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Shell-Model Description of Rotational Motion in Odd-Mass Nuclei.

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Shell-model description of rotational motion in odd-mass nuclei

Naqvi, Husney Ahmed, Ph.D.
The Louisiana State University and Agricultural and Mechanical Col., 1992
SHELL-MODEL DESCRIPTION OF ROTATIONAL MOTION IN ODD-MASS NUCLEI

A Dissertation
Submitted to the Graduate Faculty of the
Louisiana State University and
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in partial fulfillment of the
requirements for the degree of
Doctor of Philosophy

in

The Department of Physics and Astronomy

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In memory of my mother
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ABSTRACT

An algebraic shell-model realization of a quantum rotor for integral and half-integral angular momenta is introduced. The underlying symmetry of the theory is the $\text{SU}(3) \supset \text{SO}(3)$ group structure. The algebraic model reproduces the eigenvalues of the quantum rotor hamiltonian well for normal shell-model configurations; the mapping is exact for small values of the angular momentum in large $\text{SU}(3)$ representations. A shell-model hamiltonian using this algebraic realization of the quantum rotor and other non-central one-body interactions is used to reproduce the experimental spectra of representative even and odd-mass $d$-$s$-shell nuclei.
CHAPTER 1
INTRODUCTION

The main objective of any basic science is to understand observed phenomena in terms of general concepts and underlying principles. There are usually two extreme approaches to scientific development and discovery. One proceeds from the general to the specific, reducing the number of hypothesis needed to explain experimentally observed results as one progresses, and the other, not necessarily motivated by theory, sets out to explore new and unexpected phenomena. As we will see in what follows, an understanding of nuclear phenomena, in particular the structure of odd-A nuclei which is the topic of this thesis, requires one to use the full range of scientific development and discovery protocols. While the physics of complex nuclear systems resists sophisticated many-body analyses, it shows intriguing regularities that seem to favor simple collective model descriptions.

We begin our account by looking back to what was perhaps the most important single step towards our understanding of nuclear structure, namely the discovery of the neutron as a basic constituent of nuclear matter by Chadwick in 1932 (Cha 32) which opened the door to research in modern nuclear physics. After the discovery of the neutron, Heisenberg (Hei 32b; Hei 32a; Hei 32c) and Ivanenko (Iva 32) independently proposed models of nuclear structure with neutrons and protons as basic building blocks of their theories. A problem with these earliest theories was an inability to cope with the fact
that there is no apparent force center as in the atomic case so the new quantum mechanics could not be adopted in a straightforward manner. Even today, with the notion of a self-consistent mean field an accepted strategy, the lack of a well-defined central potential causes problems. In addition, of course, particle physicists have now established that the nucleons themselves have quark or quark-like substructures. Nonetheless, for most low-energy structure phenomena nucleons can still be considered to be the elementary constituents of nuclei.

As suggested above, one of the most fundamental of all nuclear physics problems, namely, the exact nature of the force that binds nucleons together inside the nucleus, remains unresolved. It is therefore not possible to calculate nuclear properties from a fundamental interaction as is done in atomic physics for example. While the general form of the interaction may be obtained from nucleon-nucleon scattering experiments, the parameters of the interaction must be renormalized to account for the fact that inside the nucleus many of the open channels are blocked due to the presence of other nucleons. The usual way of proceeding is to fit the parameters of a proposed potential form so calculated eigenvalues, electromagnetic transition rates, and particle transfer strengths are in agreement with experimental results. This method, though in principle reasonable, is not very satisfactory because the renormalization is strong so the potential inside the nucleus is very different from that which is used to obtain good fits to nucleon-nucleon scattering data.

Due to the difficulties and shortcomings of a general approach, different models have been proposed which do not involve a detailed form for the interaction potential. Most modern theories of nuclear structure start from one
of two very different premises. The simplest and most successful of these emphasizes the collective motion of the nucleus. The liquid drop and various geometrical models, which employ the Bohr-Mottelson hamiltonian form, are the backbone of such analyses. The other extreme builds on the independent particle picture of nuclear structure. Here the derivative theories are large shell-model analyses, and most recently, the development and use of algebraic techniques that focus on collective degrees-of-freedom. The most successful of these approaches are the unified model (Boh 52; BohMot 53), which adds particle degrees-of-freedom to the geometrical picture, and the symplectic model which partitions the full shell-model space up into it collective subspaces (RosRow 77; RowRos 82)

Collective phenomena in nuclei stems from the coherent motion of a sizable fraction of the total number of nucleons in a nucleus. An obvious example is the fission process. The liquid drop model was developed by N. Bohr and J. Wheeler (BohWhe 39; HilWhe 53) to explain the phenomena of nuclear fission. The basic assumption of the model is that the nucleons are so strongly interacting with one another that they lose their individual identity and dissolve into a system that can be described best in terms of a few common collective variables. The geometric model developed by A. Bohr and B. Mottelson (BohMot 53) is based upon the same assumption. It considers the nucleus to be a quantum droplet having coupled rotational (3) and vibrational (2) degrees-of-freedom. The rotational motion is characterized in terms of its moments of inertia and flow type which can be rigid or irrotational or some combination depending upon the application. The Bohr-Mottelson geometrical
model and its various derivatives (GneMos 69; GneMos 70) have been confirmed by many experimental results.

The single-particle model which represents the opposite extreme, on the other hand, considers the nucleons to move independently of one another within the nucleus. The nuclear shell model, which embraces this concept and is analogous to the atomic shell model, was originally suggested by Elsasser in 1934 (Els 34) and later developed by Mayer and by Jensen, Haxel and Suess in 1949 (HexJen 49; May 49) makes the assumption that the nucleons move independently in an averaged potential. For any particular nucleon the potential is the average field it experiences due to interactions with all the other nucleons. Although this simple model seems to ignore the possibility of collective motion, it successfully predicts magic numbers and the ground state spin and parities of nuclei throughout the periodic table.

In their simplest form the liquid drop and single-particle pictures are clearly distinct theories. Accordingly, the success of these simple versions is very limited. For example the single-particle shell model is unable to explain enhanced transition probabilities between low-lying states of deformed systems or their large quadrupole moments which are readily reproduced by collective models. On the other hand the collective models cannot account for magic numbers or the properties of odd-A nuclei. The limited success of these models forced the development of more complicated versions of each, and as feasible, the unification of these approaches. For example, the particle structure of the nucleus along with its collective motion was taken into account by the Nilsson model (Nil 55) which puts nucleons into a deformed potential well that is allowed to rotate adiabatically. Likewise for the shell model,
interactions between pairs of particles have been included and where different configurations lie close together, as for instance in $^{10}$Be (EllFlo 55), their mixing has been taken into consideration.

The real challenge facing nuclear physics is to see which collective properties, particularly rotational features, can emerge from a shell-model description of nuclei. Elliott and his collaborators (Ell 58; EllHar 63; EllWil 68) studied this problem using group theoretical techniques. With that work as background, Draayer and his co-workers (LesDra 86) have gone on to show explicitly how rotational excitations can be understood to emerge within the shell-model framework. These features survive in other more complicated algebraic theories like the symplectic model (RosRow 77; RowRos 82) and offer an opportunity for a deeper understanding of the origin of collective rotational phenomena in nuclei. Leschber's work, however, was confined to even-even nuclei with zero spin and integral total angular momentum $J$ values.

The purpose of this research is to extend the work of Leschber to odd-$A$ nuclei, which means the theory must be extended to half integral-values of $J$ and non-zero values for the spin $S$. In the next chapter the ground work is laid down and the various nuclear models of relevance to the development which have been mentioned only briefly here are discussed in more detail. In the third chapter the algebraic realization of triaxial rotor hamiltonian for integral values of $J$ is reviewed and extended to include half-integral $J$ values. Two operators, $K^2_L$ and $K^2_J$, are developed to show $K_L$-band and $K_J$-band splitting in even-$A$ and odd-$A$ nuclei, respectively. In the fourth chapter a single-particle shell-model picture of the Nilsson hamiltonian is developed. Then, in the same chapter, an algebraic realization of the Nilsson rotor-plus-particle hamiltonian
is given and the success of the model demonstrated by showing the results of its application to odd-A nuclei like $^{21}\text{Ne}$. Experimentally determined spectra are compared and matched with those given by this and some other theoretical calculations. In the final chapter some results of this work are summarized and some possible follow-up research projects are suggested.

The main objective of this research is to show how rotational motion can be found in and emerge from shell-model analyses. It is an attempt to bring two very distinct and different models of nuclear structure closer together. Although this is an important problem which has been dealt with many times in the past by other researchers using a variety of different means, our approach is unique because the connection between the macroscopic and microscopic theories of nuclear structure is reduced to an elementary mapping between hamiltonian forms of the two theories. Though in some ways this is only a small part of a very complex scientific challenge, it is a significant part since it establishes in a clear and unambiguous manner a connection between two characteristically different types of quantum phenomena, single-particle and collective motions. With this in hand, it seems reasonable to readdress the matter of the microscopic origin of collective motion, starting with the nucleon-nucleon interaction which might include, for example, the forgotten quark degrees-of-freedom. Nonetheless, we acknowledge that our knowledge of how the nucleus is constructed remains in its early stages.
CHAPTER 2
NUCLEAR MODELS

Since our object is to develop a theory that will bridge the gap between the collective and single-particle interpretations of nuclear structure, it is appropriate to begin with a description of the simplest models representing these two extreme pictures, i.e., the geometrical model and the shell model. We will then turn our attention to schemes like the Nilsson model that represent early attempts to unify these approaches. The final topic of this chapter on nuclear models will be a discussion of algebraic techniques, in particular we will describe Elliott's SU(3) model.

2.1. Collective (Geometric) Model

It is clear from experimental observations that rotation is an important excitation mode in nuclei. A. Bohr and B. Mottelson developed the geometrical model of the nucleus to explain this phenomena. According to this theory the nucleus is assumed to be a uniform distribution of nuclear matter with a well-defined surface, and vibrational and rotational degrees-of-freedom. In this model nuclei can have a deformed equilibrium shape. For small deviations from a spherical shape the nuclear surface is given in terms of spherical coordinates \((R, \theta, \phi)\) in the lab frame by the following quadrupole expansion:
\[ R(\theta, \phi) = R_0 \left[ 1 + \sum_{\mu=2}^{2} a_{\mu}^* Y_{2\mu}(\theta, \phi) \right], \]  
(2.1)

where

\[ R_0 = r_0 A^{1/3} \text{ with } r_0 = 1.2 \text{ fm}, \]  
(2.2)

and the parameters \( a_{\mu} \) describe the shape of the nucleus. A change in the shape of the nucleus is given in terms of a change in these shape parameters which obey the following relation because \( R(\theta, \phi) \) is real:

\[ a_{\mu}^* = (-1)^\mu a_{\mu}. \]  
(2.3)

As the notation indicates, the shape parameters form the components of a rank 2 spherical tensor.

