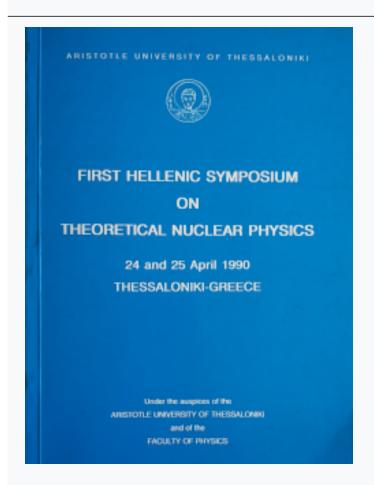




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A Democratic Mapping between the Shell Model and the IBM1

L.D. Skouras¹, P. Van Isacker² and M.A. Nagarajan²

Abstract: A method is proposed to connect states of the shell model and the interacting boson model and derive the boson model hamiltonian from shell-model data. This novel mapping technique is based on the properties of the shell-model overlap matrix. An application to the $f_{7/2}$ shell is presented and the results of the new mapping are compared with the standard OAI results.

1. Introduction

The method that has been most widely used to connect the interacting boson model¹) (IBM) with the shell model is the Otsuka-Arima-Iachello or OAI mapping ²). It is a seniority-based state mapping, that is, the seniority classification of shell-model states is carried over onto a similar classification of boson states. The boson images of fermion operators are then determined by computing matrix elements between shell-model states with good seniority.

We propose an alternative mapping method which is based on the diagonalization of a shell-model overlap matrix. Whereas the OAI method implicitly assumes an ordering of states according to the number of correlated S pairs, this hierarchy is absent from our method where all shell-model states that are mapped onto corresponding boson states are treated on an equal footing. One thus could describe our mapping method as being "democratic." The formalism can be used without making reference to a specific system of interacting bosons and is applicable equally well to odd-mass nuclei in the context of the interacting boson-fermion model³) (IBFM).

A test of the mapping is presented for the $f_{7/2}$ shell⁴). Since we consider neutrons and protons in the same valence shell, isospin is of vital importance and we map the shell model onto an isospin invariant version of the interacting boson model, the IBM-3⁵), and its extension to odd-mass nuclei, the IBFM-3⁶).

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2. A mapping from the IBM and IBFM into the shell model

We assume we have solved the eigenvalue problem for a two-fermion system,

$$H|2\Gamma\alpha\rangle = E_{2\Gamma\alpha}|2\Gamma\alpha\rangle,\tag{1}$$

where by $|n\Gamma\alpha\rangle$ we represent the eigenvectors of the shell-model hamiltonian for a n-fermion system. In this notation Γ stands for the pair J,T if isospin formalism is used, or, simply for J if the particles are identical. On the other hand, the index α distinguishes the various eigenvectors that belong to the same $(n\Gamma)$ set.

From the above set (1) of two-fermion eigenvectors we select some that are made to correspond with single-boson states,

$$|\Psi_{\Gamma\alpha}\rangle \iff |2\Gamma\alpha\rangle.$$
 (2)

The correspondence (2) defines the one-boson energies,

$$H^B|\Psi_{\Gamma\alpha}\rangle = E^B_{\Gamma\alpha}|\Psi_{\Gamma\alpha}\rangle,$$
 (3)

where

$$E_{\Gamma\alpha}^B = E_{2\Gamma\alpha}.\tag{4}$$

We now construct boson-fermion states $|\Psi_{\Gamma_1\alpha_1}, \gamma_1; \Gamma\rangle$ and the symmetric and normalized two-boson states $|\Psi_{\Gamma_1\alpha_1}, \Psi_{\Gamma_2\alpha_2}; \Gamma\rangle$ and, as in (2), we associate them with three- and four-fermion states,

$$|\Psi_{\Gamma_{1}\alpha_{1}}, \gamma; \Gamma\rangle \longleftrightarrow |2\Gamma_{1}\alpha_{1}, \gamma; \Gamma\rangle,$$

$$|\Psi_{\Gamma_{1}\alpha_{1}}, \Psi_{\Gamma_{2}\alpha_{2}}; \Gamma\rangle \longleftrightarrow |2\Gamma_{1}\alpha_{1}, 2\Gamma_{2}\alpha_{2}; \Gamma\rangle.$$
 (5)

The problem with the mapping in eq. (5) is that the states on the lhs of these relations form orthonormal sets while those on the rhs do not. Hence the states cannot directly be associated with each other and in the following we describe a mapping method that deals with this nonorthonormality problem.

