SYMPLECTIC SHELL-MODEL CALCULATION FOR $^{25}$Mg

G. ROSENSTEEL

Department of Physics and Quantum Theory Group, Tulane University, New Orleans, Louisiana 70118, USA

and

J.P. DRAAYER and K.J. WEEKS

Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA

Received 19 September 1983
(Revised 7 November 1983)

Abstract: The symplectic shell model, which incorporates major shell-configuration mixing as required by the nuclear quadrupole degree of freedom, is applied to $^{25}$Mg. The model interaction is a sum of six terms, two built from generators of the symplectic algebra, and four from generators of the embedded Elliott SU(3) subalgebra. By adjusting the six parameters of the interaction, both the calculated spectrum and the absolute E2 transition rates for the ground and $\gamma$-bands are found to be in good agreement with experiment. In particular, the $\gamma$-band is properly positioned and the interband rates are adequately reproduced. No effective charge is employed.

1. Introduction

The symplectic shell model is a fully microscopic generalization of the Bohr-Mottelson collective model which is compatible with the harmonic oscillator shell model. It is an extension of the conventional oscillator shell model that incorporates core excitations into the model space as dictated by the quadrupole degrees of freedom of the geometrical Bohr-Mottelson model. As a consequence, microscopic wave functions in the symplectic model space can give absolute E2 transition rates and static quadrupole moments in accord with their enhanced experimental values without employing an effective charge.

In this paper, the symplectic collective model is applied to $^{25}$Mg. For this nucleus, both a rotational ground band $(K^*=0^+)$ and a $\gamma$-band $(K^*=2^+)$ have been identified. Its ground band $(J=0, 2, 4, 6, 8)$ yields strong E2 transition rates in the 20 MeV excitation range with energy levels approximately obeying the rotational $I(I+1)$ rule. The $\gamma$-band $(J=2, 3, 4, 5, 6, 7)$ exhibits similarly enhanced E2 transitions while the interband rates are of single-particle magnitude.

Some of these features are explained rather straightforwardly in the Elliott SU(3) model. The leading SU(3) irreducible representations, $(\lambda, \mu) = (8, 4)$, contains a $K^*=0^+$ band with a cutoff at $J=8$ and a $K^*=2^+$ $\gamma$-band. Using an effective...
charge, the calculated intra-band transitions are in reasonable accord with experiment. However, the SU(3) model fails in two important respects. Firstly, it does not accurately reproduce the inter-band transitions. Secondly, although experiment shows there is a large gap (2.87 MeV) between the two low-lying $J^* = 2^+$ states, the simple SU(3) model predicts these states to be degenerate. In varying degrees, these same two difficulties emerge in realistic calculations in the sd shell, be they large shell-model diagonalizations [1] or projected Hartree-Fock solutions [3-5].

Using the symplectic collective model with an extended su(3) → so(3) effective interaction, we were able to correct these two problems. We found that the E2 transitions, including the interband rates, predicted by the symplectic model by and large track the available experimental data. These predicted absolute rates were calculated using microscopic wave functions, but no effective charge. Moreover, we also released the observed energy gap between the two states.

The plan of the article is to first define the model space and the interaction. Next, the results for $^{24}$Mg are surveyed. Finally, we discuss their ramifications.

2. Model space

The symplectic model space carries an irreducible representation of the symplectic Lie algebra sp(3, R), or sp(6, R) as it is sometimes denoted. This space is generated from a starting Elliott u(3) representation, at the 0th major oscillator shell, by successively acting on it with the mass quadrupole-monopole moment operators. This creates model states at oscillator excitation energies $n = 0, 2, 4, 6, \ldots, h\omega$, which we view as a vertical slice of collective states contained in the complete antisymmetrized many-nucleon Hilbert space. A most convenient labelling for the states of this slice is provided by the Elliott scheme.

The Elliott u(3) algebra is spanned by the operators

$$C_{ij} = \frac{1}{2} \left( \sigma^i \sigma^j + \delta_{ij} \right),$$

where i,j are cartesian indices, a range over the A particles, $c_{ij} = 2^{-1/4}(x_i + i y_i)$ is the harmonic oscillator boson, and the two-body $1/\Lambda$ term removes spurious c.c. excitations. The harmonic oscillator Hamiltonian is $H_0 = \sum \epsilon \sigma_i$.

