AN EXACT DIAGONALIZATION OF THE QUADRUPOLE AND PAIRING FORCES IN THE NUCLEAR d-s SHELL

by

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Abstract: The pairing plus quadrupole interaction have been diagonalized for four identical particles in the \( N = 2 \) shell of the harmonic oscillator. The states of the basic representation are classified according to the \( SU3 \) coupling scheme. The energy levels and wave functions are calculated for different values of the relative intensity of the two forces. The results are compared with the predictions of the vibrational and asymmetric rotor models.

1. INTRODUCTION

Many properties of nuclei at low energies can be explained with a model which considers the particles out of closed shell as moving independently in a single-particle potential and interacting through an effective residual force.

The residual interaction considered in this paper has been proposed by Bohr and Mottelson (1, 2, 3, 4). It has a long range component (quadrupole interaction) which produces the level scheme corresponding to ellipsoidal deformations, and a short range one (pairing interaction) which gives rise to the “seniority” scheme.

There are different approximations used in order to deal with this Hamiltonian. The more usual of them are:

a) The quasi-particle formalism which approximately diagonalizes the pairing interaction.

b) The quasi-boson method. It is used in order to treat the effects of the quadrupole force which has not been incorporated into the single particle field.
c) The deformation of the central field, which is produced by the long range component and which gives rise to collective degrees of freedom. The corresponding parameters are calculated through the "cranking model".

Although these approximations are very useful, it seems convenient to perform an exact calculation in order to obtain a more detailed insight on the effects of the residual forces and corresponding collective level schemes. This is done in the present paper. We have solved the Hamiltonian for the case of four identical particles in the $N = 2$ shell of the harmonic oscillator.

Pairing and quadrupole forces have different symmetries. The first is invariant with respect to the symplectic group and the second one is the Casimir operator of the $SU_3$ group.

We use the $SU_3$ coupling scheme because the pairing force has simpler matrix elements than the quadrupole force.

In order to classify the states of an harmonic oscillator shell, Elliott (6) introduces the chain of subgroups

$$SU_s \supset SU_3 \supset R_3 \supset R_2$$

where $s$ is the shell degeneracy.

Corresponding to the $SU_3$, $R_3$ and $R_2$ representations, the states are labelled by the pair of numbers $(\lambda \mu)$, the angular momentum $L$ and its projection $M$, respectively.

Weyl's theorem states that if we label the states according to irreducible representations of $SU_s$ we are labelling at the same time according to the representations of the symmetric group $\Pi_n$ ($n =$ number of particles). This is done through the partitions $[f]$.

The wave functions must be totally antisymmetric: this fact determines the relation between the permutation symmetries of the spatial and the spin wave components. Therefore, once $S$ is fixed, we know which irreducible representations of $\Pi_n$ are possible.

We are interested then in the possible values of $\lambda$ and $\mu$ which are compatible with a given $[f]$, and in $L$ values which are compatible with each $(\lambda \mu)$. Elliott has obtained these values of $(\lambda \mu)$ for the $N = 2$ shell and most of the $N = 3$ shell.

The representations of $R_3$, which occur in the representation $(\lambda \mu)$ of $SU_3$ are given by:

$$L = K, K + 1, K + 2, \quad K + \max (\lambda \mu) \quad (1a)$$
where the integer $K$ is

$$K = \min(\lambda \mu) - 2, \ldots, 1 \text{ or } 0$$  \hspace{1cm} (1b)$$

except when $K = 0$ in which case

$$L = \max(\lambda \mu), \max(\lambda \mu) - 2, \ldots, 1 \text{ or } 0$$  \hspace{1cm} (1c)$$

The structure of the Casimir operator of the $SU3$ group is

$$\hat{G}(\lambda \mu) = \frac{3}{4} \hat{Q} \cdot \hat{Q} + \frac{1}{4} \hat{L} \cdot \hat{L}$$  \hspace{1cm} (2)$$

with eigenvalues

$$g(\lambda \mu) = (\lambda^2 + \mu^2 + \lambda \mu) + 3(\lambda + \mu)$$  \hspace{1cm} (2a)$$

From here we obtain an expression of the quadrupole interaction

$$\hat{Q} \cdot \hat{Q} = 4 \hat{G}(\lambda \mu) - 3 \hat{L} \cdot \hat{L}$$

with eigenfunctions having definite values of $(\lambda \mu)$ and $L$.

2. CALCULATIONS

We have constructed the wave functions of four identical particles, which have total spin $S = 0$, using the Hill-Wheeler projection integrals

$$\Psi((\lambda \mu) L M K) = \frac{2L + 1}{c((\lambda \mu) L, K)} \int D^{\mu \kappa} (\Omega) \mathcal{L}_\Omega((\lambda \mu)) d\Omega$$  \hspace{1cm} (3)$$

where $\mathcal{L}_\Omega$ is the intrinsic wave function referred to a rotated frame and $c((\lambda \mu) L, K)$ is a normalization factor.

