-model code OXBASH,[19] indeed display sequences of levels that can be grouped into rotational bands. In this paper a detailed analysis of the six-particle system ($n=3$) is presented. The corresponding spectrum of levels with $J\le 16$ in the three lowest bands is shown on the left of Fig. 1; above $E=-2.80$ units, many other levels occur and these are not shown. The levels shown appear to form rotational bands with $K=0$, 12, and 2, which can be understood from a Nilsson diagram[20] and indicate oblate deformation.

The Hamiltonian [Eq. (7)] is capable of mixing seniority, and analysis of the eigenstates reveals that this generally occurs.

B. Results for the *SD* and *SDG* subspaces

1. Pair content of the low-energy eigenfunctions

The numbers of states for each angular momentum J (≤ 12) in the full $j=\frac{17}{2}$ shell-model space and the *SD* and *SDG* pair subspaces are compared in Table I. It is seen that the *SD* subspace accounts for only a small fraction of the full basis space, while for low angular momentum the *SDG* subspace exhausts a significant fraction.

The suitability of the pair subspaces for describing the low-energy rotational motion can be measured by the extent to which the corresponding eigenstates lie within these subspaces. The *SD* and *SDG* fractions of each level ($J\le 12$) in the ground ($K=0$) and $K=2$ bands (Fig. 1) are shown in Table II. It is seen that these two bands give very different results:

The low-spin ground-band levels are well described by the *SD* subspace. Note that the small improvements obtained by adding G pairs correspond to a subspace which is larger by a factor of around 3–4 (Table I). It is clear that the *SD* components are the most important for describing these levels. For higher spin ($J>6$) the *SD* subspace is of course not relevant; however, for these levels even the addition of G pairs does not allow a good description, and the continuous decrease in *SDG* occupancy can be contrasted with the reasonable fractions exhausted by the *SD* subspace up to its maximum spin ($J=6$).

The low-spin $K=2$ band levels do not lie predominantly within the *SD* subspace. For these eigenstates, the addition of G pairs is necessary for the pair-based truncation to be reasonable.

2. SD and SDG spectra

We now use the degrees of freedom investigated in Sec. III B 1 to calculate energy spectra. This will indicate how the errors in overlaps are related to the errors in energies. Spectra for each subspace are obtained by simply diagonalizing the appropriate submatrix of the shell-model

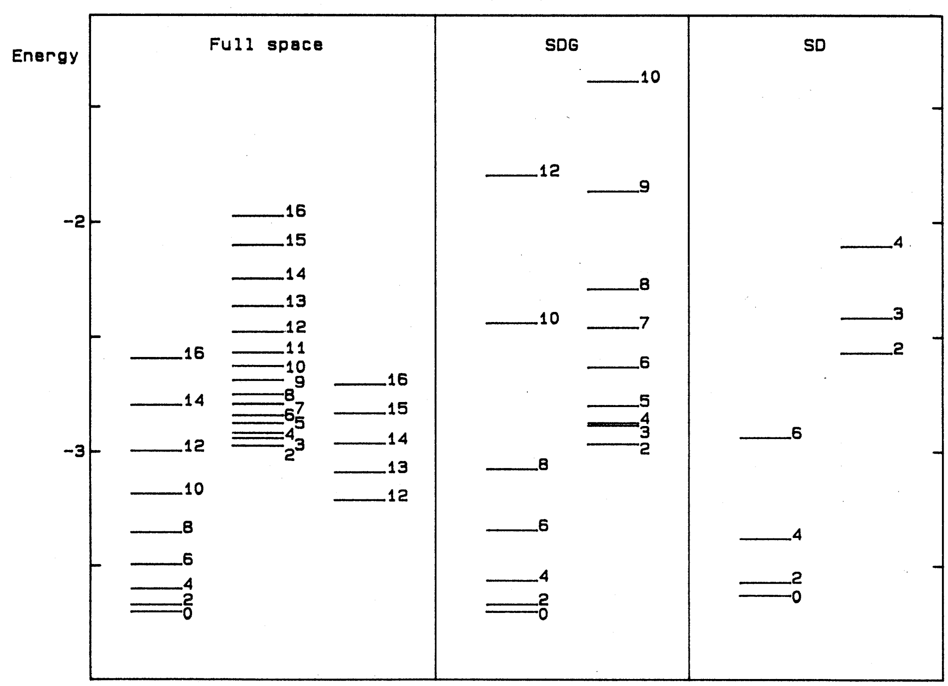

FIG. 1. Energy spectrum for six identical nucleons in a $j=\frac{17}{2}$ shell with $H=-Q\cdot Q$ (see text), and spectra corresponding to a restriction to *SDG*, and to *SD*, pairs.