The eigenspaces of $H_0$, the major oscillator shells, are viewed as horizontal layers of independent-particle states. In the Elliott scheme, each horizontal layer is subdivided further according to its permutation symmetry and, finally, into irreducible representation spaces of su(3). Each of these u(3) spaces also belongs to some vertical slice.

The starting point for a vertical slice is a u(3) space $[N_0, \lambda_{afe}]$, which is annihilated by the $2h\omega$ lowering operator of the symplectic Lie algebra,

$$B_0 = \frac{1}{2} \sum \epsilon \sigma^i \sigma^j = -\frac{1}{2A} \left( \sum \epsilon \sigma_i \right) \left( \sum \epsilon \sigma_j \right).$$
These special starting representations appear naturally in the shell model. For example, in the case of $^{28}$Mg, consider the horizontal layer belonging to the smallest possible oscillator eigenvalue $N, h_n = 62.5 h_n$. This layer is composed of state vectors with a closed $^{16}$O core plus eight nucleons distributed in the 2d10 shell. Since the 3s shell is filled completely, $B_6$ annihilates every vector in this layer. Hence, every $\text{v}(3)$ representation in this layer is a starting representation for a vertical slice.

A vertical slice is defined to be an irreducible representation space for the symplectic Lie algebra. Each slice is constructed from its unique starting $v(3)$ representation space by the successive application of the $2h_n$ raising operator of $\text{sp}(3, \mathbb{R})$.

$$A_h = \frac{1}{2} \sum_i c_i \frac{\partial}{\partial c_i} - \frac{1}{2A} \left( \sum_i c_i \right) \left( \sum_i c_i \right)^2.$$  

(3)

Note that $A_h$ is the adjoint of $B_6$.

In order to construct a basis for the slice which is symmetry-adapted to the Elliott scheme, we exploit the fact that the raising operator is a $(2, 0, 0)$ at(3) tensor operator. Then, the product of raising operators may be coupled to good total at(3) symmetry, $(n_1, n_2, n_3)$. However, since the $A_h$ commute among themselves, only totally symmetric couplings are non-zero. Thus, we are restricted to tensors for which $n_1, n_2, n_3$ are even, non-negative integers satisfying $n_1 \gg n_2 \gg n_3$ (ref. 18).

A complete infinite-dimensional basis for a slice is given by coupling symmetric products of raising operators to the starting representation.

$$[\{n_1, n_2, n_3\}], (3) \times \text{LM} = [\{A \otimes A \otimes \cdots \otimes A\}]^{m_1 n_2 n_3} \otimes [N, (\lambda \mu)],$$  

(4)

where $m$ is the multiplicity of $(\lambda \mu)$ in the at(3) tensor product $(n_1 - n_2 - n_3) \otimes (\lambda \mu)$ and $\lambda$ is the Vergados multiplicity label for the angular momentum $\text{LM}$ in the representation $(\lambda \mu)$ (ref. 27).

Finally, we couple these vectors to spin-isospin states whose permutation symmetry corresponds to the original starting $v(3)$ representation, thereby forming state vectors with good total angular momentum $J$ and isospin $T$. Note that a vector given by (4) belongs to the oscillator layer $[N, + (n_1 + n_2 + n_3)]h_n$.

The physical interpretation of the vertical slices depends upon the realization that a representation forms an invariant subspace for the algebra and group. Thus, the matrix elements of $\text{sp}(3, \mathbb{R})$ generate connecting different slices much vanish. But any Bohr-Mottelson geometrical collective operator is contained in the symplectic algebra via its subalgebras, the mass quadrupole collective algebra (27), the cm(3) algebra (27) and the at(3, R) algebra (27). For example, the mass quadrupole-monopole tensor

$$Q_J = \frac{1}{2} \left( x_i - X / x_i - X_i \right),$$  

(5a)