For the present case the $SU3 \supset R3$ chain is not sufficient to give a complete classification of the states and we cannot use fractional parentage coefficient techniques. In order to perform a complete classification, the parameter $K$ is introduced by (3). This parameter $K$ is an approximately good quantum number and can be interpreted as the projection of the angular momentum on the $z$-axis of the rotated frame.
The complete set of wave functions is given in table 1. The intrinsic wave function introduced in (3) must satisfy the system of equations

\[ A_{xy} \chi = A_{yx} \chi = A_{zy} \chi = 0 \]
\[ (A_{zz} - A_{yy}) \chi = \mu \chi \]
\[ (2A_{zz} - A_{xx} - A_{yy}) \chi = (2 \lambda + \mu) \chi \]

where

\[ A_{ij} = \frac{1}{\sqrt{2}} (a_i + a_j + a_i^+ a_j) \]

and the operator \( a_i^+ = \frac{1}{\sqrt{2}} (x_i + i p_i) \) creates one quantum of the harmonic oscillator in the \( i \)-direction (\( i = x, y \) or \( z \)).

We can obtain functions which satisfy the conditions (4) using the fact that the SU3 group classifies the quanta of the harmonic oscillator and that for each irreducible representation \( (\lambda \mu) \) corresponds a Young tableaux according to Weyl’s theorem. For example, the wave function \( \chi (42) \) is given by

\[
\chi(42) = \begin{vmatrix}
    a_x^+(1) & a_y^+(1) \\
    a_y^+(2) & a_z^+(2)
\end{vmatrix}
\begin{vmatrix}
    a_z^+(3) \\
    a_x^+(4)
\end{vmatrix}
\begin{vmatrix}
    a_x^+(4)
\end{vmatrix}
\begin{vmatrix}
    | 0 >
\end{vmatrix}
\]

\[ (5) \]

\[ \text{Figure 1} \]

Young tableaux corresponding to the representation \( (42) \) of the SU3 group.

where \(| 0 >\) indicates the state in which the four particles are in the ground state of the harmonic oscillator. The Young tableaux associated with the representation \( (42) \) is given in fig. 1.
In the Schrödinger representation $\chi(\lambda \mu)$ is expressed as a linear combination of products of four harmonic oscillator functions. In the spherical basis it becomes

$$
\chi_{\mu} (\lambda \mu) = \sum_{\nu l} a_{\nu l} \varphi_{\nu} (l_{1} r_{1}) \varphi_{\nu} (l_{2} r_{2}) \varphi_{\nu} (l_{3} r_{3}) \varphi_{\nu} (l_{4} r_{4}) = 
$$

$$
= \sum_{\nu l} a_{\nu l} \sum_{m} D_{\nu m_{1}}^{l_{1}*} D_{\nu m_{2}}^{l_{2}*} D_{\nu m_{3}}^{l_{3}*} D_{\nu m_{4}}^{l_{4}*} \varphi(l_{1} m_{1}) \times
\varphi(l_{2} m_{2}) \varphi(l_{3} m_{3}) \varphi(l_{4} m_{4})
$$

(6)

by evaluating the Hill-Wheeler integral we obtain

$$
\psi ((\lambda \mu) L M K) = \frac{2L+1}{c ((\lambda \mu) L, K)} \int D_{MK}^{L}(\Omega) \chi_{\mu} (\lambda \mu) d\Omega
$$

$$
= \frac{2L+1}{c ((\lambda \mu) L, K)} \sum_{\nu l} a_{\nu l} \sum_{m} \left[ \int D_{MK}^{L} D_{\nu m_{1}}^{l_{1}*} D_{\nu m_{2}}^{l_{2}*} D_{\nu m_{3}}^{l_{3}*} D_{\nu m_{4}}^{l_{4}*} \varphi(l_{1} m_{1}) \varphi(l_{2} m_{2}) \varphi(l_{3} m_{3}) \varphi(l_{4} m_{4}) \right]
$$

(7)

The second equation is deduced from the symmetry properties of the rotation matrices $D$.

The following step is to reduce the obtained set of functions with respect to the symmetric group $\Pi_{s}$. We use the Young operators in order to perform this calculation.

The totally antisymmetric wave functions can be expressed by

$$
\psi ((\lambda \mu), L, M = 0, K, S = 0, M_{s} = 0) =
$$

$$
= \frac{1}{\sqrt{2}} \{ \psi ([f] (\lambda \mu), L, M = 0, K | r_{1}) \varphi ([f] S = 0, M_{s} = 0 | r_{1}) 
$$

$$
- \psi ([f] (\lambda \mu), L, M = 0, K | r_{2}) \varphi ([f] S = 0, M_{s} = 0 | r_{2})
$$

(8)

where $r_{i}$ states for a particular standard tableaux.
The nonorthogonality of the wave functions labelled by different $K$ in the $(42)$ representation has been overcome through a Schmidt orthogonalization process.

We then diagonalize the proposed Hamiltonian

$$H = H_0 + H_q + H_p$$

(9)

in the basis given by the complete set of functions (8).

