SHELL MODEL DESCRIPTION

of the

COLLECTIVE MODEL POTENTIAL

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ABSTRACT

The purpose of this paper is to give a shell model interpretation of the collective model potential energy surface. This will be done in three steps: First, a mapping between the shape variables \( (\delta, \gamma) \) of the collective model and the irreducible representation labels \( (\lambda, \mu) \) of the SU(3) shell model is given. Secondly, a pseudo symplectic scheme for heavy deformed nuclei, an extension of the SU(3) model that includes major shell mixing as generated by the quadrupole-quadrupole interaction, is introduced. And third, a correspondence between the expectation value of a simple shell model hamiltonian and the collective model potential energy surface is established. The results suggest that the sharp rise in the collective model potential energy surface for deformations greater than the equilibrium value is a shell feature that can be duplicated with a two-body interaction. The exclusion principle plays an essential role in the argument.

1. Mapping: \( (\delta, \gamma) \to (\lambda, \mu) \)

A relation between \( (\delta, \gamma) \) and \( (\lambda, \mu) \) can be established by requiring the invariants of SU(3) and the triaxial quantum rotor to map onto one another. Before doing this, however, the fact that these two theories yield similar results for observables needs to be established.

First consider the triaxial quantum rotor hamiltonian,

\[
H_{\text{ROT}} = A_{12}^2 + A_{23}^2 + A_{31}^2 . \tag{1}
\]

Here \( \ell \) is the projection of the total angular momentum on the \( \omega \)-th body-fixed symmetry axis and \( A_{ \omega } \) is the corresponding inertia parameter. This hamiltonian can be rewritten in a frame independent form by introducing three special rotational scalars:
\[ L^2 = L_a^2 + L_b^2 + L_c^2, \]  
(2a)  
\[ X_3 = L_{aab}^3 + L_{bab}^3 + \lambda_1 \lambda_2 \lambda_3, \]  
(2b)  
\[ X_4 = L_{aab}^4 + L_{bab}^4 + \lambda_1 \lambda_2 \lambda_3 \lambda_4, \]  
(2c)

where \( L_a \) and \( Q_c \) are cartesian forms for the angular momentum and collective mass quadrupole operators, respectively. The last expression given on the right in (2) is the form these operators take in the body-fixed, principal-axis system: \( Q_{ab}^c = < Q_{ab}^c > \). In making this substitution we have assumed that the eigenvalues of \( Q_c \) are sharp.

Equations (2) can be solved for \( L_a \) in terms of \( L_c \) and \( X_3 \).

Specifically, if \( D_a = 2 \alpha_a^3 + \lambda_1 \lambda_2 \lambda_3 \), then

\[ L_a^2 = (\lambda_1 \lambda_2 \lambda_3) L_c^2 + (\lambda_2) X_3 + (\lambda_3) X_4 D_a. \]  
(3)

Substituting this result into (1) yields a new form for the rotor hamiltonian,

\[ H_{ROT} = \alpha L^2 + b X_3 + c X_4, \]  
(4)

where the parameters \( a, b \) and \( c \) depend on the inertia parameters and the eigenvalues of \( Q_c \),

\[ a = \frac{\lambda_1 \lambda_2 \lambda_3}{D_a}, \]  
\[ b = \frac{\lambda_2}{D_a}, \]  
\[ c = \frac{\lambda_3}{D_a}. \]  
(5a, 5b, 5c)

It is important to emphasize that these two forms for the rotor hamiltonian, (1) and (4), yield the same results.

Now consider the corresponding SU(3) hamiltonian,

\[ H_{SU3} = \alpha L^2 + b X_3 + c X_4. \]  
(6)

Here the operators \( X_3^a \) and \( X_4^a \) are given by (2) but with \( Q_c \) replaced by \( Q^a \), the algebraic mass quadrupole operator. The operator \( Q^a \) differs from \( Q_c \) by being symmetrized in the coordinate and momentum variables so its matrix elements vanish between states belonging to different major shells of the oscillator while at the same time reproducing all matrix elements of \( Q_c \) within a shell. The operators \( L \) and \( Q^a \) generate SU(3) which is a compact group with finite dimensional representations while \( L \) and \( Q_c \) are generators of the semidirect product \( T \times SO(3) \) which has infinite dimensional representations. In Figure 1 the eigenvalue spectrum of \( H_{SU3} \) is compared with that of \( H_{ROT} \) for rotor parameters that give a best fit to members of the ground and lowest K=2 band in \(^{168}\text{Er} \).