where $X_i = (1/A) \sum_{i=1}^{A} x_i$, is the c.m., is given by

$$Q_J = A_h + B_6 + \frac{1}{2}(C'_0 + C_0).$$  

(5b)
In our work on $^{24}\text{Mg}$, we have selected the vertical slice constructed from the "leading" starting representation. This is the $\text{su}(3)$ representation from the lowest layer, $N_0 = 62.5$, with the most symmetric spatial permutation symmetry consistent with the Pauli principle, $|J| = 44$, and which has the maximal possible $\text{su}(3)$ Casimir operator value, $(\lambda_{\mu_{\rho}}) = (8, 4)$. This leading $\text{su}(3)$ representation is identical to the Elliott choice $7^{13} 14$.

In the course of our numerical calculations, we discovered that we could safely truncate this infinite-dimensional slice and, nevertheless, obtained converged eigenstates. We included all $\text{su}(3)$ representations from the leading slice up to and including $\hbar\omega$ of excitation energy above the parent Elliott configuration. In addition, the stretched $\text{su}(3)$ representations at the $n\hbar\omega$ level, viz. $(\lambda_n = n, \mu_n)$, for $n = 8, 10, 12, 14, 16, 18$ and $20$ were included. The resulting total number of $\text{su}(3)$ representations in this model space is 88. The dimensions of the angular momentum subspaces for $J = 0, 1, 2, 3, 4, 5, 6, 7$ and 8 are 39, 124, 125, 192, 185, 219, 196, and 208.

3. Interaction

The model hamiltonian was taken to be the harmonic oscillator plus a quadrupole collective potential and an $\text{su}(3)$ residual interaction,

\[ H = \hbar \omega H_0 + V_{\text{col}} + V_{\text{res}}. \]  

Since these three terms are constructed from symplectic generators, the slices are invariant subspaces for $H$. Therefore, each exact eigenstate must lie completely in its own slice.

The collective quadrupole potential is, in general, a function of the Bohr-Mottelson shape parameters $\beta$ and $\gamma$. Any such function can be written in terms of the (dimensionless) quadratic and cubic rotational scalars in the microproscopic quadrupole moment $^{24}$-26$, which to their leading orders in the deformation $\beta$ are given by $^{27}$$
\begin{align*}
\alpha_1 &= (3/20\pi)A^2(R/h\omega)^2\beta^2, \\
\alpha_2 &= (1/20\pi)A^2(R/h\omega)^2\beta^2 \cos 3\gamma,
\end{align*}

where $R = 1.2 \times A^{1/3}$ fm is the nuclear radius and $h = (44/\hbar\omega)^{1/2}$ fm is the oscillator length.

In the present work, we have chosen a particularly simple form for the collective potential which is $\gamma$-independent,

\[ V_{\text{col}} = h\alpha_1 + h_\beta(a_2)^2. \]  

In order for $V_{\text{col}}$ to define a potential well, we require $h_\beta$ to be negative and $h_\alpha$ positive.

The collective potential mixes states from different major shells. It is directly responsible for bringing in the coherent admixtures of states which together form
nuclear wave functions with the requisite deformation. Indeed, \( a_2 = \frac{1}{2} Q^{(2)} - Q^{(3)} \) has non-zero matrix elements connecting states differing by 0, 2 and 4 oscillator quanta.

Lastly, we need to incorporate into \( H \) non-collective aspects of the nuclear force via the residual interaction. But these forces, primarily pairing and spin-orbit terms, act across horizontal layers and, consequently, break symplectic symmetry. In previous work on \(^{208}\text{Pb}\), we accounted for this by expanding the model space to encompass a large number of \( su(3) \) representations at the 0th horizontal layer\(^{27}\).

However, in the present work on \(^{26}\text{Mg}\), we have opted for the restriction to a single \( su(3) \) representation space at the 0th layer at the expense of the need for an effective interaction for \( V_{\text{res}} \). This alternate solution was shown to be successful for rare-earth nuclei in the pseudo-\( su(3) \) scheme by two of the authors\(^{28}\).