The hamiltonian of the nuclear system is constructed either directly in terms of these shape parameters and their conjugate momenta or in terms of another body-fixed frame of reference set that are related to the lab frame parameters as follows:

\[ a_{\mu} = \sum_{\nu} D_{\mu\nu}^2(\Omega) \alpha_{\nu}, \]  
(2.4)

where \( D_{\mu\nu}^2 \) is a rotational matrix and \( \Omega \) denotes the three Euler angles that specify the orientation of the body-fixed frame with respect to the lab frame. In the principal axis frame \( \alpha_{-1} = \alpha_1 = 0 \) and \( \alpha_{-2} = \alpha_2 \). The \( a_{\mu} \) can therefore be replaced by two other more physical parameters \( \beta \) and \( \gamma \) as:
\[ \alpha_0 = \beta \cos \gamma. \]  \hspace{1cm} (2.5)

\[ \alpha_2 = \sqrt{2} \beta \sin \gamma. \]  \hspace{1cm} (2.6)

One can easily see that the $\beta$ represents the total deformation of the nucleus ($0 \leq \beta \leq \infty$) and $\gamma$ gives the deviation from axial symmetry ($0^\circ \leq \gamma \leq 60^\circ$). For a prolate shape $\gamma = 0^\circ$ while for oblate shape $\gamma = 60^\circ$. There are only two independent and rotationally invariant quantities in this representation:

\[ (\alpha \times \alpha)^0 = \beta^2/2, \]  \hspace{1cm} (2.7)

\[ (\alpha \times \alpha \times \alpha)^0 = \sqrt{2/35} \beta^2 \cos 3\gamma. \]  \hspace{1cm} (2.8)

The Hamiltonian is a rotational scalar so the geometrical model uses a form built with polynomials in these scalar quantities. We will not go into details of how the Hamiltonian is constructed and diagonalized to obtain desired results as this is readily available in textbooks. There are many enhancements to this elementary model but the basic concepts and methods remain the same.

2.2. Single-Particle Shell Model

A series of experiments established the fact that the single-particle separation energy, which is the energy needed to remove the least bound nucleon from the nucleus, is extraordinarily large for the nuclei whose proton or neutron number is 2, 8, 20, 28, 50, 82, and 126 in comparison with the other nuclei. At these so-called magic numbers effects analogous to electron shell closure in atoms (e.g. high ionization energies of inert gases) are observed.
The occurrence of these magic numbers was one of the strongest motivations for the formulation of the nuclear shell model which is analogous to the atomic shell model where there exist groups of degenerate levels with quite large energy difference in between the electron shells as a consequence of strongly attractive central Coulomb potential of the nucleus that imposes sphericity.

For nucleons in a nucleus there is a priori no such central potential, however, one can imagine one resulting from the interaction of the nucleons with one another. Before suggesting a particular form for this potential we will consider what its behavior should be in different regions. A nucleon close to the center of a nucleus (r=0) should experience a uniform field because it is completely surrounded by other nucleons. This force grows stronger as a nucleon moves away from the surface (r=R_0) into the interior region of the nucleus. Since nuclear forces are short range the potential should be zero for large distances (r>>R_0). One potential which not only satisfies these conditions quit well but also produces very reasonable density distributions is Wood-Saxon potential (WooSax 54):

\[ V_{WS}(r) = -V_0 \left[ 1 + \exp \left( \frac{r-R_0}{a} \right) \right]^{-1}. \]  

(2.9)

where

\[ R_0 = r_0 A^{1/3}; \quad V_0 \sim 50 \text{ (MeV)}; \quad a \sim 0.5 \text{ (fm)}; \quad r_0 = 1.2 \text{ (fm)}. \]  

(2.10)
The eigenfunctions of Wood-Saxon potential cannot be given in closed form. To avoid this difficulty and to simplify the calculations either a harmonic oscillator potential $V_{\text{HO}}$ or square-well potential $V_{\text{SW}}$ approximation is used:

\[ V_{\text{HO}} = -V_0 \left[ 1 - \left( \frac{r}{R_0} \right)^2 \right] = \frac{m\omega_0^2}{2} (r^2 - R_0^2), \tag{2.11} \]

\[ V_{\text{SW}} = -V_0 \quad \text{for } r \leq R_0 \]
\[ = 0 \quad \text{for } r > R_0. \tag{2.12} \]

Note that the $V_{\text{WS}}$, $V_{\text{HO}}$, and $V_{\text{SW}}$ are spherically symmetric potentials. We will discuss deformed potentials later. The solution of the eigenvalue problem for the harmonic oscillator potential gives rise to equidistant energy levels with energy $\epsilon(N)$ given by:

\[ \epsilon(N) = \hbar \omega_0 (N+3/2) - V_0, \tag{2.13} \]

with

\[ N = 2(n-1) + l, \quad n=1, 2, 3, \ldots \quad l, \quad \text{and} \quad l=0, 1, 2, \ldots \tag{2.14} \]

where $N$ is the total number of oscillator quanta, $n$ is the radial quantum number, $l$ is the angular momentum, and $\omega_0$ is the oscillator frequency. Levels with the same $N$ belong to the same oscillator shell. From eq. (2.14) we see that an oscillator shell only contains either even or odd $l$ values, which means only states with the same parity. Furthermore, levels in the same oscillator shell with different $n$ and $l$ values are $d(N)$-fold degenerate.
\[ d(N) = \frac{(N+1)(N+2)}{2}. \quad (2.15) \]

The degeneracy of the various \( l \) values is removed in the square well case. The actual energies lie between the limits given by harmonic oscillator and square well potentials. The actual situation can be simulated best by adding an \( I\cdot I \) term with eigenvalues \( I(I+1) \) that favors the high \( l \) values over lower ones to the harmonic oscillator form. The levels are filled, as is done in the atomic case, in accordance with Pauli principle. The \( N \)-th oscillator shell can accommodate \( d(N) \) protons and \( d(N) \) neutrons and as shown in fig. 2.1 both these potentials can explain the occurrence of the magic numbers like 2, 8, and 20 but not the higher ones. This deficiency in the model was removed by Mayer and by Haxel, Jensen and Suess (HexJen 49; May 49) who took into account the spin degree-of-freedom and added a strong spin-orbit interaction \( I\cdot s \) to the hamiltonian. Since \( I\cdot s = \frac{1}{2}[j^2 - l^2 - s^2] \) this interaction is diagonal in a \( jj \)-coupled but not an \( ls \)-coupled basis and the single-particle states are characterized by the quantum numbers \( j, j_z, l, \) and \( s \) instead of \( l, l_z, s, \) and \( s_z \). The effect of inclusion of spin-orbit term on the energy levels given in fig. 2.1 is shown in fig. 2.2. If the other terms in the hamiltonian remain the same the inclusion of the spin-orbit term in the hamiltonian removes the degeneracy of the doublets \( j = l \pm 1/2 \). The splitting \( \Delta \varepsilon(l) \) is easily shown to be:

\[ \Delta \varepsilon(l) = 2l+1. \quad (2.16) \]
Figure 2.1. Level scheme of the harmonic oscillator (eq. (2.11), l.h.s.) and of the infinite square well (eq. (2.12), r.h.s., with \( V_0 = \infty \)). Levels with the same \( N \) and different radial quantum numbers \( n \) and angular momentum \( l \) are degenerate. The levels are specified by \((n,l)\) where the usual spectroscopic symbols (s,p,d,f,...) are used to denote the orbital angular momentum \((l = 0,1,2,3...,\) respectively). The radial degeneracy of the harmonic oscillator is removed for the square-well potential. The true energies lie between the limits given by these two potentials.
Figure 2.2. Schematic energy level diagram for the single-particle shell-model hamiltonian. The left-hand side indicates how the degenerate levels of a shell of the spherical oscillator \((l = N, N-2, \ldots, 1 \text{ or } 0)\) are split by the \(l^2\) term. The \(l\cdot s\) term removes the remaining (spin) degeneracy and in this case the levels are specified by \((nlj)\). The number of nucleons a particular orbital can accommodate is given in parentheses next and to the right of the corresponding level. The numbers on the far right (in parentheses) are running totals while the numbers on the far right (not in parentheses) are the magic numbers.
Experimental results show that the $j = l - 1/2$ level is energetically above the $j = l + 1/2$ level when an attractive spin-orbit interaction is added to yield the desired results. Eq. (2.16) also suggests that the splitting will be larger for higher $l$ values. We can now see with the help of the energy level scheme given in fig. 2.2 that it is easy to explain the occurrence of almost all magic numbers. This is the main success of the single-particle shell model.

If pairing between nucleons is also taken into account then the ground state spin of all even-even nuclei is predicted to be zero and that for odd-$A$ nuclei is predicted to be the spin of the last odd nucleon. Experimental results show that ground state spins are in accordance with this extended single-particle shell-model picture. In spite of its great success in predicting the magic numbers and ground state spins, however, the single-particle picture has some serious shortcomings. For instance it is unable to explain the rotational bands and very large quadrupole moments in the region far from closed shells, i.e, $A \sim 25$ (Al, Mg), $150 < A < 190$ (rare earth nuclei), and $A > 220$ (the actinides). We will see in the next section how a deformed single-particle potential can be used to overcome this difficulty.

2.3. Nilsson Model

As discussed in the previous sections, the geometrical model and the simplest spherical shell-model picture focus respectively on the collective and single-particle behavior of nucleons in nuclei. Nilsson developed a model for odd-$A$ nuclei that considers the nucleus as an even-$A$ core plus a single nucleon outside the core. While the equilibrium shape of the core for nuclei near
major shell closures is spherical, with the addition of valence nucleon it assumes a deformed shape. In general the coupling of the collective modes of this deformed shape and the individual particle modes of the valence nucleon is complicated. The situation simplifies in regions far from a closed shell where the core acquires a stable deformation. It is then possible to approximately separate the intrinsic motion of the extra-core nucleon from the core which can rotate and vibrate. The assumption of a stable deformed nuclear shape is confirmed by experimental observations, such as large quadrupole moments, strongly enhanced quadrupole transition probabilities, and single-particle energies which depend on the details of the deformation.

The wave function of the combined system can be written as a product $\Psi = D_{\text{rot}} \phi_{\text{vib}} \chi$. Here $D_{\text{rot}}$ represents the collective rotational motion of the system and is characterized by the total angular momentum as given by $I^2$ with its eigenvalue $I(I+1)$, the projection M of $I$ on the space-fixed $z'$-axis, and the projection K of $I$ on the body-fixed $z$-axis. The function $\chi$ represents the intrinsic motion of the extra-core nucleon; in the case of an axially symmetric system it is characterized by the projection of the particle's angular momentum $J$ on the symmetry (z) axis of the nucleus. The function $\phi_{\text{vib}}$ characterizes the vibrations of core about its equilibrium shape. The relationship of the angular momenta and axes to one another is shown in fig. 2.3.