In order to simultaneously discuss the three- and four-fermion cases, we denote by $|B_i\rangle$ the boson-fermion and two-boson states that appear on the lhs of (5). Similarly, we denote by $|F_i\rangle$ the fermion states that appear on the rhs of (5). Thus eq. (5) reads in the new notation

$$|B_i\rangle \longleftrightarrow |F_i\rangle, \quad i = 1, 2, \dots, d,$$
 (6)

where d denotes the dimension of the space for a given set $\{n\Gamma\}$. As pointed out previously, the $|B_i\rangle$ form an orthonormal set while the $|F_i\rangle$ do not,

$$\langle B_i|B_j\rangle = \delta_{ij}, \quad \langle F_i|F_j\rangle \neq \delta_{ij}, \quad i,j=1,2,\ldots,d.$$
 (7)

Our mapping method requires the determination of the matrix elements

$$P_{ij} \equiv \langle F_i | F_i \rangle, \quad H_{ij} \equiv \langle F_i | H | F_j \rangle, \quad i, j = 1, 2, \dots, d.$$
 (8)

These matrix elements can be determined either directly or, in a more elegant manner, from the solutions of the eigenvalue problem:

$$H|n\Gamma\alpha\rangle = E_{n\Gamma\alpha}|n\Gamma\alpha\rangle \tag{9}$$

Thus, if we obtain all solutions of (9) for n = 3, 4 and for all Γ , we can then use the quantum-mechanical relations

$$I = \sum_{\Gamma_{\alpha}} |n\Gamma_{\alpha}\rangle \langle n\Gamma_{\alpha}|, \quad H = \sum_{\Gamma_{\alpha}} |n\Gamma_{\alpha}\rangle E_{n\Gamma_{\alpha}} \langle n\Gamma_{\alpha}|, \tag{10}$$

to determine

$$P_{ij} = \sum_{\Gamma\alpha} \langle F_i | n\Gamma\alpha \rangle \langle n\Gamma\alpha | F_j \rangle, \quad H_{ij} = \sum_{\Gamma\alpha} \langle F_i | n\Gamma\alpha \rangle E_{n\Gamma\alpha} \langle n\Gamma\alpha | F_j \rangle.$$
 (11)

As eq. (11) shows, the only quantities required for the determination of the P and H matrices, defined in (8), are the overlaps $\langle F_i|n\Gamma\alpha\rangle$ which can be obtained from the solutions of (9).

Let us now consider the transformation from the nonorthonormal basis $|F_i\rangle$ to an orthogonal basis $|X_k\rangle$ obtained by diagonalizing the overlap matrix P. The diagonalization yields the eigenvalues p_k and the transformation coefficients $\langle F_i|X_k\rangle \equiv \langle X_k|F_i\rangle$, defined by

$$P|X_{k}\rangle = p_{k}|X_{k}\rangle,$$

$$|X_{k}\rangle = \sum_{i} \langle F_{i}|X_{k}\rangle |F_{i}\rangle, \quad k = 1, 2, \dots, d.$$
(12)

The eigenvectors $|X_k\rangle$ form an orthogonal basis since

$$\langle X_k | X_l \rangle = \sum_{ij} \langle X_k | F_i \rangle \langle F_i | F_j \rangle \langle F_j | X_l \rangle = p_k \delta_{kl}, \quad k, l = 1, 2, \dots, d.$$
 (13)

and this relation can be viewed as a property satisfied by the coefficients $\langle F_i|X_k\rangle$. Since these coefficients result from a matrix diagonalization, they also satisfy the orthonormality property

$$\sum_{i} \langle X_k | F_i \rangle \langle F_i | X_l \rangle = \delta_{kl}, \quad k, l = 1, 2, \dots, d.$$
 (14)

Equation (14) can be viewed as a special case of (13), namely one in which the original basis $|F_i\rangle$ was properly orthonormalized.