The effective residual interaction must be a rotationally invariant function of the \( su(3) \) generators. Every such function can be expressed in terms of the \( su(3) = su(2) \) \( \times \) \( sl(2) \) integrality basis. Judd et al.\(^{29}\) have proved that there are five independent rotational scalars in this integrality basis. These are the second and third order Casimir invariants of \( sl(3) \), which are just constants within an \( su(3) \) representation, the square of the angular momentum \( L^2 \), which is independent of \( \lambda \) but produces an \( L(L+1) \) splitting, and two scalars \( X_5 = L^5 \langle C^5 \rangle \) and \( X_6 = L^6 \langle C^6 \rangle \) which have both an \( L \)- and \( \lambda \)-dependence. We furthermore restricted \( V_{\text{res}} \) to be a polynomial function of degree four in the integrality basis. Thus, we chose the following form for the residual interaction:

\[
V_{\text{res}} = \kappa_5 X_5 + \kappa_6 X_6 + \gamma_5 Y^5 + \gamma_6 Y^6 .
\]  

(9)

4. Results for \(^{26}\text{Mg}\)

The phenomenological hamiltonian was diagonalized in the model space of the leading vertical slice. The two parameters of the collective quadrupole potential and the four parameters of the residual \( su(3) \) effective interaction were adjusted in order to produce a good fit to both the energy spectrum (10 observed collective levels) and the \( B(E2) \) rates (17 experimental transitions). We fixed \( \hbar \omega = (45/\hbar^2 c^2) = 12.6 \text{ MeV} \).

Although there is an interdependence, each of the interaction terms has an important primary role to play. \( X_5 = L^5 \langle C^5 \rangle \) together with \( X_6 = L^6 \langle C^6 \rangle \) with the two low-lying \( 2^+ \) states is the degree required by experiment and, hence, properly positions the \( \gamma \)-band. \( L^2 \) and \( L^3 \) allow us to reproduce the spectrum of the ground band. Varying \( X_5 = L^5 \langle C^5 \rangle \) also adjusts the moment of inertia of the \( \gamma \)-band. Finally, \( \gamma_5 \) and \( \gamma_6 \) are necessary to obtain the requisite deformation for the absolute \( B(E2) \) rates. After searching for an overall good fit to the data, we found, \( \beta_2 = -0.2, \lambda_0 = 0.00072, \kappa_5 = 0.0071, \kappa_6 = -0.00145, \gamma_5 = 0.194, \gamma_6 = -0.000465 \).
In fig. 1, the resulting symplectic eigenvalues are compared with experiment. The salient feature is the correct location of the $\gamma$-band in our model. A variety of other microscopic models have failed to reproduce this attribute of the spectrum $^{35-37}$. However, the decisive test of the efficacy of the symplectic model is its capacity for predicting absolute $B(E2)$ rates in accord with experiment. In the sp(3, R) model, these rates are computed using the microscopic quadrupole tensor and microscopic wave functions. No effective charge is employed in the symplectic collective model. In table 1, all available experimental E2 transition rates are compared with their theoretical values in the sp(3, R) model as well as with several other models cited in ref. 14. Clearly, the overall sp(3, R) results are excellent. Although projected Hartree–Fock calculations $^{35-37}$ and shell-model diagonalizations in an su(3) basis $^{38}$...
do a good job with the collective intraband rates, only the symplectic model also tracks the interband transitions with an accuracy comparable to that found for the intraband rates.

Another significant test of the symplectic model wave functions is given by their static quadrupole moments. Experimentally, the static moment of the $\text{Er}^2^+$ state is $-0.178 \pm 0.013 \text{ e } b$ (ref. 25). In our work, we found a moment of $-0.184 \text{ e } b$.

Considerable insight into the physical nature of the symplectic eigenfunctions is provided by exploring their relationship with the rotational model. In the rotational model, the static quadrupole moment in the intrinsic frame $Q_6^0$ is a constant for each $K$-band state, it is related to the static moment in the lab frame by

$$Q_6^0 = \frac{3K^2 - I(I+1)}{(J+1)(2J+3)} Q_6^e. \tag{10}$$

For the symplectic eigenfunctions, we have computed the expectations $\langle Q_6^0 \rangle$ and inferred from (10) the corresponding intrinsic moments. In fig. 2, the calculated intrinsic moment is plotted versus the total angular momentum. Since $Q_6^e$ is not
constant throughout a band, the rotational model is not applicable. Indeed the intrinsic moment of the symplectic eigenstates decreases linearly as the square of the total angular momentum in the ground band and fluctuates about 0.65 \( \epsilon \cdot b \) in the \( \gamma \)-band.