We now turn our attention to the deformed potential seen by the extra-core nucleon, considering its form first. As previously noted, the harmonic oscillator hamiltonian with the $I\cdot s$ and $I\cdot h$ terms added is a good starting point for a shell-model theory. Nilsson used the same scheme but replaced the isotropic oscillator with a deformed harmonic potential. He started with the
Figure 2.3. The projection of the total angular momentum $I$ of an odd-$A$ nucleus on the laboratory (space-fixed) $z'$-axis ($M$) and body-fixed $z$-axis ($K$). The quantum number $\Omega$ is the projection of the angular momentum $j$ of the odd nucleon on the body-fixed $z$-axis. The angular momentum of the core is given by $R = I - j$. This means $K = \Lambda + \Omega$ where $\Lambda$ is the projection of the core on the body-fixed $z$-axis. The quantum numbers $K$ and $\Omega$ are constants of the motion if the nucleus has axial symmetry. For deformed systems, $j^2$ is not a constant of the motion.
axially symmetric case which was later extended to include asymmetric shapes. The density distribution of the deformed system is assumed to have an ellipsoidal shape and in analogy with the spherical case the average particle potential can be represented by an anisotropic harmonic oscillator:

\[ H_0 = -\frac{\hbar^2}{2m} \nabla^2 + \frac{m}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \tag{2.17} \]

where the three frequencies, \( \omega_x, \omega_y, \) and \( \omega_z \) are chosen proportional to the inverse of the half axes \( a_x, a_y, \) and \( a_z \) of the ellipsoid:

\[ \omega_x = \tilde{\omega}_o R_o/a_x, \quad \omega_y = \tilde{\omega}_o R_o/a_y, \quad \text{and} \quad \omega_z = \tilde{\omega}_o R_o/a_z, \tag{2.18} \]

where \( R_o \) is the mean radius and \( \tilde{\omega}_o = (\omega_x \omega_y \omega_z)^{1/3}. \)

For the case of an axially symmetric shape the \( z \)-axis is chosen as the symmetry axis and a deformation parameter \( \delta \) is defined such that:

\[ \omega^2_x = \omega^2_y = \omega^2_z(\delta) \left( 1 + \frac{2}{3} \delta \right), \quad \omega^2_z = \omega^2_z(\delta) \left( 1 - \frac{2}{4} \delta \right) \tag{2.19} \]

where \( \omega_o(\delta) \) can be found using the assumption of constant volume and is given up to the quadratic term in \( \delta \) as:

\[ \omega_o(\delta) = \tilde{\omega}_o \left( 1 + \frac{2}{3} \delta^2 \right) \quad \text{and} \quad \hbar \tilde{\omega}_o = \eta A^{-1/3} \text{MeV}. \tag{2.20} \]

In this expression \( \eta \) is a constant determined in principle through a comparison of theoretical and experimental spectra but generally taken as simply \( \eta = 41. \)
The parameter $\delta$ is related to the parameter $\beta$ of eqs. (2.5) and (2.6) as:

$$\delta = \frac{3}{2} \sqrt{\frac{3}{4\pi}} \beta.$$  \hfill (2.21)

Positive (negative) $\delta$ correspond to a prolate (oblate) shape.

Nilsson introduced a deformation dependent oscillator length and used dimensionless coordinates $r' = [m\omega_0(\delta)/(\hbar\omega)]^{1/2} r$ to give the hamiltonian as:

$$H_0(\beta) = \hbar \omega_0(\delta) [ -\frac{1}{2} V' + \frac{1}{2} r'^2 - \beta r'^2 Y_{20}(\theta',\phi')].$$  \hfill (2.22)

The total hamiltonian $H_p$ of the extra-core particle can now be written as:

$$H_p = \hbar \omega_0(\delta) [ -\frac{1}{2} V' + \frac{1}{2} r'^2 - \beta r'^2 Y_{20}(\theta',\phi') + C \cdot s + D l^2].$$  \hfill (2.23)

Defining two new parameters $\kappa$ and $\mu$, $H_p$ can be rewritten as:

$$H_p = H_h - \hbar \omega_0(\delta) [ \beta r'^2 Y_{20}(\theta',\phi') + 2\kappa l \cdot s + \mu l^2],$$  \hfill (2.24)

where

$$H_h = \frac{\hbar \omega_0(\delta)}{2} (-V' + r'^2), \quad \kappa = -C/2\hbar \bar{\omega}_0 \text{ and } \mu = 2D/C.$$  \hfill (2.25)

The hamiltonian $H_p$ can be diagonalized in the representation $|Nlmms_m> \text{ which diagonalizes the operators } H_h, I^2, s^2, I_z \text{ and } s_z \text{ with eigenvalues } (N+3/2), l(l+1), s(s+1), m_l, \text{ and } m_s, \text{ respectively. An alternative basis is } |Nljms_m> \text{ which diagonalizes } H_h, I^2, s^2, j^2 \text{ and } j_z \text{ with eigenvalues } (N+3/2), l(l+1), s(s+1), m_l, \text{ and } m_s \text{ respectively.}$
j(j+1) and $\Omega$, respectively. In both these representations $\beta r^2 Y_{20}$ is not diagonal. This term not only mixes the terms with different $j$ values but $N$ is not a good quantum number. The $\beta r^2 Y_{20}$ term couples states with $N$ to those with $N\pm 2$ as well as $N$. The off diagonal elements, though comparable in size to the diagonal elements, are small compared to $2\hbar \omega$ therefore $N$ is usually taken as a good quantum number. For large deformation the $l s$ and $l^2$ can be neglected in comparison with $\beta r^2 Y_{20}$ and then the so-called asymptotic quantum numbers $\Omega \pi [N n z m_l]$ are good quantum numbers. The energy levels for a particle in a Nilsson potential can be found in any standard text of nuclear physics.

The $\mu$ and $\kappa$ values are usually determined so that for zero deformation the level scheme is the same as for spherical nuclei. An interesting empirical result is that $\mu$ (which measures the relative strength of the $l^2$ and $l s$ terms) is roughly $N$ independent and nearly equal to 0.5 which is the value required for good pseudo-spin symmetry. This result and its significance to nuclear structure vis-a-vis the pseudo-spin concept are discussed in Section 2.5. So far we considered the particle and the rotational motion to be independent of each another; the coupling between the particle and rotational motion has been ignored. This coupling and what it means in terms of nuclear structure will be discussed in Chapter 3 where the rotor hamiltonian and rotational motion are considered in greater detail.
2.4. Elliott SU(3) Model

Despite its many successes, the shell-model scheme (extended in the usual way from the simple single-particle picture to a complex many-particle theory) is not suitable for many situations. One difficulty, for instance, is the extraordinarily large model space dimensions one encounters. For example, if one divides the 32 nucleons in $^{32}\text{S}$ into an inert $^{16}\text{O}$ core and 16 valance nucleons and the valance space includes the (ds) and (fp) shells there are $4 \times 10^{12}$ states with $J=2$. If the space is restricted to the (ds) shell only, the number of $J=2$ state drops to 1206 (Les 87). The diagonalization of matrices that are this large is not only difficult but unnecessary because there are only about 10 such states observed in the $^{32}\text{S}$ spectrum. The use of dynamical symmetries proves to be very helpful in avoiding these difficulties.

The dynamical symmetry approach to nuclear structure exploits special symmetries and the theory of Lie groups to reduce model spaces to reasonable sizes. A discussion of the theory of Lie groups is given in Appendix A. In short, the model space is defined by a group chain $G \supset G_i \supset H$ where the system is assumed to have an exact symmetry $H$ (like angular momentum) and a conserved symmetry $G$ (like the unitary group associated with a change in the single-particle basis). The choice of the intermediate groups $G_i$ depends upon the nature of problem. A basis state $\Psi$ for this chain is given as follows:

$$\Psi = |g\alpha[g_i\beta[h]\rangle, \quad (2.26)$$
where \( g, g_i, \) and \( h \) are the labels of the irreducible representations (irreps) of the groups \( G, G_i, \) and \( H \) respectively and \( \alpha \) and \( \beta \) are multiplicities in the reductions.

Elliott (Ell 58; Har 68) used the \( SU(3) \supset SO(3) \) group chain to explain the rotational spectra of light nuclei \((16 < A < 28)\) from a shell-model prospective. Later on this model was extended to the pseudo \( SU(3) \) model (AriHar 69; DraWee 84a; HecAdl 69; RatDra 73) and applied to heavy nuclei in the rare earth and actinide regions. The basic idea behind the model is the classification of nuclear states according to the unitary group \( SU(3) \) of the three-dimensional isotropic harmonic oscillator, as well as the permutation group \( S_A \) that enters because of the antisymmetrization requirement for fermions and the rotation group in three dimension \( SO(3) \) which is an exact symmetry. The properties of these groups are discussed in many standard textbooks. Here we will discuss their use in labelling shell-model configurations.

First, in the single-particle shell-model picture the closed shell is considered to be an inert core and the nuclear properties are determined only by the \( m \) valence nucleons outside this inert core. Second, the valence space is limited to one shell only. For an oscillator shell \( N \) there are \( d=(N+1)(N+2)/2 \) spatial states and four spin (\( S \)) isospin (\( T \)) states (i.e \([S_z,T_z] = \{1/2,1/2\}, \{1/2,-1/2\}, \{-1/2,1/2\}, \{-1/2,-1/2\}\)) so the total valence space consists of \( D=2(N+1)(N+2) \) single-particle levels. Since the \( m \)-particle state must be antisymmetric under permutation of particles it must transform like the \([1^m]\) irrep of \( U(D) \). The states can be labelled by additional quantum numbers from subgroups of this \( U(D) \) group. The wave function is separated into its spatial and spin-isospin parts: \( U(D) \supset U(d) \otimes U(4) \). A full classification of the states
can be obtained through the irreps of subgroups U(d) and U(4) as is shown schematically in fig. 2.4. The two parts are labelled by conjugate Young patterns, \([f(d)]\) and \([\overline{f(d)}]\) because the product wavefunction is antisymmetric. The U(4) group can further be separated into intrinsic spin (S) and isospin (T) parts. For a particular \([\overline{f(d)}]\) there are states with different spin-isospin values, some occurring multiple times. This (ST) multiplicity in \([\overline{f(d)}]\) is denoted by \(\beta\).

The SU(3) group is a subgroup of \(U(3) \subset U(4)\), the space part of U(D). The irrep of U(3) for an \(m\)-particle state in the \(N\)-th oscillator shell are given by a Young diagram with \(mN\) (total number of quanta) boxes and at the most three rows, which describes the distribution of the \(mN\) quanta in the three spatial directions. The representation labels of SU(3) equivalent to a partition \([f_1 f_2 f_3]\) of U(3) are \(\lambda = f_1 - f_2\) and \(\mu = f_2 - f_3\). There may be more than one irrep of SU(3) labelled by the same \((\lambda \mu)\) in a U(d) irrep. This is where the \(\alpha\) multiplicity of \((\lambda \mu)\) enters. SU(3) has two subgroup chains, namely SU(3) \(\supset\) SU(2) \(\times\) U(1) and SU(3) \(\supset\) SO(3). The group of rotations in three dimensions SO(3) is required for angular momentum conservation and to explain the rotational behavior.

The irreps of SO(3) are labelled by the orbital angular momentum \(L\). The angular momentum operators form a subalgebra of SU(3) so basis states can be labelled by the SU(3) \(\supset\) SO(3) chain. The values of \(L\) for a given \((\lambda \mu)\) are found by the following rule:

\[
L = K, K+1, K+2, \ldots, (\lambda + \mu) - K ,
\]

(2.27)
Figure 2.4. Schematic diagram showing the breakup of the full model space for \( m \) nucleons into irreps of \( U(d) \otimes U(4) \) and subgroups of these symmetries, where \( d = (N+1)(N+2)/2 \) is the spatial degeneracy of the \( N \)-th oscillator shell and 4 denotes the spin-isospin degrees-of-freedom. As required by the Pauli principle, the \( U(D) \) irrep must be the totally antisymmetric representation \([1^m]\), where \( D = 4d \) is the dimensionality of the full model space. From this it follows that the irreps \( [f(d)] = [f_1 f_2 \ldots f_d] \) of \( U(d) \) specifying the spatial symmetry, and the irrep \( [	ilde{f}(d)] = [\tilde{f}_1 \tilde{f}_2 \tilde{f}_3 \tilde{f}_4] \) of \( U(4) \) labeling the complimentary spin-isospin symmetry, must be related by row-column interchange of the associated Young shapes (Ham 62; Hec 73). Further reduction of the spatial symmetry yields the quantum labels \((X,p)\) of \( SU(3) \) and \( K \) of \( SO(3) \) with multiplicities \( \alpha \) and \( K \) (Ell 58); and for the spin-isospin \( [\tilde{f}(d)] \) symmetry the quantum numbers \((S,T)\) of \( SU_S(2) \otimes SU_T(2) \) with multiplicity \( \beta \). The last step includes the coupling of the orbital and spin angular momenta to total angular momentum \( J = L + S \) of the \( SU_J(2) \) group.
where the integer \( K = \min(\lambda, \mu), \) \( \min(\lambda, \mu) - 2, \ldots, 1 \) or 0, with the exception that if \( K = 0, \)

\[
L = K, K+1, K+2, \ldots, (\lambda + \mu) - K ,
\]