TABLE I. Number of six-particle states in the full $j=\frac{17}{2}$ space, and in the SDG and SD subspaces, for each value of the angular momentum $J \leq 12$.

Space	J = 0	1	2	3	4	5	6	7	8	9	10	11	12
$(\frac{17}{2})^6$	8	4	16	14	26	21	34	28	37	33	40	33	41
$(SDG)^3$	7	2	11	7	13	6	10	4	5	2	2		1
$(SD)^3$	3		3	1	2		1						

Hamiltonian (the "bare" interaction). The errors then indicate the extent of renormalization that would be required to compensate for the inadequacy of the chosen restrictions.

Spectra appropriate for restriction to the SDG and SD subspaces are shown in Fig. 1 alongside the exact results. At the qualitative level, the rotational nature of the exact calculation is seen to be preserved; sets of levels corresponding to rotational bands with $K=0$ and 2 are apparent in both truncated calculations, although the $K=12$ band is of course not present in either. Quantitatively, the bandhead energies are well reproduced, excepting that of the $K=2$ band in the SD calculation. However, there are significant errors in the moments of inertia for both subspaces. The binding energies, excitation energies of the $K=2$ band, and effective moments of inertia obtained by fitting to the levels with $J \leq 4$ are presented in Table III. It is seen that the deviations are correlated to the results presented in Table II, and that the errors in the moment of inertia are much larger than those for the wave functions.

C. SU(3) symmetry in the SD subspace

Squared overlaps of the shell-model eigenstates with the SD subspace states defined by the sd IBM SU(3) subgroup[1] [see text following Eq. (6)] are displayed in Table II below the total SD content. The (60) representation exhausts the SD component of the ground band, and thus gives a good description of the lowest eigenvectors in the exact calculation. Similarly, the (22) representation also exhausts the (smaller) SD components of the $K=2$ band. Thus the SU(3) "symmetry," which corresponds only to a particular mixing of seniority, is seen to have some validity, as for $j=\frac{13}{2}$,[14] although there is no shell-model SU(3) algebra.

IV. CONCLUSION

The suitability of the SD pair approach to rotational motion has been investigated for a model system consisting of six identical particles in a $j=\frac{17}{2}$ shell interacting through a quadrupole force. That such a model is a reasonable one with which to study rotational motion is suggested by the clear appearance of rotational bands and by the strong mixing of the shell-model seniority. This calculation differs from most other investigations of pair construction for exactly solvable models[11–13] in that the content of the relevant pair subspaces in the rotational eigenstates has been explicitly considered in order to identify the degrees of freedom which constitute their major "building blocks" and those which are not of primary importance but do significantly perturb the spectrum.

In this model calculation, it is found that S and D pairs do allow an accurate construction of the ground-band

TABLE II. SDG and SD occupancies, and SU(3) decomposition of the SD content, for levels in the (a) ground ($K=0$) and (b) $K=2$ bands.

(a)

	J = 0	2	4	6	8	10	12
SDG	1.000	0.999	0.981	0.916	0.761	0.445	0.139
SD	0.969	0.945	0.867	0.627			
(60)	0.947	0.944	0.863	0.627			
(22)	0.003	0.001	0.004				
(00)	0.019						

(b)

	J = 2	3	4	5	6	7	8	9	10	11	12
SDG	0.995	0.958	0.962	0.945	0.785	0.658	0.338	0.081	0.086		0.060
SD	0.576	0.497	0.240		0.146						
(60)	0.000		0.001		0.146						
(22)	0.576	0.497	0.239								

TABLE III. Binding energies, $K=2$ excitation energies, and effective moments of inertia for the $J\leq 4$ members of the $K=0$ and 2 bands, for the exact, *SDG*, and *SD* calculations.