The deformation \( \beta \) of a state is determined in a model-independent way from the expectation of \( a_{1} = \frac{1}{4} Q^{21} - Q^{22} \) via (7). In fig. 3, we see that the deformation of both bands decreases linearly with the square of the total angular momentum. Of course, if the rotational model were relevant, \( \beta \) would be constant for each band. This linear behavior would be expected had the space been truncated severely.

Fig. 3. The dimensionless deformation parameter \( \beta \) is plotted versus the total angular momentum.
to the 00s shell, since \( a_s \) is given then by the difference of the \( u^2 \) Casimir invariant and \( \mathcal{L} \). However, the contribution of the 00s space to \( \mathcal{L} \) in our multishell-model space accounts only for about 25\% of its expectation. The raising of this expectation up to its experimentally observed enhanced value is due to the coherent superposition of core-excited basis wave functions.

But, since the rotational model is evidently not applicable, can we even sensibly talk about an intrinsic deformation? The answer to this depends upon whether or not the fluctuations in \( \beta \) are small, i.e. is \( \Delta \beta = \frac{1}{2} \left( \langle a_s^2 \rangle - \langle a_s \rangle^2 \right)^{1/2} \) small compared to \( \langle a_s \rangle \), or, using (7), is \( \Delta \beta \) small compared to \( \beta \)? For the states of both bands, the fluctuation was determined to be approximately the same \( \Delta \beta = 0.2 \). Hence, the concept of an intrinsic nuclear shape for the symplectic eigenstates is blurred by the fluctuations, but not obliterated.

The axial symmetry \( \gamma \) of the intrinsic state is measured by the expectation of the cubic quadrupole invariant \( a_s \) using (7). We found that \( \gamma \) increases with angular momentum from 15\% for the ground state to 19\% at the top of both bands. This is similar to that required in an axisymmetric rotor calculation (9).

The \( K \) quantum number was found to be good in our symplectic calculations. From (10), the rotational model predicts that the \( K^* = 2^-, J = 3 \) state has a vanishing static quadrupole moment. In the spr(3, R) model, the moment of the state is very small, \(-0.001 \). Inspection of the wave functions of the ground band in table 2 shows that the Vargason quantum number \( \kappa \) is excellent.

Another obvious approximate symmetry evident from table 2 is the stretched or spr(1, R) symmetry (11). At each \( \ell \)-shell layer, the stretched state \( (\ell + \kappa, \mu) \) dominates the wave function. Unfortunately, the spr(2, R) scheme (3) was not found to select the next most important spr(3) representations after spr(3, R).

A striking characteristic of the symplectic model is the competition between the kinetic and potential energies. In the pure rotational model, excitation energies are entirely kinetic. The observed \( LL + 1 \) spectrum is explained as the rotation of the nucleus with some intrinsic inertia tensor. On the other hand, energies in either a conventional Hartree-Fock or shell-model calculation have kinetic contribution, since the kinetic energy is a constant within a major oscillator shell. Here the \( LL + 1 \) spectrum emerges as a consequence of the is-shell quadrupole-quadrupole potential which is a sum of the \( u^2 \) Casimir invariant and \( L^2 \). However, in the spr(3, R) model as is evident from fig. 4, both the kinetic energy and the potential energy are comparable. Note that the exact kinetic energy operator is in the symplectic algebra.