(2.27)

where the integer \( K = \min(\lambda, \mu), \) \( \min(\lambda, \mu) - 2, \ldots, 1 \) or 0, with the exception that if \( K = 0, \)

\[
L = (\lambda + \mu), (\lambda + \mu) - 2, (\lambda + \mu) - 4, \ldots, 1 \) or 0 . \]

(2.28)

It is clear from these expressions that a particular \( L \) value can occur several times within an irrep \( (\lambda, \mu) \). The parameter \( K \) not only serves as a multiplicity label but corresponds to the projection of the angular momentum on the symmetry axis in the rotational model. This means that states with the same \( L \) values belong to different \( K \) bands which are, however, cut off at some upper limit. A state with spin \( S, \) isospin \( T, \) orbital angular momentum \( L \) and total angular momentum \( J = L + S \) is given in this framework as:

\[
\Psi = \sum_{M_L, M_s} \left\langle L M_L; S M_S; L M_M \right| \left[ 1^m \right] \left[ f(d) \right] \alpha(\lambda, \mu) K L M_L; \left[ f(d) \right] \beta S M_S T M_T \right\rangle
\]

\[
= \left\langle 1^m \right| \left[ f(d) \right] \alpha(\lambda, \mu) K L ; \left[ f(d) \right] \beta S T M_T ; J M \right\rangle . \]  

(2.29)

The spatial basis states can also be labelled according to the chain \( SU(3) \supset SU(2) \otimes U(1) \) as \( l(\lambda, \mu) e \Lambda \nu >. \) The \( \Lambda \) and \( \nu \) labels specify respectively the \( SU(2) \) irrep and its projection while \( e, \) which is the eigenvalue of \( Q_0, \) labels the \( U(1) \) irrep. The state with \( e = e_{\text{max}} = 2\lambda + \mu \) and \( \nu = \nu_{\text{max}} = \mu \)
is called the highest-weight state and corresponds to the distribution of the quanta for which the deformation of the system is maximum. Elliott showed that all the spatial states \( |\lambda,\mu\rangle_{KLM}\) can be projected from the highest-weight state using the Hill-Wheeler projection technique:

\[
|\lambda,\mu\rangle_{KLM} = \frac{(2L+1)}{a[\lambda,\mu]_{L,K}} \int d(\Omega) \, D_{MK}^* (\Omega) \, R(\Omega) \, |\lambda,\mu\rangle_{\max} |\alpha_{\max}\rangle, \tag{2.30}
\]

where \( R(\Omega) \) is the rotation operator and \( a[\lambda,\mu]_{L,K} \) are normalization coefficients. (The labels \([1^m][f(d)]\alpha \) are suppressed (2.30) because they are not affected by the projection.) Since these \( |\lambda,\mu\rangle_{KLM}\) states are projected from an intrinsic state with maximum deformation, they are close to the eigenstates of systems with well-defined deformation.

Elliott (EllWil 68) also showed that the LS-coupled basis states given in (2.29) can be expressed as a sum over projections \( K_j = K + K_S \) of another set of projected functions defined by

\[
|\gamma K_S K_J M\rangle = \frac{(2J+1)}{a[\lambda,\mu]_{SK_S K_J}} \int D_{MK}^* (\Omega) \, \Phi_{\Omega}(\gamma K_S) d\Omega \tag{2.31}
\]

where the intrinsic function \( \Phi_{\Omega}(\gamma K_S) \) in this expression involves the spin and its projection \( K_S \) along the body-fixed symmetry axis in addition to a spatial part. In (2.31), the symbol \( \gamma = [1^m][f(d)]\alpha(\lambda\mu)\beta(ST) \) and the coefficients \( a[\lambda,\mu]_{SK_S K_J} \) are chosen to ensure normalization. For a given \( S \) and \( (\lambda,\mu) \), the labels \( K_S, K_J, \) and \( J \) in the basis (2.31) are restricted (EllWil 68) as follows:
\[ K_S = S, (S - 1), \ldots, -S, \]
\[ K_J = K_S + K_L \geq 0, \text{ where } K_L = \mu, (\mu - 2), \ldots, -\mu, \quad (2.32) \]
\[ J = K_J, K_J + 1, \ldots, (\lambda + \mu + S), \]

with the exception that for \( K_J = 0 \), \( K_L \geq 0 \) only, and if \( K_J = K_S = K_L = 0 \), then \( J \) is even or odd as \( \lambda + S \) is even or odd. The states defined by (2.31) is not only lacking orthogonality, but is also overcomplete, a complication which occurs for high values of \( J \).

We suggest a modification to rule (2.32) with the upper limit on \( J \) values changed from \( (\lambda + \mu + S) \) to \( J_{\text{max}} \) defined by

\[
J_{\text{max}} = (\lambda + \mu + 1) - 2 |K_L| + K \quad \text{when } K_L > 0 \text{ and } K \geq (S - K_L) \\
= (\lambda + \mu + 1) - 1 |K_L| + 2K - S \quad \text{when } K_L > 0 \text{ and } K < (S - K_L) \\
= (\lambda + \mu) - |K_L| + 2K - S \quad \text{when } K_L \leq 0. \quad (2.33)
\]

Although the assignment of the maximum value of \( J \) for each \( K_J \) label is not unique, this makes no real difference because the \( K_J \) label serves only to distinguish the multiple occurrences of \( J \). The rule (2.32) (EllWil 68) with (2.33) not only removes the redundancy in the \( J \) values and restricts them to only those values which are possible to form from the angular momentum coupling formula \( J = L + S, L+ S - 1, \ldots, |L - S| \), but also gives the correct dimensionality \( \{d[(\lambda, \mu)S] = (2S+1)(\lambda+\mu+2)(\lambda+1)(\mu+1)/2 \} \) of the states in an \( SU(3) \) irrep \( (\lambda, \mu) \) for a fixed value of \( S \).

While the task of reducing the huge model space can be achieved by partitioning the space into smaller subspaces using group symmetries, one can go even further. Elliott (Ell 66) showed that the long-range nucleon-nucleon
interaction is determined by a quadrupole-quadrupole force which can be written in terms of generators of SU(3) as follows:

\[ Q^a Q^a = 4 C_2 - 3L^2, \]  

(2.34)

where \( C_2 \) is the second degree Casimir operator of SU(3) and has eigenvalue \( (\lambda^2 + \mu^2 + \lambda\mu + 3\lambda + 3\mu) \). It can now be seen that within a single irrep of SU(3) the eigenvalue of the operator \( Q^a Q^a \) is given by \( 4\langle C_2 \rangle - 3L(L+1) \), which means that the quadrupole-quadrupole interaction gives rise to a rotational spectrum. Since rotational spectra are found at low-lying energies the irrep with maximum \( \langle C_2 \rangle \) dominates the low-lying energy region. This irrep is called the leading irrep and can be found by maximizing \( \langle C_2 \rangle \). It is easy to see how through the application of algebraic methods we can partition full space into many small subspaces and out of these how the most dominant set of states can be identified and as a result how the computational requirements can be reduced.

Here we have used group symmetries to help in the selection of a physically meaningful and manageable basis for a shell-model theory of nuclear structure. A second required step in the algebraic treatment using dynamical symmetries is the construction of a model hamiltonian using generators of the same symmetry groups used in the basis selection. This problem will be considered in Chapter 3 where a model hamiltonian for a triaxial rotor is formed using SO(3) scalar combinations of generators of SU(3).
2.5. **Pseudo-spin Symmetry for A > 100.**

As previously noted, the three-dimensional isotropic harmonic oscillator, \( H_0 \), with the 1-body \( l \cdot s \) and \( l^2 \) interactions included is a good approximation for the nuclear single-particle hamiltonian \( H \):

\[
H = H_0 + C l \cdot s + Dl^2.
\]  

(2.35)

The strength \( C \) of the \( l \cdot s \) term (with eigenvalue \( \langle l \cdot s \rangle = \frac{1}{2} l(l+1) - l(l+1) - s(s+1) \)) that is required to get shell closures at the magic numbers is so large that for heavy \( (A > 28) \) nuclei the underlying \( SU(3) \) symmetry of the oscillator is destroyed. This means Elliott's \( SU(3) \) model cannot be applied to heavy nuclei. In particular, the \( j_{\text{max}} = N+1/2 \) state of the \( N \)-th shell is pushed down among the orbitals of the next lower shell. The \( N \)-th oscillator shell therefore includes — in addition to the normal-parity \( j = 1/2, 3/2, ..., N-1/2 \) orbitals — a unique-parity \( j = N+3/2 \) intruder level from the shell immediately above. These normal-parity orbitals of the \( N \)-th oscillator shell can be organized into levels of a pseudo oscillator shell with \( \bar{N} = N - 1 \).

As an example, consider the \( N = 4 \) shell. It consists of the \( (1g_9/2, 1g_7/2, 2d_5/2, 2d_3/2, 3s_1/2) \) orbitals. The \( 1g_9/2 \) orbital of this set is pushed down among the levels of the \( N = 3 \) shell and the remaining normal-parity levels can be relabelled and identified as the four levels \( (1\bar{f}_7/2, 1\bar{f}_5/2, 2\bar{p}_3/2, 2\bar{p}_1/2) \) of an \( \bar{N} = 3 \) shell. The complete shell is then comprised of these four (\( \bar{N} = 3 \)) normal-parity orbitals along with the unique-parity \( i_{11/2} \) intruder level from the \( N = 5 \) shell above. This situation is illustrated in fig. 2.5. This mapping of
Figure 2.5. Diagram showing how the levels of a shell-model hamiltonian [fig. (2.2)] can be relabelled as normal and unique-parity orbitals of a pseudo oscillator shell. The highest j level of the N-th oscillator shell is pushed down among the orbitals of the next lower shell. The j = N+3/2 intruder level from the next higher shell penetrates down into the valence space (normal parity levels) and has a different (unique) parity.
normal-parity single-particle orbitals defines the pseudo coupling scheme and has the following simple form:

\[ |N(\tilde{I}, \tilde{s}) \tilde{J} \tilde{m}> = U_{N j m, N \tilde{J} \tilde{m}} (I, \tilde{T}) |N(l, s) j m>, \]

\[ U_{N j m, N \tilde{J} \tilde{m}} (I, \tilde{T}) = \delta_{N-1, N} \delta_{j, \tilde{J}} \delta_{m, \tilde{m}} \delta_{l \pm 1/2, \tilde{T} \pm 1/2}. \quad (2.36) \]

It can be seen from the structure of \( U_{N j m, N \tilde{J} \tilde{m}} (I, \tilde{T}) \) that the transformation is simply a relabeling of the basis states with all levels of the \( N \)-th shell, less the one with \( j = N+1/2 \), associated with levels of \( \tilde{N} \)-th shell of another pseudo oscillator with algebraic properties that are identical to those of normal oscillator, where \( \tilde{N} = N-1 \). This unitary transformation must be applied to all quantities, both the operators and their matrix elements, to maintain the physics of the problem.