It is important to realize that the coefficients $\langle F_i|X_k\rangle$ satisfy both relations (13) and (14). This occurs because the diagonalization method is insensitive to whether the overlap matrix was defined in an orthonormal basis or not. As will be discussed below, this property of the coefficients $\langle F_i|X_k\rangle$ is the basic point in our mapping method.

Let us now return to the results obtained by diagonalizing the overlap matrix in the nonorthonormal basis $|F_i\rangle$ and examine the following two possibilities:

Case 1: The vectors $|F_i\rangle$ are linearly independent

The condition for this case to occur is

$$p_k > 0, \quad k = 1, 2, \dots, d.$$
 (15)

In such a case it is straightforward to introduce an orthonormal basis in the fermion space, formed by the vectors

$$|X_k^F\rangle = \frac{1}{\sqrt{p_k}}|X_k\rangle, \quad k = 1, 2, \dots, d,$$
 (16)

which, as is evident from (13), satisfy

$$\langle X_k^F | X_l^F \rangle = \delta_{kl}, \quad k, l = 1, 2, \dots, d. \tag{17}$$

We now introduce the following vectors in the boson space:

$$|X_k^B\rangle = \sum_i \langle F_i | X_k \rangle |B_i\rangle, \quad k = 1, 2, \dots, d.$$
 (18)

where the coefficients $\langle F_i|X_k\rangle$ are the same as those that appear in (12). Since these coefficients satisfy (14) while, as seen in (6), the vectors $|B_i\rangle$ form an orthonormal set one can easily verify that

$$\langle X_k^B | X_l^B \rangle = \delta_{kl}, \quad k, l = 1, 2, \dots, d.$$
 (19)

Since we now are dealing with orthonormal bases in both the fermion and the boson spaces, we can formally execute the mapping

$$|X_k^B\rangle \Longleftrightarrow |X_k^F\rangle, \quad k = 1, 2, \dots, d,$$
 (20)

and use this mapping to determine the boson or boson-fermion hamiltonian by equating the matrix elements

$$\langle X_k^B | H^B | X_l^B \rangle = \langle X_k^F | H | X_l^F \rangle, \quad k, l = 1, 2, \dots, d.$$
 (21)

Matrix elements of this boson or boson-fermion hamiltonian in the original boson basis (6) in terms of the original shell-model matrix elements (8) can be found by inverting the transformations (12), (16) and (18). The final result is

$$\langle B_i | H^B | B_j \rangle = \sum_{kl} \sum_{mn} \frac{1}{\sqrt{p_k p_l}} \langle F_i | X_k \rangle \langle X_k | F_m \rangle H_{mn} \langle F_n | X_l \rangle \langle X_l | F_j \rangle. \tag{22}$$

Case 2: The vectors $|F_i\rangle$ are not linearly independent Suppose that $m \ (m < d)$ eigenvalues of the overlap matrix P are zero:

$$p_i = 0, \quad i = 1, 2, \dots, m.$$
 (23)

Equation (23) indicates that only d-m vectors $|F_i\rangle$ are linearly independent. To deal with this problem we remove from the fermion space m vectors $|F_i\rangle$, say those with $i=d-m+1,\ldots,d$, and we treat the remaining d-m vectors, which are linearly independent, as in case 1. We thus obtain the matrix elements of the hamiltonian H^B between the d-m states $|B_i\rangle$ that correspond to the linearly independent vectors of the fermion space. The remaining matrix elements of H^B are defined in the following way:

$$\langle B_i | H^B | B_j \rangle = \langle B_j | H^B | B_i \rangle = 0, \quad i = d - m, \dots, d, \quad j = 1, 2, \dots, d, \quad i \neq j,$$

$$\langle B_i | H^B | B_i \rangle = \infty, \quad i = d - m + 1, \dots, d. \tag{24}$$