	Exact	*SDG*	*SD*
$-E(0)$	3.702	3.702	3.631
$E(2)^*$	0.727	0.736	1.063
$I(0)$	99.2	71.5	39.4
$I(2)$	120.7	74.5	15.1

eigenstates for which such a description is possible ($J\leq 2n$), and clearly form a reasonable set of building blocks for these levels. States including in addition *G* pairs are much less important for $J\leq 2n$, and are also of limited relevance for larger values of J ($\leq 4n$) since high occupancies do not extend out to this limit. Indeed, it is interesting to contrast the high overlaps for the *SD* subspace out to its maximum angular momentum with the steady decrease in relevance of the *SDG* subspace. However, the eigenstates of the $K=2$ band, even those of low angular momentum, are not well described by *S* and *D* pairs alone; here the addition of states involving also *G* pairs allows a much more accurate construction. This result may be influenced by the overemphasis of higher-spin pairs in a single *j*-shell calculation, the existence of many *S* and *D* pairs in more realistic shell-model spaces providing an opportunity for greater dominance.

Although pairs with $J>2$ are not major constituents of the low-spin ground-band levels, the small admixtures do carry a significant contribution to energies (relative to the mean level spacing) as shown by the *SD*-subspace spectrum. Similarly, pairs with $J>4$ appear to be important in describing the low-spin $K=2$ level energies. Nevertheless, these low-spin pairs constitute a useful set of degrees of freedom for the description of the rotational motion of lower members of the ground and $K=2$ bands, and thus form a possible basis for a truncated calculation; the significant effects of other pairs on the spectrum would seem to be a reasonable target for perturbation theory. In contrast, renormalization would not be appropriate for shifting the energy of, say, the *SDG* $J=12$ state closer to that of the ground-band level; the smallness of the overlap between the two states (Table II) indicates that the model state is in fact describing some combination of other levels rather than the lowest eigenstate, which must then have a different structure.

The result for the ground band is counter to the view that the *SD* pair approach is not relevant when seniority is mixed,[2,6] supporting the arguments, summarized in the Introduction, that this need not be the case. We also note in this context the apparently successful applications of OAI to nuclei which, although not strongly deformed, do indicate breaking of seniority.[3–5]

The result for the $K=2$ band is of particular interest given the recent suggestions that excited (β) bands can be intruders into the space corresponding to low-spin pairs optimized for the ground band.[9,10] Here the excited ($K=2$) band levels are indeed not well described by the *SD* degree of freedom, although in contrast to the ^{156}Gd calculations,[10] in the present example the description is significantly improved on the addition of *G* pairs rather than *S'* pairs, there being only a single pair of each spin in a single *j* shell. These conclusions from a range of different systems all suggest that models based on single types of *S* and *D* pairs[1,8] may not in fact include the degrees of freedom appropriate for describing shape excitations in rotational nuclei.

The validity of the boson SU(3) in the ground-band levels reveals an SU(3) symmetry "latent" in the shell model, although there is no SU(3) algebra in the shell model itself. This appearance of symmetries realized with appropriately defined "collective modes," in this case bosons mapped from *S* and *D* pairs, is one of the major motivations for this type of work. It also suggests that studies of rotational motion restricted to shell-model systems with an explicit SU(3) algebra[8,21] are unnecessarily limited. The appearance of an SU(3) symmetry in the OAI microscopic calculation for a situation in which SU(3) would have been expected phenomenologically adds support to the use of this approach.

Finally we again stress that performing an exact calculation has enabled us to obtain unambiguous results concerning the nature of the low-energy states. If instead we had simply performed an *SD* subspace calculation (as in Refs. 3–5, 11–13), giving only the energy spectra in Fig. 1, we would not have known whether the significant errors were due to the influence of small admixtures to the chosen states (as for the ground band) or to the dominance of different degrees of freedom (as for the $K=2$ band). Analysis such as this determines the validity of a renormalization approach.

This work is being extended to more realistic models consisting of protons and neutrons in several *j* shells, and renormalization procedures for this case are also under consideration.

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