From this discussion several questions arise. First, does there exist a pseudo form for the hamiltonian having the same excitation spectrum as the normal form? Second, does there exists a simple operator form which transforms the original hamiltonian into its pseudo form? Third, is this scheme useful for heavy nuclei where the neutrons and protons fill different oscillator shells? And fourth, what is the role of intruder level? – specifically, how does the intruder level couple to its like-parity partners and to the normal-parity states resulting from the transformation? These questions have been studied by Draayer (DraNaq 90), Naqvi (NaqDra 92a), and Escher (EscBah 91).
CHAPTER 3
TRIAXIAL ROTOR MODEL

The rotor has always enjoyed a prominent role in physics. Complete results for the rotor in classical mechanics are given in the work of Sommerfeld and Klein (KleSom 97). The rotor was one of the first problems addressed with quantum methods developed independently by Heisenberg (BorHei 26; BorJor 25; Hei 25) and Schrödinger (Sch 26c; Sch 26d; Sch 26a; Sch 26b). Kramers and Ittman (Kraltm 29a; Kraltm 29b; Kraltm 30) solved the Schrödinger equation for the case of an asymmetric rotor geometry whereas O. Klein (Kle 29) solved the same problem using Heisenberg's matrix methods. This work on the rotor was extended by Ray (Ray 32) and R. G. B. Casimir (Cas 31) using algebraic techniques.

Casimir established a relationship between the eigenfunctions of the rotor and irreducible representations of the rotation group in three dimensions. This work clearly demonstrates the advantage of using algebraic techniques over analytic methods for systems where the Hamiltonian possesses a higher symmetry than rotational invariance. The dynamics of a quantum rotor found its earliest application in the fields of atomic and molecular physics. With the advent of nuclear structure data showing rotational features, it quickly became a model of choice in nuclear physics and it is now commonly applied in the study of nuclei with spectra that show rotational characteristics. Later on, in an attempt to bring the shell model and geometric models closer together, Elliott
(Ell 58) showed that a quadrupole-quadrupole interaction operating in a space partitioned into irreducible representations of SU(3) produces rotational spectra in a very simple and natural manner. Leschber (Les 87) established an explicit algebraic realization of rotor for integral values of angular momentum and zero spin using the Elliott SU(3) model. This approach is extended to include non-zero spin values and half-integral values of total angular momentum in what follows.

3.1 Hamiltonian and Bases States

The hamiltonian of a triaxial rotor $H_R$ is given by:

$$ H_R = \sum_{\alpha=1}^{3} A_\alpha I_\alpha^2. \quad (3.1) $$

where $A_\alpha = 1/2I_\alpha$ are the inertia parameters, and $I_\alpha$ are the projections of the angular momentum operator $I$ on the $\alpha$-th axis in the body-fixed frame of reference. It should be pointed out that the commutation rules for the $I_\alpha$ differ by a minus sign from those for the projections of angular momentum operator on the laboratory frame axes, $I_k$:

$$ [ I_\alpha, I_\beta ] = -i\epsilon_{\alpha\beta\gamma} I_\gamma. \quad (3.2) $$

whereas,

$$ [ I_\alpha^L, I_\beta^L ] = i\epsilon_{\alpha\beta\gamma} I_\gamma^L. \quad (3.3) $$
The inertia parameters $A_\alpha$ are chosen using the convention $A_2 \leq A_1 \leq A_3$. These conditions can be satisfied by an appropriate assignment of the numbers 1, 2, and 3 to one of the six possible permutations of the $x$, $y$, and $z$ axes shown in Table 3.1. The inertia parameters are related to the shape variables $\beta$ (2.5) and $\gamma$ (2.6) by,

$$I_\alpha \sim \beta^2 \sin^2 \left( \frac{\gamma - \frac{2}{3} \pi \alpha}{2} \right). \quad (3.4)$$

An asymmetry parameter $\kappa$, related to the inertia ellipsoid and defined by

$$\kappa = \frac{2A_1 - A_2 - A_3}{A_3 - A_2}, \quad (3.5)$$

can also be used to describe the shape: $\kappa = -1$ for $A_1 = A_2 < A_3$, a prolate shape; and $\kappa = 1$ for $A_2 < A_1 = A_3$, an oblate geometry. The value $\kappa = 0$ represents the most asymmetric case.

We now return to a consideration of the rotor Hamiltonian $H_R$ given in (3.1). The symmetry properties of this Hamiltonian, its eigenvalues and eigenfunctions, and the grouping of basis states into different classes according to their transformation properties under axis permutations have been given by Leschber (Les 87). As mentioned earlier however, Leschber's work focused only on integral values of the angular momentum and the spin $S=0$ case. Since many of those results carry over to the $S\neq0$ case (integral as well as half-integral total angular momentum) which is the focus of this work, important features of that theory will be reviewed in what follows.
Table 3.1  Different choices for the assignment of x, y, and z to $A_1$, $A_2$, and $A_3$, such that the inertia parameters satisfy the condition $A_2 \leq A_1 \leq A_3$. In the table R and L refer to right and left-handed coordinate systems, respectively.

<table>
<thead>
<tr>
<th></th>
<th>Choice I</th>
<th></th>
<th>Choice II</th>
<th></th>
<th>Choice III</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>R</td>
<td>L</td>
<td>R</td>
<td>L</td>
<td>R</td>
</tr>
<tr>
<td>x</td>
<td>$A_2$</td>
<td>$A_1$</td>
<td>$A_1$</td>
<td>$A_3$</td>
<td>$A_3$</td>
</tr>
<tr>
<td>y</td>
<td>$A_1$</td>
<td>$A_2$</td>
<td>$A_3$</td>
<td>$A_1$</td>
<td>$A_2$</td>
</tr>
<tr>
<td>z</td>
<td>$A_3$</td>
<td>$A_3$</td>
<td>$A_2$</td>
<td>$A_2$</td>
<td>$A_1$</td>
</tr>
</tbody>
</table>
The Wigner D-functions, $D^l_{K,M}$, provide a complete set of basis states for the quantum rotor. The operator $I_3$ is diagonal in this basis with eigenvalues $K (K=I, I+1, \ldots, -I)$ and the matrix elements of the $I_3^2$ are given by,

\[ [I_3^2]_{K,K} = K^2, \quad (3.6b) \]

\[ [I_3^2]_{K,K+2} = -[1^1]_{K,K+2} = \left(\frac{1}{1} \right)^{K+1} \left(1+1\right)^{K+2} \left(1-1\right)^{K} \left(1+1\right)^{K+2} \right]^{1/2}, \quad (3.6c) \]

where the labels of the angular momentum operator $I$ and its projection in the lab-frame have been omitted because they are good quantum numbers.

Matrix elements of the rotor hamiltonian in this D-function basis can be found by using eqs. (3.6) to be,

\[ [H_R]_{K,K} = \frac{1}{2} \left( A_1 + A_2 \right) \frac{1}{\left( 1 + 1 \right)} + K^2 \left( 2A_3 - A_2 - A_1 \right), \quad (3.7a) \]

\[ [H_R]_{K,K+2} = \frac{1}{2} \left( A_1 - A_2 \right) [f(I,K+1)]^{1/2}. \quad (3.7b) \]

The function $f(m,n)$ in eq. (3.7) is defined as

\[ f(m,n) = f(m,-n) = \frac{1}{4} (m-n)(m+n)(m-n+1)(m+n+1). \quad (3.8) \]
The \((2I+1)\times(2I+1)\) hamiltonian matrix \(H_R\) can be diagonalized and its eigenvalues determined. How this Hamiltonian matrix can be transformed to a simpler block-diagonal form using the invariance of \(H_R\) under rotations by \(\pi\) around the principal axes is the topic of the next section.

### 3.1.1 Even A and Integral Angular Momentum

Ray was first to recognize that \(H_R\) is invariant under \(\pi\) rotations about the principal axes. These transformations can be written as,

\[
T_\alpha = \exp(-iI\alpha); \quad \alpha = 1,2,3. \tag{3.9}
\]

The invariance means \(H_R\) commutes with \(T_\alpha\): 
\[
[\mathbf{H}_R, T_\alpha] = 0.
\]

For integral values of \(I_\alpha\) these transformations, together with the identity operation \(E\), form the \(D_2\) symmetry group (Vierergruppe) with elements \(\{E, T_1, T_2, T_3\}\). This group has four classes. The multiplication table, its irreducible representations, and the character table of \(D_2\) are given in tables 3.2, 3.3, and 3.4, respectively.

The Wigner D-functions transform under the action of \(T_\alpha\) as follows:

\[
T_1D^I_{MK} = (-1)^{I+K} D^I_{M-K},
\]

\[
T_2D^I_{MK} = (-1)^I D^I_{M-K},
\]

\[
T_3D^I_{MK} = (-1)^K D^I_{M-K}. \tag{3.10}
\]
Table 3.2  Multiplication table for the $D_2$ symmetry group.

<table>
<thead>
<tr>
<th></th>
<th>$E$</th>
<th>$A=T_1$</th>
<th>$B=T_2$</th>
<th>$AB=T_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>$E$</td>
<td>$A$</td>
<td>$B$</td>
<td>$AB$</td>
</tr>
<tr>
<td>$A$</td>
<td>$A$</td>
<td>$E$</td>
<td>$AB$</td>
<td>$B$</td>
</tr>
<tr>
<td>$B$</td>
<td>$B$</td>
<td>$AB$</td>
<td>$E$</td>
<td>$A$</td>
</tr>
<tr>
<td>$AB$</td>
<td>$AB$</td>
<td>$B$</td>
<td>$A$</td>
<td>$E$</td>
</tr>
</tbody>
</table>
Table 3.3  Irreducible representations of the D_2 symmetry group.

<table>
<thead>
<tr>
<th>Irrep</th>
<th>Element</th>
<th>E</th>
<th>A=T_1</th>
<th>B=T_2</th>
<th>AB=T_3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Γ(1)</td>
<td></td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Γ(2)</td>
<td></td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>Γ(3)</td>
<td></td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>Γ(4)</td>
<td></td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>
Table 3.4  Character table for the $D_2$ symmetry group.

<table>
<thead>
<tr>
<th>Character/Class</th>
<th>(E)</th>
<th>(A=T1)</th>
<th>(B=T2)</th>
<th>(AB=T3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi^{(1)}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\chi^{(2)}$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$\chi^{(3)}$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$\chi^{(4)}$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>
It follows from these transformation properties that functions which transform irreducibly under $D_2$ can be constructed out of combinations of the Wigner D-functions. Because the rotor Hamiltonian is invariant under $D_2$, these combinations are also appropriate basis states for the symmetric rotor:

\[
\psi_{SR}^{(\lambda \mu)KL} = \frac{2l+1}{16\pi^2(1 + \delta_{K0})} \left[ D_{MK} + (-1)^{\lambda+\mu+1} D_{M,K} \right]. \tag{3.11}
\]

In eq. (3.11), the $\lambda$ and $\mu$ are integers (even or odd) with $\mu$ even or odd as $K$ is even or odd. Acting with the elements of $D_2$ on the bases set given in eq. (3.11), and using the properties of D-functions under this group, eq. (3.10), it can be shown that these wavefunctions transform irreducibly under $D_2$, see table 3.5. Leschber (Les 87) has given a detailed account of these properties and their various consequences. Matrix elements of the rotor Hamiltonian with respect to these basis states are:

\[
\langle \psi_{SR}^{(\lambda \mu)KL} | H_R | \psi_{SR}^{(\lambda \mu)KL} \rangle = \frac{(H_R)_{K',K} + (-1)^{\lambda+\mu+1}(H_R)_{K,K'}}{\sqrt{(1+\delta_{K0})(1+\delta_{K'0})}}. \tag{3.12}
\]

The Hamiltonian matrix is block diagonal in this representation (fixed $\lambda$ and $\mu$ values) so and the task of diagonalizing the $(2l+1)\times(2l+1)$ matrix is reduced to diagonalizing smaller submatrices. The classification of the bases states into irreps of $D_2$ and the dimensions of the submatrices are given in table 3.5. The wavefunctions of the asymmetric rotor Hamiltonian can be given as:
Table 3.5. Classification of the eigenstates of a symmetric rotor according to their transformation properties under the group $D_2$. $T_\alpha$ corresponds to a rotation by $\pi$ rotations about the $\alpha$-th principal axis [see eq. (3.9)]. The total dimensionality in each case is $(2I+1)$.