Finally, to determine the matrix elements of the two-body component of H^B we need to remove the one-body contribution from the matrix elements of this operator, defined in eqs. (21) and (24). Thus, going back to the notation of eq. (5), we can write

$$\langle \Psi_{\Gamma_{1}\alpha_{1}}, \gamma; \Gamma | V | \Psi_{\Gamma'_{1}\alpha'_{1}}, \gamma'; \Gamma \rangle = \langle \Psi_{\Gamma_{1}\alpha_{1}}, \gamma; \Gamma | H^{B} | \Psi_{\Gamma'_{1}\alpha'_{1}}, \gamma'; \Gamma \rangle$$

$$- \left(E^{B}_{\Gamma_{1}\alpha_{1}} + E_{\gamma} \right) \delta_{\Gamma_{1}\Gamma'_{1}} \delta_{\alpha_{1}\alpha'_{1}} \delta_{\gamma\gamma'},$$

$$\langle \Psi_{\Gamma_{1}\alpha_{1}}, \Psi_{\Gamma_{2}\alpha_{2}}; \Gamma | V | \Psi_{\Gamma'_{1}\alpha'_{1}}, \Psi_{\Gamma'_{2}\alpha'_{2}}; \Gamma \rangle = \langle \Psi_{\Gamma_{1}\alpha_{1}}, \Psi_{\Gamma_{2}\alpha_{2}}; \Gamma | H^{B} | \Psi_{\Gamma'_{1}\alpha'_{1}}, \Psi_{\Gamma'_{2}\alpha'_{2}}; \Gamma \rangle$$

$$- \left(E^{B}_{\Gamma_{1}\alpha_{1}} + E^{B}_{\Gamma_{2}\alpha_{2}} \right) \delta_{\Gamma_{1}\Gamma'_{1}} \delta_{\alpha_{1}\alpha'_{1}} \delta_{\Gamma_{2}\Gamma'_{2}} \delta_{\alpha_{2}\alpha'_{2}}.$$

$$(25)$$

3 Test of the mapping in the $f_{7/2}$ shell

In the following we discuss an application of our mapping method to the $f_{7/2}$ shell. In this application we associate boson states to $(f_{7/2})^2$ fermion states and we deduce the boson-boson and boson-fermion interactions from the matrix elements of the fermion hamiltonian in the space of $(f_{7/2})^4$ and $(f_{7/2})^3$ states, respectively. These interactions are then used to determine the energy spectra of nuclei in the A=45-48 mass region and these results are compared with shell-model spectra and also with results of other boson model calculations based on the OAI mapping method $^{7-9}$). In order to have a meaningful comparison between the OAI and the present mapping method, we consider the same shell-model hamiltonian as the one used in the previous boson calculations. Thus, as in refs. $^{7-9}$), the $(f_{7/2})^2$ matrix elements are taken directly from the experimental data on 42 Sc.

As discussed in sect. 3, our mapping method is not restricted to any specific choice of the boson space. To demonstrate this flexibility of the method we determine the spectra of the A=45-48 nuclei for two choices. In the first we consider an sd space while in the second an sdg space. To avoid confusion we denote in the following by model-1 and model-2 the results obtained with sd and sdg bosons, respectively. Similarly, we denote by OAI the results obtained with the interaction deduced from the corresponding mapping method. Note that the sd boson space is used in both the OAI and model-1 calculations. In table 1 we compare the matrix elements of the boson-boson interaction derived in this work with those obtained using the OAI mapping. To avoid making the table too lengthy we give only those matrix elements that involve s and d bosons. Thus the list of matrix elements given in table 1 is only complete for model-1. As tables 1 shows, the model-1 matrix elements are only slightly modified by the introduction of the g boson, indicating that the s and d bosons are the more important components for the mapping from the fermion to the boson space.