5. Discussion

The addition of major shell symplectic configurations to the sd-shell-model space has enabled us to achieve a good fit to the absolute E2 transition rates in \( ^{25}\text{Mg} \) without using an effective charge. These rates are a sensitive probe of the nuclear
<table>
<thead>
<tr>
<th>$\pi$ (k, $\mu$)</th>
<th>$n$</th>
<th>0°</th>
<th>2°</th>
<th>4°</th>
<th>6°</th>
<th>8°</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 (18, 4)</td>
<td>1</td>
<td>0.677</td>
<td>0.654</td>
<td>0.780</td>
<td>0.716</td>
<td>0.710</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.003</td>
<td>0.013</td>
<td>0.034</td>
<td>0.028</td>
<td>0.027</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>0.002</td>
<td>0.012</td>
<td>0.033</td>
<td>0.028</td>
<td>0.027</td>
</tr>
<tr>
<td>2 (10, 4)</td>
<td>1</td>
<td>0.203</td>
<td>0.199</td>
<td>0.187</td>
<td>0.167</td>
<td>0.137</td>
</tr>
<tr>
<td>(5, 5)</td>
<td></td>
<td>0.001</td>
<td>0.003</td>
<td>0.007</td>
<td>0.041</td>
<td>0.091</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.001</td>
<td>0.002</td>
<td>0.003</td>
<td>0.004</td>
<td>0.004</td>
</tr>
<tr>
<td>(6, 6)</td>
<td>1</td>
<td>0.025</td>
<td>0.024</td>
<td>0.018</td>
<td>0.013</td>
<td>0.009</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.016</td>
<td>0.015</td>
<td>0.013</td>
<td>0.011</td>
<td>0.009</td>
</tr>
<tr>
<td>4 (13, 4)</td>
<td>1</td>
<td>0.016</td>
<td>0.007</td>
<td>0.015</td>
<td>0.013</td>
<td>0.012</td>
</tr>
<tr>
<td>(10, 5)</td>
<td></td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>(6, 6)</td>
<td>1</td>
<td>0.005</td>
<td>0.003</td>
<td>0.002</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>0.004</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
<td>0.001</td>
</tr>
</tbody>
</table>

* Amplitudes contributing less than 0.5% in the wave functions are omitted. The amplitudes of multiply occurring $u(3)$ irreducible representations have been summed over.
be desirable to discover a suitable subgroup classification, because of its technical simplicity and its potential for elucidating the physics.

In this paper, the parameters of the interaction have been adjusted in order to produce a good overall fit to the available experimental data. In order to achieve the requisite deformation and position the γ-band correctly, we found it necessary to include three- and four-body components in the model interaction. This does not necessarily imply the importance or even the existence of three- and four-body interactions in nuclei. It does show that the effective interaction appropriate to the symplectic model space requires such terms.

The successful positioning of the γ-band is due to the $X_1$ and $X_2$ terms in the $su(3)$ residual interaction [23]. In future work, we intend to investigate the relationship between two-body interactions in the full sd shell and these three- and four-body terms required for the effective interaction in a single $su(3)$ model space.

If the collective potential only contained the two-body term $a_2 \times \beta^2$, then there would be an infinitely deep potential well for large $\beta$. The four-body operator $(a_2)^2 \times \beta^4$ is necessary to restore stability to the collective potential. However, we have shown previously that the correlation of $(a_2)^2$ with its two-body projection in the symplectic algebra is 98% for $^{24}$Mg [ref. [23]]. Hence, we could replace $(a_2)^2$
with its two-body approximation and achieve the same result. Nevertheless, we prefer to use $\mu^2$ and maintain a clear connection with the geometrical model.

The US National Science Foundation has supported this investigation.

References

5) V.S. Vedelov, Nucl. Sci. 32 (1986) 957
13) D. Strottman, Phys. Lett. 39B (1972) 457
   A. Bohr, B. Mottelson and J. Andersen, Rev. Mod. Phys. 48 (1976) 365, and references therein
22) G. Rosenthal and D.I. Rowe, Ann. of Phys. 94 (1975) 1;
   G. Rosenthal and E. Itzig, Ann. of Phys. 121 (1979) 113;
24) J.M. Eisenberg and W. Greiner, Nuclear models (North-Holland, Amsterdam, 1975), p. 45
25) D. Chae and C. Haen, Pro. Intern. Conf. on nuclear structure studies using electron scattering
   and photo-connections (Sevres, 1972) ed. K. Shoda and P. Uss, Supplement to Research Report
   of the Laboratory of Nuclear Science, Tsukuba University, ed. 5 (1972), p. 51