<table>
<thead>
<tr>
<th>Symmetry type</th>
<th>Transformation</th>
<th>Index</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E$</td>
<td>$T_1$</td>
<td>$T_2$</td>
</tr>
<tr>
<td>$A$</td>
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<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$B_3$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_2$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>$B_1$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>

Total Dimensionality  $2I+1$  $2I+1$
\[ \Psi^{(\lambda \mu)\lambda l}_{K M} = \sum_{K \geq 0} C^{(\lambda \mu)\lambda l}_{K} \Psi^{(\lambda \mu)\lambda l}_{SR M}, \]  

(3.13)

where the prime over the summation sign means that the sum is over only even or odd values of \( K \).

So far nothing has been said about the spin degree-of-freedom; only the spin \( S=0 \) case has been considered. When the rotor is assigned a spin, there are a total of \((2L+1) \times (2L+1) \times (2S+1)\) basis states for each \((L,S)\) combination, where we assume that \( L \) does not itself involve the spin. If the total angular momentum of the system \((I=L+S)\) and spin \((S)\) are invariant symmetries of the hamiltonian, the dimensionality of the model spaces will be determined by the number of different ways a particular \((I,S)\) combination can be formed: \( d = \Sigma (2L+1) \times (2L+1) \times (2S+1), \) where the sum \((\Sigma)\) runs over all \( L \) values in the range \( |I-S| \) to \( I+S \). This is a weak-coupling picture, where the total angular momentum \((I)\) results from the coupling of an "orbital" part \((L)\) to the "spin" part \((S)\). When the \( I_\alpha \) in \( H_R \) are taken to be components of the total angular momentum (so half-integral as well as integral \( I \) values can be realized), one has a strong-coupling scenario. In this case the basis states are again Wigner \( D \)-functions but for integral or half-integral, representations, as appropriate. The integral case is a straightforward extension of the \( S=0 \) scenario, whereas if half-integral angular momentum is also included the hamiltonian displays another symmetry which is the subject of the next section.
3.1.2 Odd A and Half-integral Angular Momentum

It can be easily verified that the hamiltonian $H_R$ is not invariant under the $T_\alpha$ transformations of (3.9) for half-integral values of angular momentum. When acting on wavefunctions with half-integral angular momentum, the $T_\alpha$ follow the following multiplication rules:

$$T_\alpha T_\beta = -T_\beta T_\alpha = T_\gamma,$$

$$T^2_\alpha = \exp(-2i\pi I_\alpha) = -1 , \quad (3.14)$$

where $\alpha$, $\beta$, and $\gamma$ are permuted cyclically and can have values 1, 2, and 3. These properties indicate that the $T_\alpha$ (with half-integral $I_\alpha$ values included) together with the identity are elements of another group structure with eight members: \{E, $T_1, T_2, T_3, -E, -T_1, -T_2, -T_3$\).

The rotor hamiltonian with integral and half-integral angular momentum values is invariant under the operation of the members of this new larger symmetry group. As for the case of integral angular momentum values, the invariance of $H_R$ under this set of transformations means the basis states for the problem should be divided into classes which transform irreducibly under this new group, because when this is done the hamiltonian matrix will be block diagonal with zero matrix elements between basis states belonging to different irreps. So what is this new group? It is a realization of the quaternion group which has five classes and therefore five different irreducible representations. Four of the five irreps are one dimensional whereas the fifth is a faithful two-dimensional representation. Acting with the elements of quaternion group on
bases (3.10), and using the transformation properties of the D functions under elements of this group when both integral and half-integral values of angular momentum are allowed, it can be shown that the wavefunctions transform irreducibly under quaternion group. The wavefunctions with integral values of angular momentum transform irreducibly according to the four one-dimensional irreps whereas those with half-integral angular momentum transform according to the one two-dimensional irrep. The class structure, its irreps, and the characters of the quaternion group are given in tables 3.6. and 3.7.

3.2. SU(3) Image of the Triaxial Rotor

In this section we will establish a connection between the rotor and shell-model pictures. This was done for the S=0 case by Leschber; our results are for the more general case when S≠0, with half-integral as well as integral S values taken into consideration. The theory is applicable to both even-A and odd-A nuclei and will lead to the notion of an extended collective model picture — one that includes S(integer)>0 configurations for even-A systems and a generalized Nilsson picture with S(half-integer)>1/2 for odd-A nuclei.

3.2.1 Algebraic Connection

A shell-model image of the rotor hamiltonian (3.1) can be realized most simply by rewriting H_R in a frame independent representation by introducing three rotational scalars, J^2, Y_3^c and Y_4^c, given by
Table 3.6 Irreducible representations of the quaternion group.

<table>
<thead>
<tr>
<th>Irrep \ Element</th>
<th>E</th>
<th>i</th>
<th>j</th>
<th>k</th>
<th>$i^2=j^2=k^2$</th>
<th>$j^3$</th>
<th>$j^3$</th>
<th>$k^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma(1)$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\Gamma(2)$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$\Gamma(3)$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$\Gamma(4)$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
<tr>
<td>$\Gamma(5)$</td>
<td>$\begin{pmatrix} 1 &amp; 0 \ 0 &amp; 1 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; -i \ -i &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; -1 \ -1 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} i &amp; 0 \ 0 &amp; -i \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; i \ i &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} 0 &amp; 1 \ 1 &amp; 0 \end{pmatrix}$</td>
<td>$\begin{pmatrix} i &amp; 0 \ 0 &amp; -i \end{pmatrix}$</td>
<td></td>
</tr>
</tbody>
</table>
Table 3.7  Character table for the quaternion group.

<table>
<thead>
<tr>
<th>Character</th>
<th>Element</th>
<th>E</th>
<th>(i,i^3)</th>
<th>(j,j^3)</th>
<th>(k,k^3)</th>
<th>(i^2=j^2=k^2=E)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\chi^{(1)})</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\chi^{(2)})</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\chi^{(3)})</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\chi^{(4)})</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>(\chi^{(5)})</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-2</td>
</tr>
</tbody>
</table>
\[
J^2 = \sum_{\alpha} J_{\alpha}^2 = \sum_{\alpha} I_{\alpha}^2, \\
Y_3^5 = \sum_{\alpha,\beta} J_{\alpha} Q_{\alpha \beta} J_{\beta} = \sum_{\alpha} \lambda_{\alpha} I_{\alpha}^2, \\
Y_4^5 = \sum_{\alpha,\beta,\gamma} J_{\alpha} Q_{\alpha \beta} Q_{\beta \gamma} J_{\gamma} = \sum_{\alpha} \lambda_{\alpha} I_{\alpha}^2, \\
\]

(3.15)

where \( J_\alpha \) and \( Q_{\alpha \beta} \) are the Cartesian components of the total angular momentum and full collective quadrupole operators, respectively, and the \( \lambda_\alpha \) are the eigenvalues of \( Q^c \) in the body-fixed, principal-axis system: \( (Q_{\alpha \beta}^c)^{BF/PA} = \lambda_{\alpha} \delta_{\alpha \beta} \). The microscopic expressions for \( J_\alpha \) and \( Q_{\alpha \beta}^c \) are

\[
J_\alpha = \sum_i j_\alpha (i) \\
Q_{\alpha \beta}^c = \sum_i q_{\alpha \beta} (i) \\
\]

(3.16)

where \( j_\alpha \) and \( q_{\alpha \beta} \) are the Cartesian components of the single-particle total angular momentum \( (\vec{j} = \vec{j}_s + \vec{j}_p) \) and collective quadrupole \( (q_{\alpha \beta} = x_{\alpha \beta} - \frac{1}{3} r_2 \delta_{\alpha \beta}) \) operators, respectively, and the sum extends over all particles of the system.

Equations (3.15) can be solved for the \( I_j^2 \)'s to obtain

\[
I_j^2 = (\lambda_1 \lambda_2 \lambda_3 J^2 + \lambda_j^2 Y_3^5 + \lambda_1 Y_4^5) / (2 \lambda_1^3 + \lambda_1 \lambda_2 \lambda_3) \\
\]

(3.17)

and the corresponding hamiltonian is then given as

\[
H_{\text{ROT}} = a J^2 + b Y_3^5 + c Y_4^5, \\
\]

(3.18)
where

\[
\begin{align*}
    a &= \sum_{i=1}^{3} a_i A_i, \quad a_i = \lambda_1 \lambda_2 \lambda_3 / D_i, \\
    b &= \sum_{i=1}^{3} b_i A_i, \quad b_i = \lambda_i^2 / D_i, \\
    c &= \sum_{i=1}^{3} c_i A_i, \quad c_i = \lambda_i / D_i,
\end{align*}
\]

and

\[
D_i = 2 \lambda_i^3 + \lambda_1 \lambda_2 \lambda_3.
\]

Having obtained these expressions for \(a, b, \) and \(c\) in terms of the \(A_i\)'s, note that in a shell-model framework \(Q_{\alpha \beta}^c\) has nonzero matrix elements between oscillator shells that differ by \(\pm 2\) quanta, that is, between shells with principal quantum numbers \(n\) and \(n' = n \pm 2\). This means that \(Y_3^c\), which involves one \(Q^c\), and \(Y_4^c\), which involves two, have matrix elements coupling shells that differ by \(\Delta n = \pm 2\) and \(\Delta n = \pm 2 \& \pm 4\) quanta, respectively. Since the off-diagonal \(n' = n \pm 2\) matrix elements of \(Q^c\) are comparable in size to the diagonal \(n' = n\) ones, even small multipliers for \(Y_3^c\) and \(Y_4^c\) in the hamiltonian can generate strong mixing among different major shells. Of course, the magnitude of these off-diagonal \(n' \neq n\) couplings are to be compared with the corresponding shell separation energy, \(2\hbar \omega\) for the \(\Delta n = \pm 2\) and \(4\hbar \omega\) for the \(\Delta n = \pm 4\) cases, that is generated by the underlying harmonic oscillator hamiltonian.

One way to resolve this matter and at the same time gain a consistent shell-model description of rotational motion is to simply set the off-diagonal \(\Delta n \neq 0\) matrix elements to zero and thereby transform \(Q_{\alpha \beta}^c\) into the algebraic quadrupole operator \(Q_{\alpha \beta}^a\) of Elliott (Ell 58; EllHar 63; EllWil 68) who has...
shown that this $Q^{a}_{\alpha\beta}$ together with the angular momentum operators $L_\alpha$ generate the SU(3) algebra. The shell-model hamiltonian then takes the form

$$H_{SU3} = H_0 + aJ^2 + bY_3^3 + cY_4^4$$

(3.21)

To complete the mapping from $H_{ROT}$ to $H_{SU3}$, shell-model expressions for the $\lambda_i$'s are required. Since SU(3) is a rank two group it has two invariants (Casimir operators) that are usually labelled $C_2(\lambda,\mu)$ and $C_3(\lambda,\mu)$ with eigenvalues $(\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu)$ and $(\lambda-\mu)(\lambda+2\mu+3)(2\lambda+\mu+3)$, respectively. Here $\lambda$ and $\mu$ are irreducible representation (irrep) labels of SU(3) with $\lambda+\mu$ and $\mu$ specifying, respectively, the number of boxes in first and second row of a Young diagram labelling of the irrep.