The parameters of \( H_{SU3} \) were taken directly from \( H_{ROT} \), no adjustments or rescaling was done. Results are for the leading pseudo SU(3) representation of \(^{168}\text{Er} \), \( (\lambda, \nu) = (30, 8) \). Numerous other results, including comparisons for electromagnetic transitions, confirm that \( H_{SU3} \) is the shell model image of \( H_{ROT} \).

Having established this equivalence, we can now legitimately invoke a correspondence between invariant measures of the two theories. The logic behind this requirement, using a classical mechanics analogy, is very simple: constants of the motion of two theories used to describe the same physical phenomena should agree. The invariants of the rotor are traces of the square and the cube of the quadrupole matrix. The expectation values of these invariant operators are given by

\[ \lambda_1 = (\mu-1)/3, \]  
\[ \lambda_2 = (\mu+2)/3, \]  
\[ \lambda_3 = (2\mu+3)/3. \]
\[
<\text{tr}[(Q^2)^2]> = \frac{3}{2} k^2 a^2 , \\
<\text{tr}[(Q^3)^2]> = \frac{1}{4} k^3 a^3 \cos(3\nu) , 
\]
where \( k = \sqrt{\frac{A}{r^2}} \) with \( A \) the number of nucleons and \( r^2 \) the dimensionless root-mean-square radius. The expectation value of the second and third order invariants of SU(3) are given in terms of \( \lambda \) and \( \nu \) by
\[
C_2 = \frac{2}{3} (\nu^2 + \lambda^2 + 2\lambda^2 + 3\nu + 3\lambda) , \\
C_3 = \frac{1}{9} (\lambda^2 - \nu^2)(2\lambda^2 + 3\lambda + 3\nu + 3) .
\]
There is a preferred linear mapping between these two sets that lets the shell model picture duplicate the collective model geometry,
\[
\gamma = \tan\left[\frac{\pi}{2} (\nu+1)\right] ,
\]
or in Cartesian form,
\[
ka = k_0 \cos(\gamma) = (2\lambda + \nu + 3)/3 , \\
ka = k_0 \sin(\gamma) = (\nu+1)/\sqrt{3} .
\]
These results show that each \((\lambda,\nu)\) corresponds to a unique value for the pair \((a,\gamma)\). Since \(a\) and \(\gamma\) are SU(3) irrep labels, they can only be non-negative integers. This interpretation is contrary to a liquid drop picture where \(a\) and \(\gamma\) are taken to be continuous variables. The constraint derives from the fact that nucleons are made up of fermions that obey the Pauli Principle.

2. Pseudo Symplectic Model

For nuclei with \( A \geq 40 \) the single particle spin-orbit interaction scrambles levels of the oscillator and destroys the simple SU(3) picture. Also, the neutron excess grows with \( A \) so for heavy deformed nuclei the valence protons and neutrons occupy different shells. This situation, which at first appears to be an extremely unhappy one, upon closer scrutiny is really not so bad because another symmetry emerges that is even better than the one that applies for light nuclei: the pseudo SU(3) scheme. When this new realization of SU(3) is extended to include major shell mixing as generated by the quadrupole operator, one obtains the pseudo symplectic model.

The logic of the pseudo SU(3) scheme can best be understood pictorially. In Figure 2, the effect of spin-orbit splitting on single particles levels of the spherical shell model is shown in schematic form. Levels grouped together on the left form shells of the normal oscillator while those grouped together on the right are shells of a pseudo oscillator. Specifically, the highest \( J \) state of each normal oscillator shell is associated with the shell immediately below it. The \( J \) values of the states that remain, when grouped together, are the same as the \( J \) values of a oscillator shell of one less quanta. Of course, the \( \lambda \) values are different but since \( \lambda \) and \( s \) are not good quantum numbers they can be realized differently, and, in particular, in terms of pseudo \( \lambda \) and \( s \) labels of a new pseudo SU(3) scheme:
1. Decoupling parameters
2. Alpha particle transfer strengths
3. Backbending ($^{138}$Ba)
4. Forking ($^{48}$Ge)
5. Strong coupling limit and $Q_sQ_v$
6. Unique parity spin sequences
7. Collective modes: $E2$ & $M1$, $M3$

The earliest (latest) of these carries a 1973 (1987) publication date. Though conceptually simple, applications of the scheme are challenging because SU(3) rather than SU(2) is the basic symmetry and the shell model technology for it is nontrivial.