At first sight the matrix elements in the OAI and model-1 columns of table 1 appear to be quite similar. However, a more careful study reveals significant differences between the two interactions. These differences are most pronounced for the (J,T)=(4,0) and (0,0) matrix elements. In the first case the OAI method produces a matrix element which is almost 1.4 Mev more attractive than the one found with our mapping method. On the other hand, the two methods produce almost identical diagonal (J,T)=(0,0) matrix elements, but in the OAI method the diagonal interaction in the s^2 state is the most attractive one while in the democratic method this value is assigned to the d^2 diagonal matrix element.

To test the democratic mapping we now use the matrix elements of the boson and boson-fermion hamiltonians derived with this technique and calculate the energy spectra of nuclei in the A = 45-48 mass region. A selection of these spectra is shown

Table 1
Matrix elements $\langle ab; JT|V|cd; JT \rangle$ (in Mev)

\overline{a}	b	c	d	J	\overline{T}	OAI	Model-1	Model-2
\bar{s}	s	s	s	0	0	-7.20	-6.61	-6.13
				0	2	0.21	0.21	0.21
s	s	d	d	0	0	-2.09	-2.44	-2.55
				0	2	0	0	0
s	d	s	d	2	0	-8.29	-7.86	-7.34
				2	1	-4.46	-3.92	-3.98
				2	2	0.21	0.44	0.44
s	d	d	d	2	0	0.96	1.24	1.26
				2	2	0	-0.67	-0.67
d	d	d	d	0	0	-6.65	-7.19	-7.28
				2	0	-6.60	-6.63	-6.40
	6.			4	0	-8.50	-7.13	-6.63
				1	1	-5.62	-5.12	-5.12
				3	1	-5.28	-4.43	-4.43
				0	2	∞	∞	∞
				2	2	0.71	0.45	0.45
				4	2	-0.38	-0.29	-0.36

in figs. 1-3 and compared with the shell-model and OAI results.

Figure 1 shows that the three IBFM-3 calculations for ⁴⁵Ti are in satisfactory agreement with the shell-model spectrum, which here, as also in the following figures, plays the role of experiment. Most shell-model states up to about 3.5 Mev excitation appear also in the boson-fermion spectra and the differences in the excitation energies do not, generally, exceed 500 Kev.

Figure 2 shows the energy spectra for 46 Ti. All three IBM-3 spectra are in satisfactory agreement with the shell-model spectrum. The OAI results account for all shell-model states up to about 3.7 Mev excitation with the exception of the second J=4 state at 3 Mev. However, the OAI spectrum is somewhat compressed and especially the J=1,3 states occur at lower energies than the corresponding shell-model states. They are correctly reproduced in model-1 which, on the other hand, has trouble in getting the first J=4. Also, it fails to account for the second J=4 and the first J=6 levels which it predicts at 5.04 and 5.28 Mev, respectively. Finally, as fig. 2 shows, model-2 accounts for all fermion levels up to 4 Mev excitation with the exception of the second J=6 state. However, as with the OAI mapping, the spectrum

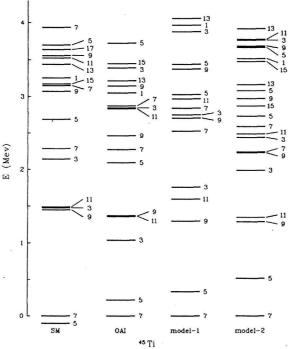


Figure 1: A comparison of shell-model and IBFM spectra for ⁴⁵Ti. All levels are labelled by 2J.

obtained using model-2 is compressed compared to the shell-model spectrum.