The symmetry group of the rotor is the semi-direct product group $T_5 \ltimes SU(2)$ generated by the five independent components of the quadrupole operator and the three components of the angular momentum $J$ where $J = I = L + S$. Using the fact that the generators of the $T_5$ and SU(3) algebras act in different spaces we have, as is shown schematically in fig. 3.1., that $[T_5 \ltimes SO_L(3)] \otimes SU_S(2) \rightarrow T_5 \ltimes [SO_L(3) \otimes SU_S(2)] \rightarrow T_5 \ltimes SU(2)$. For the special case when spin is zero, the $T_5 \ltimes SU(2)$ symmetry group of the rotor reduces to $T_5 \ltimes SO_L(3)$. The symmetry group of the rotor has two invariants, namely $\text{Tr}[(Q^c)^2]$ and $\text{Tr}[(Q^c)^3]$ with eigenvalues $(\lambda_1^2+\lambda_2^2+\lambda_3^2)$ and $\lambda_1\lambda_2\lambda_3$, respectively. By requiring a linear relation between the invariants of the rotor and SU(3) $\supset SO_L(3)$ groups and insisting on the geometrical interpretation of the $\beta$ and $\gamma$ shape variables of the collective model, the following expressions for the $\lambda_i$'s in terms of $\lambda$ and $\mu$ can be determined (CasDra 88).
Figure 3.1. Schematic diagram showing the mapping between the symmetry group of rotor and $SU(3) \rightarrow SO(3)$.
\[ \begin{align*}
\lambda_1 &= \frac{\mu - \lambda}{3} \\
\lambda_2 &= \frac{- (\lambda + 2 \mu + 3)}{3} \\
\lambda_3 &= \frac{2 \lambda + \mu + 3}{3}
\end{align*} \tag{3.22} \]

This completes the \( H_{\text{ROT}} \leftrightarrow H_{\text{SU3}} \) mapping.

### 3.2.2 Matrix Elements

In this section, explicit expressions are given for matrix elements of the \( Y_3^a \) and \( Y_4^a \) operators (and therefore for the hamiltonian) in the angular-momentum-projected (Ell 58) and orthonormalized (Ver 68) basis of the SU(3) \( \supset \) SO(3) coupling scheme:

\[
| m[f\alpha(\lambda,\mu)\kappa L][\tilde{f}]\beta STM_T;JM_J \rangle = | \gamma(\lambda,\mu)\kappa LSJ M_J \rangle,
\]

\[ \gamma = m[f\alpha][\tilde{f}]\beta TM_T, \tag{3.23} \]

where

- \( m = \) total number of particles in \( N \)-th oscillator shell
- \([f] = U[(N+1)(N+2)/2] \) spatial symmetry label
- \( \alpha = \) multiplicity of the \((\lambda,\mu)\) irrep in \([f]\)
- \((\lambda,\mu) = \) SU(3) irrep label
- \( \kappa = \) multiplicity of \( L \) in \((\lambda,\mu)\)
- \( L = \) total orbital angular momentum
- \([\tilde{f}] = U(4) \) spin-isospin symmetry label conjugate to \([f]\)
- \( S = \) total spin
- \( T = \) total isospin
\[ M_T = \text{isospin projection} \]

Notice that the multiplicity label \( \kappa \) is different from \( K \) given in eq. (2.29). This is due to the fact that basis states identified in eq. (2.29) are not orthonormalized (Ell 58) whereas the use here of \( \kappa \) rather than \( K \) indicates an orthonormalized basis. (Ver 68).

Matrix elements of the \( Y^a \)'s can be determined in terms of reduced \( SU(3) \supset SO(3) \) coupling coefficients (also called isoscalar factors) and \( SU(2) \) recoupling coefficients (DraRos 85). Since computer programs for evaluating these coefficients are available (AkiDra 73) numerical results for cases of interest can be generated.

It can be easily shown that

\[
Y_3 = \sum_{\alpha, \beta} J_\alpha Q_{\alpha \beta} J_\beta = \frac{\sqrt{30}}{6} \left[ (J \times Q)^1 \times J \right]^0
\]

and

\[
Y_4 = \sum_{\alpha, \beta, \gamma} J_\alpha Q_{\alpha \beta} Q_{\beta \gamma} J_\gamma = \frac{\sqrt{3}}{18} \left[ (J \times Q)^1 \times [Q \times J]^1 \right]^0. \tag{3.25}
\]

Since the reduced matrix elements of \( Q^a \) are known, the reduced matrix elements of \( [J \times Q^a]^1 \times J \) and \( [J \times Q^a]^k \times [Q^a \times J]^k \) \( (k = 1 \text{ for } Y_4^a) \) and therefore of \( Y_3^a \) and \( Y_4^a \), which are diagonal in all but \( \kappa \) and \( L \), can be calculated. They are given by
\[
\langle \gamma(\lambda, \mu) \kappa L SJ \parallel Y \parallel \gamma(\lambda, \mu) \kappa' L' SJ \rangle
\]
\[
= \sqrt{\frac{5}{6}} J(J + 1)(2J + 1) W(J1J1;J2) \times
\]
\[
\langle (\lambda, \mu) \kappa L J \parallel Q^* \parallel (\lambda, \mu) \kappa' L' J \rangle
\]
\[
= (-1)^{J'} \sqrt{\frac{10}{3}} J(J + 1)(2J + 1) \sqrt{C_2(\lambda, \mu)(2L + 1)} \times
\]
\[
W(J1J1;J2) W(SJL2;L'J) \langle (\lambda, \mu) \kappa' L';(1,1)12 \parallel (\lambda, \mu) \kappa L \parallel_p = 1 \rangle \quad (3.26)
\]

and

\[
\langle \gamma(\lambda, \mu) \kappa LSJ \parallel Y \parallel \gamma(\lambda, \mu) \kappa' L' SJ \rangle = \frac{5}{6} J(J+1)(2J+1) \sum_{\kappa' L' J'} (-1)^{J'} [W(1J2J;J1)]^2 \times
\]
\[
\langle (\lambda, \mu) \kappa LSJ \parallel Q^* \parallel (\lambda, \mu) \kappa'' L'' SJ \parallel (\lambda, \mu) \kappa'' L'' SJ \parallel Q^* \parallel (\lambda, \mu) \kappa' L' SJ \rangle
\]
\[
= \frac{10}{3} J(J + 1)(2J + 1) C_2(\lambda, \mu) \sum_{\kappa'' L'' J''} (-1)^{L''+1} [(2J''+1)(2L''+1)(2L+1) \times
\]
\[
[W(1J2J'';J1)]^2 W(SJ''L2;L''J) W(SJ''L'2;L''J) \times
\]
\[
\langle (\lambda, \mu) \kappa' L';(1,1)12 \parallel (\lambda, \mu) \kappa'' L'' \parallel_p = 1 \times (\lambda, \mu) \kappa'' L'' ;(1,1)12 \parallel (\lambda, \mu) \kappa L \parallel_p = 1 \rangle \quad (3.27)
\]

where in the last forms given for eqs. (3.26) and (3.27) the result
\[
\langle (\lambda,\mu)k\ell s|Q^a| (\lambda,\mu)k'\ell' s' \rangle = (-1)^{\mu} 2\sqrt{c_2}(\lambda,\mu)(2\ell+1)(2\ell'+1) \times \\
W(S\ell\ell';|LJ>(\lambda,\mu)k\ell s=|1,1)12|| (\lambda,\mu)k\ell s= b_1 \quad (3.28)
\]

was used. The phase factor \((-1)^{\mu} = -1\) if \(\mu \neq 0\) and \(+1\) if \(\mu = 0\) is required for consistency with the definition of the SU(3) \(\supset SO(3)\) coupling coefficients (AkiDra 73; DraAki 73; DraRos 85). In these reduced matrix element expressions the \(W's\) are SU(2) Racah coefficients, the \(\langle (\lambda,\mu)k\ell s;|L0,\mu0)K0L0|| (\lambda,\mu)k\ell s= b_1\rangle\) denote SU(3) \(\supset SO(3)\) coupling coefficients that enter as they do because \(Q^a\) is a generator of SU(3) with tensor character \((\lambda_0,\mu_0)K0L0 = (1,1)12\), \(C_2(\lambda,\mu)\) is the second order Casimir operator of SU(3) defined earlier, and the additional state labels, see (3.23), have been suppressed as they must be the same in the bra and ket for a nonvanishing result. These expressions suffice for constructing a matrix representation of \(H_{SU3}\) which can then be diagonalized, as is done in the next section, to obtain eigenvalues and eigenvectors.

3.2.3 Eigenvalue Comparisons

So what have we accomplished? The hamiltonian of an asymmetric rotor for integral and half-integral values of angular momentum has been rewritten in a frame-independent form and we have shown that a similar hamiltonian can be constructed out of products of SU(3) generators that are SO(3) scalar operators (members of the so-called SU(3) \(\supset SO(3)\) integrity basis). In section 3.2.1, formulae were given that relate parameters of the rotor and a shell-model hamiltonian. In this section we demonstrated by using those
formulae that $H_{SU3}$ [eq. (3.23)] reproduces the asymmetric rotor results for odd-A (half-integral angular momenta) cases. Spectra were determined for the rotor hamiltonian $H_R$ with asymmetry parameters $\kappa = \pm 1$, 0 by fixing the inertia parameters to be $A_2 = 1$, $A_3 = 3$, and $A_4 = 3$ ($\kappa = +1$), $1$ ($\kappa = -1$), and $2$ ($\kappa = 0$). The matrix representation of $H_{SU3}$ was calculated and its eigenvalues were determined in the leading normal-SU(3) irrep (Ell 58; EllHar 63; EllWil 68) for $^{25}$Mg [(\(\lambda,\mu\)) = (9,3); $S=\frac{3}{2}$] and the leading pseudo-SU(3) irreps (CasDra 87; DraWee 84a) for $^{159}$Dy [(\(\lambda,\mu\)) = (28,6); $S=\frac{1}{2}$] and $^{165}$Er [(\(\lambda,\mu\)) = (29,8); $S=\frac{1}{2}$]. The results obtained for the $K_j = 1/2$, $3/2$, and $5/2$ bands in these three cases are compared with the corresponding rotor results in figs. 3.2 - 3.10. These plots illustrate the success of the $H_{ROT} \leftrightarrow H_{SU3}$ mapping.

Before proceeding with a detailed discussion of these results, however, we will introduce two microscopic operators which can be used to describe and reproduce the energy splitting of $K_L$-bands ($S=0$) and $K_J$-bands ($S\neq0$) that is a characteristic feature of strongly deformed even-A and odd-A nuclei, respectively. As the $K_L$-band case follows from the $K_J$-band results by setting $S=0$, the discussion will be proceed from the general to the special. For the $K_L$-band case, explicit analytic results with no sums are given for matrix elements of the $X^a$ operators, and therefore for the operator that generates $K_L$-band splitting. While it should be possible to give analytic results in the $S\neq0$ case as well, these have not been worked out since it appears there is little new to be learnt in doing so and for applications it is unnecessary because the numerical results are easy to generate from the results for the $Y^a$ operators, eqs. (3.26), (3.27), and (3.28).
Figure 3.2. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1,A_2,A_3;\kappa) = (2,1,3; 0)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) $\supset$ SO(3) scheme for the leading SU(3) representation $(\lambda,\mu) = (9,3)$ of $^{25}\text{Mg}$. 
Figure 3.3. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1, A_2, A_3; \kappa) = (1,1,3;-1)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) ⊃ SO(3) scheme for the leading SU(3) representation $(\lambda, \mu) = (9,3)$ of $^{25}\text{Mg}$. 