The pseudo symplectic model is nothing more than the pseudo SU(3) scheme extended by including those major shell admixed configuration at $2n\hbar\omega$ ($n=1,2,\ldots$) that couple strongly to low-lying $O\hbar\omega$ configurations through the collective quadrupole-quadrupole interaction. It is a natural extension of the symplectic model, also known as the microscopic collective model, to heavy deformed nuclei. The purpose of the symplectic enhancement is to generate more realistic eigenstates, ones that reproduce, for example, $E2$ transition strengths without the necessity of introducing an effective charge.

To illustrate the importance of quadrupole mixing we applied a simplified version of the model to an analysis of the $d$-shell nuclei $^{20,22,24}$Ne and $^{23,24}$Mg. The simplifying assumption involves replacing the six ($t=0$ & $=2$) $2\hbar\omega$ raising (lowering) operators of $Sp(6,R)$ by $S$ and $D$ boson creation (annihilation) operator with the same tensor properties.\(^7\) Formally this corresponds to a contraction of $Sp(6,R)$. The resultant symmetry algebra is $U_q(6) \times U_F(3)$ where "h" denotes the boson algebra and "F" the $O\hbar\omega$ shell model group which has fermion statistics. The physics of this approximation is simple: shells above (below) the valence one are nearly empty (full) so the action of boson creation (annihilation) operators with the same tensorial properties as their fermion counterparts will, for all practical purposes, be the same. In other words, Pauli blocking plays an insignificant role in couplings to configurations of the $\pm 2\hbar\omega$ shells.
In Figure 3, a comparison of calculated and experimental E2 transition strengths in $^{20}$Ne is shown. The results are for a calculation which included $\pi n \pi \nu$ configurations with $n=1,2,\ldots,6$ built on the $(\lambda,\nu) = (8,0)$ representation of the $\Omega \pi \nu$ space. The Hamiltonian that was used is simply

$$H = H_0 - \frac{1}{2} \alpha \vec{Q} \cdot \vec{Q} + a L^2 + b \lambda^2 + c \lambda^4$$

(14)

where $H_0$ is the oscillator with $\Omega = 13.2$ MeV and $\alpha = 0.058$ MeV. In the case of $^{20}$Ne the parameters $a$, $b$, and $c$ are not uniquely determined because there is no $\pi \pi \pi$ band. Note that while the calculation reproduces the data, even to the falling off of strength observed in the $J^\pi = 0^+ - 6^+$ transition, artificially increasing $\Omega$ destroys this agreement. The result labelled “INFINITE” is equivalent to a $\Omega \pi \nu$ calculation. No effective charge was used. Whereas it may appear from the results that an effective charge can be used to duplicate the effect of the major shell admixture, this is not the case because the structure of the calculated eigenstates change significantly.

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Figure 4. Experimental and calculated $[\nu_\beta(6) \times \nu_\alpha(3)]$ spectra for $^{24}$Mg. Parameters of the Hamiltonian are $\Omega = 12.6$ and $\alpha = 0.0438$ for the shell and quadrupole-quadrupole terms, respectively, and $a = 0.130$, $b = -0.0408$, and $c = -0.00521$ for the residual SU(3) parts. All quantities are given in MeV.

Figure 5. Intensity profile in the $\Omega \pi \nu$ ($N_\pi=0$), $2 \Omega \pi \omega$ ($N_\pi=1$), $4 \Omega \pi \nu$ ($N_\nu=2$) and higher levels for members of the ground band of $^{24}$Mg.
of the resultant $V$ as a function of $a$ and $\gamma$ is the PES of the GGM.

Terms in $V$ of order 4 (6) or greater in $a$ are required to obtain a nonzero equilibrium $\rho_0 (r_0)$ deformation value. Furthermore, it is clear that if $V_{03}$ enters with a negative sign there must be a positive $V_{02}$ or $V_{01}$ to balance it so the potential does not go to negative infinity for large $a$, etc. In other words, all the familiar problems encountered whenever polynomial expansions are used, enter in the theory. One purpose of this discussion is to point out that these high-order terms are necessary because the GGM does not address the particle dynamics properly. Specifically, it ignores the elementary but important fact that nucleic are made up of fermions that obey the exclusion principle. Another complementary purpose is to show that stable nonzero equilibrium values for the deformation arise naturally within the framework of the shell model with no more than two-body interactions.