The quadrupole component of the Hamiltonian is given by

$$H_q = -\kappa \sum_{i,j} \sum_m (-)^m r_i^2 r_j^2 Y^2_m \left(\theta_i \phi_i\right) Y^2_{-m} \left(\theta_j \phi_j\right)$$

(9a)

and the pairing component $H_p$ is defined by the non-vanishing matrix elements

$$\langle \left(l_i \ m_i\right) \left(l_j m_j\right) | V_{ij} | \left(l'_i m'_i\right) \left(l'_j m'_j\right) \rangle =$$

$$= -G \delta_{m_i-m'_j} \delta_{l_i-l'_j} \delta_{i_i-i'_j} \delta_{i'_i-i'_j} \langle (-)^{l_i+l_j+m_i+m_j} \rangle$$

(9b)

The quadrupole interaction is diagonal in the chosen basis, meanwhile the pairing force mixes the states with the same $L$ but belonging to different representations $(\lambda \mu)$.

We obtain the energies and the corresponding eigenfunctions for different values of the ratio $\frac{G}{\kappa}$ between the strengths of the forces. The results are given in Table 2 in which we have indicated with $(42) K = 2$ the eigenvector coefficient corresponding to the wave function which is orthogonal to the $(42) K = 0$ one.

We know that for $\frac{G}{\kappa} = \infty$ we have the seniority scheme and that for $\frac{G}{\kappa} = 0$ we obtain the rotational extreme. With the results corresponding to intermediate values it is possible to determine the regions in which the nuclear motion can be interpreted in terms of the different collective models.

In fig. 2 we give the resulting energies as a function of $\frac{G}{\kappa}$. The error is estimated to be $0.2\%$ for each level because the obtained trace for the $L = 0$ matrix in the pairing extreme is $-13.97 \ G$ and it must be $-14 \ G^{(2)}$. 
3. DISCUSSION

The levels obtained in the quadrupole extreme correspond to a rigid rotator as can be seen in fig. 2. Applying expressions of reference (7), the three inertial parameters result equal. We may assume that for a sufficiently small departure from rigid rotator, the rotational behaviour will remain valid with a perturbation term of the form

$$H' = b L^4$$

In references (7, 8), the coefficient $b$ has been given the same value to all the levels of the same rotational band. We have found that a unique value of $b$ does not give agreement with our results, however small is the departure from the extreme $\frac{G}{\kappa} = 0$.

In no case an axially symmetric rotation can be obtained for the ground state.

The triplet predicted by the vibrational model appears for the value of $\frac{G}{\kappa} = 2\alpha$, the center of gravity of the 0, 2, 4 levels being 12% lower than twice the energy of the first $2^+$ level. However the presence of a $3^+$ level at this energy disturbs the vibrational picture.

The overlaps of the functions belonging to the $(42)$ representation are

$$< (42) 200 | (42) 202 > = 0.06285$$
$$< (42) 400 | (42) 402 > = 0.29786$$

To realize the influence of the nonorthogonality in the label $K$ we performed the diagonalization with the nonorthogonal wave functions and the results are compared with the correct ones in fig. 3.

As Elliott states, the lowest states have the main contribution from the $(42)$ representation. However, there is a rather important part corresponding to higher representations, which increases as $\frac{G}{\kappa}$ does.

We want to thank Dr. Rebeca Ch. de Guber for kindly making available to us the computing facilities of the Instituto de Cálculo (Universidad de Buenos Aires).
Ver leyenda en la pág. n° 122
Plot of the results of the diagonalization for the nonorthogonal wave functions (b), compared with the correct ones (a).

**TABLE 1**

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#### Quadrupole extreme

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| 2   | 0.6515 | 0.014      | 0.039      | -0.429 | -0.902| -0.003 |
| 2   | 0.5392 | -0.040     | 0.042      | 0.902  | -0.423| 0.006  |
| 2   | 0.2262 | 0.390      | -0.919     | 0.036  | -0.051| 0.001  |
| 2   | 0.1736 | 0.920      | 0.391      | 0.080  | 0.017 | 0.013  |
| 3   | 0.7788 |           | 0          | 1      | -     |       |
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| 4   | 0.8982 | 0.000      | 0.046      | 0.993  | 0.106 |       |
| 4   | 0.4600 | -1.000     | -0.001     | 0.000  | 0.000 |       |
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Pairing extreme

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<th>$(31)$</th>
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REFERENCES


(7) C. A. MALLMANN, Nuclear Physics 24 (1961) 535


(9) J. P. ELLIOTT, Lectures given at “Escuela Latinoamericana de Física-México 1962” (Universidad de México, México, D.F.)

Explicación de la Fig. 2

Plot of the energy levels as a function of the ratio between the strength of the forces. The values of $\frac{G}{\kappa}$ are given in units of $\frac{1}{3.1} \left(\frac{MW}{k}\right)^{-2}$. For each value of $\frac{G}{E}$ the energy unit is the difference between the lowest and the highest level. The states are characterized by the value of the angular momentum $L$. When two angular momenta are written in the same line, the corresponding levels are degenerated.