Figure 3 shows the spectra for 48 Cr. The three IBM-3 calculations fail to account for the second shell-model J=4 state and, in addition, the J=6 state is absent from model-1. The remaining levels are correctly obtained in model-1. On the other hand, the model-2 calculation, although it does predict a J=6 state, produces excitation energies which are in less satisfactory agreement with the shell-model than the model-1 results. As fig. 3 shows, the OAI matrix elements lead to a compressed energy spectrum, in particular for states with high J. The most characteristic example of this behavior is the J=8 state which in the OAI spectrum appears at about 3.3 Mev while in the shell model this state is predicted above 5 Mev.

Summarizing the comparison between the OAI and the democratic mapping methods, we observe that the first produces better results in nuclei that have few extra particles compared to those used to deduce the boson and boson-fermion hamiltonians. However, the second method becomes superior in nuclei with more valence

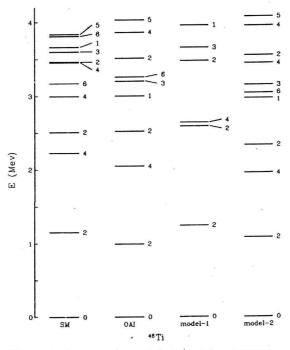


Figure 2: A comparison of shell-model and IBFM spectra for ⁴⁶Ti.

particles. The treatment of renormalization effects (coming mainly from the G pair) is responsible for this difference, as can be illustrated with the example of the J=4 states in 44 Ti (see table 1). Analyzing the shell-model structure of the lowest J=4 state, one finds 7) it to be an almost equal mixture of D^2 and SG components. The OAI exactly reproduces the energy of this state and it does this in spite of the fact that only s and d bosons are considered in the mapping. The s,d interaction matrix elements derived in the OAI approximation must therefore in some way incorporate the effect of the g boson. The democratic mapping method works differently. The first J=4 state in the model-1 calculation fits the average energy of the first and second shell-model J=4 states and it does so because D^2 is equally shared between them. Thus the diagonal d^2 , J=4, T=0 interactions are different, -8.50 MeV in OAI and -7.13 MeV in model-1 (see table 1), because the former includes a g boson renormalization whereas the latter does not. Clearly, the renormalized results will be better for small particle numbers. However, as the particle number increases, the G pair admixtures in the shell-model wave functions tend to decrease (at least for

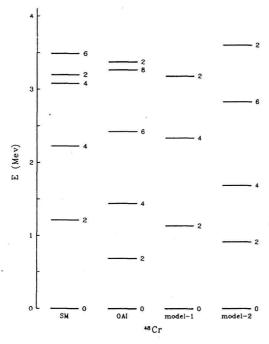


Figure 3: A comparison of shell-model and IBFM spectra for ⁴⁸Cr.

low-spin states) and hence the renormalized results will overpredict the g boson effect and give worse results.

4. Conclusions

In this paper we introduced a new method to determine the boson and boson-fermion hamiltonians from shell-model data. The method is based on the properties of the overlap matrix in the basis of nonorthogonal shell-model states onto which the boson states are mapped. In contrast to previous mapping methods ^{6,7}), which assume a hierarchy of states according to the number of correlated S pairs, the method proposed here treats all mapped shell-model states on an equal footing and can thus be characterized as "democratic."

The democratic mapping method was tested in the $f_{7/2}$ shell. This test proved successful since we obtained energy spectra for even-even and odd-mass A = 45-48

nuclei which compared well with the shell model. The democratic mapping method was also compared with the OAI mapping and turned out to give similar—if not slightly better—results.

The main advantage of the democratic mapping method is that it can be readily applied to more realistic multi-shell configurations which are more difficult to treat with other mapping techniques. In addition, extensions of the method are easily incorporated. We showed already in this paper how the method can be used to deal with any choice of boson space. Another extension concerns the introduction of higher-order terms in the boson hamiltonian, which can be obtained via a mapping of states containing more than two bosons. Such terms, which effectively would correct for the Pauli effects, could improve significantly the agreement between the shell-model and IB(F)M results. Having shown in this paper that the democratic mapping method gives sensible results in a simple test case, we believe it can now be used to study those more complex situations.

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