Now reconsider the $^{24}$Mg calculation. The $O_{hw}$ SU(3) representations are (1s)$^2$(1p)$^{12}$ (2s1d)$^8$ particle configurations. They are determined by a U(6) - SU(3) group plethysm. For example, the most symmetric spatial symmetry (1f) = [444444] contains the following SU(3) irreps with $L = 0$ states: $(1,1) = (8,4), (4,6), (0,8), (6,2)^2, (2,4)^2, (4,0)^2$ and (0,2) where the superscript labels multiplicity. Of all the allowed irreps, including those in less symmetric spatial symmetries, the (8,4) yields the maximum value for $a$ and for this SU(3) irrep $\gamma = 20.6^o$, see (9).

The expectation value of $H$ for $^{24}$Mg between basis states of the $U_0 (6) \times U_3 (3)$ model are plotted as a function of $a$ in Figure 6. The solid curve traces out the locus of minimum expectation values in the $O_{hw}$ space for $a < a_0$ and connects leading irreps of the $2\Omega_w, 4\Omega_w, \ldots$, spaces in the products $(2,0)^n \times (8,4)$ for $a > a_0$. The $\gamma$ values range from 46.1° for the (0,2) irrep, to 20.6° for the (8,4), and 15.6° for the (12,4). A point to be noted is that the slow rise to the left of the minimum ($a < a_0$) is a $O_{hw}$ phenomena while the sharp rise beyond the minimum ($a > a_0$) is primarily due to the shell structure. SU(3) irreps with $a > a_0$ only exist in higher shells. If $x$ is set to zero, all irreps of the n-th shell would lie at $n\Omega_w$. The actual position of the irreps is lower than this because $Q^2 - Q^2$ increases the binding energy.
of the system. The strength of $Q^2:Q^2$ must be large enough to build in the required coherence yet small enough so the shell structure established by $H_0$ is not destroyed. Note that the matrix elements of $L^2$, $x^a_3$ and $x^a_4$ are all zero in $J=N^2$ states so the shape of the potential is determined solely by the allowed representations of $SU(3)$ and the parameters $\mu_\omega$ and $\gamma$. A trivial divergence can be overcome by removing the major-shell, trace-equivalent part of $Q^2:Q^2$. This was done in the calculation.

A general microscopic (shell model) interpretation of the macroscopic (collective model) PES concept can now be given. A schematic plot of the expectation value of the hamiltonian, $\langle H \rangle$, versus the deformation, $\gamma$, that indicates how things go is given in Figure 7. In each major shell the allowed $SU(3)$ representations fall into a conical band with terminus defined by the leading $SU(3)$ irrep, that is, the $(\lambda_1,\lambda_2)$ for which $\gamma$ as given by (4) is a maximum. The PES corresponds to the envelope that is defined for $\gamma < \gamma_0$ by the irreps of the $D\omega_\omega$ shell that lie lowest in energy and for $\gamma > \gamma_0$ by leading $SU(3)$ irreps of the higher shells. Of course, $SU(3)$ is not an exact symmetry so $(\lambda_1,\lambda_2)$ mixing occurs both within and among the shells. This mixing blurs the boundaries but so long as $SU(3)$ is a reasonably good symmetry the argument applies. Regions below and to the left (right) of the enveloping curve for $\gamma < \gamma_0$ ($\gamma > \gamma_0$) are forbidden domains due to the Pauli Principle. The equilibrium value for the deformation, $\gamma_0$, is determined by a complicated convolution of intrashell and intershell dynamics.

In conclusion, the results show that the sharp rise in the PES for $\gamma > \gamma_0$ is a shell model feature that can be reproduced with a simple two-body interaction. The GGM requires high-order terms in the potential
to get stable nonzero equilibrium deformation values because there is no other mechanism for building the exclusion principle into the theory. The importance of the shell admixtures in low-lying eigenstates is signaled by enhanced $E2$ transition strengths. Typically, in low-lying eigenstates the summed intensities of shell admixed configurations is between 30% and 40%. This percentage is much too large to be ignored in any realistic microscopic theory of nuclear structure.

References


6. In addition to 3 and 5 above, see:
   
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