$(\lambda, \mu) = (9,3)$

$\kappa = -1$
Figure 3.4. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1, A_2, A_3; \kappa) = (3, 1, 3; +1)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.2)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) $\supset$ SO(3) scheme for the leading SU(3) representation $(\lambda, \mu) = (9, 3)$ of $^{25}$Mg.
Figure 3.5. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1, A_2, A_3; \kappa) = (2, 1, 3; 0)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) ⊗ SO(3) scheme for the leading pseudo-SU(3) representation $(\lambda, \mu) = (28, 6)$ of the rare earth nucleus $^{159}$Dy.
Figure 3.6. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1,A_2,A_3;\kappa) = (1,1,3;-1)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) $\supset$ SO(3) scheme for the leading pseudo-SU(3) representation $(\lambda,\mu) = (28,6)$ of the rare earth nucleus $^{159}$Dy.
Figure 3.7. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1,A_2,A_3;\kappa) = (3,1,3;+1)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) ⊇ SO(3) scheme for the leading pseudo-SU(3) representation $(\lambda,\mu) = (28,6)$ of the rare earth nucleus $^{159}\text{Dy}$. 
Figure 3.8. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1,A_2,A_3;k) = (2,1,3; 0)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott $SU(3) \supset SO(3)$ scheme for the leading pseudo-$SU(3)$ representation $(\lambda, \mu) = (29,8)$ of the rare earth nucleus $^{165}$Er.
Figure 3.9. Eigenvalues of the rotor hamiltonian $H_R$ [eq. (3.1)] with $(A_1, A_2, A_3; \kappa) = (1, 1, 3; -1)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3) $\supset$ SO(3) scheme for the leading pseudo-SU(3) representation $(\lambda, \mu) = (29, 8)$ of the rare earth nucleus $^{165}$Er.
Figure 3.10. Eigenvalues of the rotor Hamiltonian $H_R$ [eq. (3.1)] with $(A_1, A_2, A_3; \kappa) = (3, 1, 3; +1)$ compared with the eigenvalues of its algebraic image $H_{SU3}$ [eq. (3.21)] in angular-momentum projected and spin-coupled basis states of the Elliott SU(3)$\supset$SO(3) scheme for the leading pseudo-SU(3) representation $(\lambda, \mu) = (29, 8)$ of the rare earth nucleus $^{165}$Er.
3.3 $\mathcal{K}_j^3$ Operator

Large $K_j$-band splitting is observed in the spectra of most odd-$A$ nuclei, where $K_j = K_L + K_S$ is the projection of the total angular momentum ($J = L + S$) on the principal symmetry axis of the system. A simple and tractable shell model description for this energy splitting, as for the collective model, can be given by introducing a $\mathcal{K}_j^3$ operator which is the SU(3) image of $I_3^3$, where $I_3$, as defined earlier, is the projection of the total angular momentum $I$ on the body-fixed symmetry axis. An algebraic expression for the $\mathcal{K}_j^3$ operator and analytic results for its matrix elements in the Elliott SU(3) basis are given in the following sections. In addition, it is applied to some specific light and heavy nuclei to illustrate its usefulness in shell-model applications.

3.3.1 Algebraic Expression for the $\mathcal{K}_j^3$ Operator

Since the $\mathcal{K}_j^3$ operator is the SU(3) shell-model image of $I_3^3$, its algebraic expression can be easily obtained by setting $A_1 = A_2 = 0$ and $A_3 = 1$ in eq. (3.1). Using eqs. (3.19), (3.20), and (3.21) we get

$$\mathcal{K}_j^3 = \left( \lambda_1 \lambda_2 J^2 + \lambda_3 Y_3^3 + Y_3^2 \right) / (2\lambda_3^2 + \lambda_1 \lambda_2),$$

(3.29)

where the $\lambda_i$'s are given in (3.22).
3.3.2 Matrix Elements of the $\mathcal{K}_3^2$ Operator

The form of the $\mathcal{K}_3^2$ operator [eq. (3.29)] suggests that its matrix representation in the bases of eq. (3.23) can be obtained using expressions for matrix elements of the $\mathcal{Y}_3^a$ and $\mathcal{Y}_4^a$ operators given in eqs. (3.26), (3.27), and (3.28). Since these expressions only involve SU(3) isoscalar factors and SU(2) recoupling coefficients, and very general codes for calculating these coupling and recoupling coefficients are available, the matrix elements of the $\mathcal{K}_3^2$ operator can be easily determined for any given set of state labels.

3.3.3 Applications to $^{25}\text{Mg}$, $^{159}\text{Dy}$, and $^{165}\text{Er}$

To test the $\mathcal{K}_3^2$ operator, its matrix representation was calculated and its eigenvalues determined in the leading normal–SU(3) irrep (Ell 58; EllHar 63; EllWil 68) for $^{25}\text{Mg}$ $[\lambda, \mu] = (9,3); S=\frac{1}{2}]$ and the leading pseudo–SU(3) irreps (CasDra 87; DraWee 84a) for $^{159}\text{Dy}$ $[\lambda, \mu] = (28,6); S=\frac{1}{2}]$ and $^{165}\text{Er}$ $[\lambda, \mu] = (29,8); S=\frac{1}{2}]$. The results are shown in figs. 3.11, 3.12, and 3.13, respectively where the eigenvalues of $\mathcal{K}_3^2$ are plotted as a function of the total angular momentum $J$. It is clear from these curves that the shell-model $\mathcal{K}_3^2$ operator really does generate $K_f$–band splitting. For the lowest $J$ values in each band the calculated eigenvalues are almost equal to the collective model value: $\left(\frac{1}{2}\right)^2, \left(\frac{3}{2}\right)^2, \left(\frac{5}{2}\right)^2,$ etc. For higher $J$ values, however, the eigenvalues fall off smoothly with increasing angular momentum such that the eigenvalue of the last member of each band almost reaches down to the lowest $\left(\frac{1}{2}\right)^2$ value. In fact, a question can be raised concerning this; namely, with which band(s)
Figure 3.11. Eigenvalues of the $K^2_J$ operator in angular-momentum projected and spin-coupled basis states for the leading SU(3) representation of $^{25}\text{Mg}$, namely, $(\lambda,\mu) = (9,3)$. Note that whereas for the $K_J = 1/2$ band the eigenvalues of $K^2_J$ are very nearly $1/2^2 = 1/2$, even for the largest $J$ values, the eigenvalues for $K_J = 3/2, 5/2, \text{etc.}$, fall off from the corresponding $K^2_J$ values with the fall off more pronounced the higher the $K_J$ and $J$. This fall off from the expected rotor values is due to the fact that SU(3) is a compact group with finite dimensional irreps while the symmetry group of the rotor, $T_5 \cong SO(3)$, is non-compact and has infinite dimensional representations, specifically, the $K_J$ bands with $J = K_J, K_J+1, \ldots$ do not terminate.
Figure 3.12 Eigenvalues of the $\mathcal{K}_J^2$ operator in angular-momentum projected and spin-coupled basis states for the leading pseudo SU(3) representation of the rare-earth nucleus $^{159}$Dy, namely, $(\lambda, \mu) = (28,6)$. Note that as seen in fig. (3.11) for the $^{25}$Mg case, the eigenvalues of $\mathcal{K}_J^2$ for $K_J = \frac{1}{2}$ are very nearly $\hbar^2 = \frac{4}{4}$, but the values for the higher $K_J$'s fall off from the expected rotor values with the fall off being more pronounced the higher the $K_J$ and $J$. However in this case, the fall off is not as sharp as for $^{25}$Mg because the dimensionality, $d(\lambda, \mu) = \frac{1}{2}(\lambda+\mu+2)(\lambda+1)(\mu+1)$, of the leading representation for $^{25}$Mg, $[d(9,3) = 280]$ is much smaller than for leading representation for $^{159}$Dy $[d(28,6) = 3654]$. 

$^{159}$Dy : ODD - A
( $\lambda, \mu$ ) = (28, 6)
Figure 3.13. Eigenvalues of the $\mathcal{K}_j^2$ operator in angular-momentum projected and spin-coupled basis states for the leading pseudo SU(3) representation of the rare-earth nucleus $^{165}$Er, namely, $(\lambda, \mu) = (29,8)$. The eigenvalues of $\mathcal{K}_j^2$ follow the same pattern as for the $^{25}$Mg [figure (3.11)] and $^{159}$Dy [figure (3.12)] cases. Because the dimensionality of the $(29,8)$ irrep is 5265, the fall off for higher $\mathcal{K}_j^2$ values from the rotor $\mathcal{K}_j^2$ results is slower and occurs for higher $J$ values than in the $^{159}$Dy case.
should the highest \( J \) values be associated? In particular, should the \( J = \lambda + \mu + \frac{1}{2} \) state be associated with the \( K_J = \frac{1}{2} \) or \( K_J = \mu + \frac{1}{2} \) band? Fortunately, the choice makes no difference insofar as calculations are concern because the \( K_J \) label serves only to distinguish multiple occurrences of the \( J \) values. Nonetheless, the \( B(E2) \) transition strengths suggest that the first occurrence of a given \( J \) value should be associated with the lowest \( K_J = \frac{1}{2} \) band, the second with the \( K_J = \frac{3}{2} \) band, etc.

One reason for the fall-off of the eigenvalues of the \( K_J^2 \) operator with increasing \( J \) values within a band is that SU(3) is a compact group with finite dimensional irreps, \( d(\lambda, \mu) = \frac{1}{2}(\lambda + \mu + 2)(\lambda + 1)(\mu + 1) \), as compared with irreps of the corresponding non-compact \( T_5 \wedge SO(3) \) rotor symmetry group which are infinite dimensional. This conclusion is even more obvious upon comparing the results for \( ^{25}\text{Mg} \) with those for \( ^{165}\text{Er} \) and \( ^{159}\text{Dy} \). The dimensionality for \( ^{25}\text{Mg} \) \([d(9,3) = 280]\) is far less than the dimensionalities \([d(28,6) = 3654 \text{ and } d(29,8) = 5265]\) for the leading irreps for \( ^{159}\text{Dy} \) and \( ^{165}\text{Er} \), respectively. These results illustrate that the shell-model \( K_J^2 \) operator reproduces as best possible in finite dimensional SU(3) irreps the \( K_J \)-band splitting generated by \( I_J^2 \) in the case of the quantum rotor. Indeed, one can show analytically, starting with the forms given in eqs. (3.26) and (3.27) for matrix elements of the \( Y^a \) operators and employing logic similar to that used in next section for the \( K_L^2 \) case, that the condition \( J \ll \min(\lambda, \mu) \) suffices to insure that the SU(3) and rotor matrix representations are the same. Again, however, a less stringent but more qualitative condition can be given, namely, for small \( J \) values in large dimensional \((\lambda, \mu)\) representations the \( K_J^2 \) operator has very nearly the same eigenvalues as \( I_J^2 \).
To explore the potential usefulness of the $K^2$ operator in shell model analyses, a comparison was made of the spectrum for $^{21}\text{Ne}$ that was generated using a shell-model hamiltonian consisting of the usual $^{17}\text{O}$ single-particle energies with $Q\cdot Q$, $J^2$ and the $K^2$ operator as residual interactions with the experimental results and results generated in another full $ds$-shell calculation using a realistic interaction that was fit to the experimental data. The results of this analysis, which are given in the next chapter, confirm the claim that the $K^2$ operator can be used in shell-model calculations for odd-$A$ nuclei with $S \neq 0$ to achieve observed $K_J$-band splitting.

3.4 $K^2$ Operator

A simplification of the $K^2$ can be done to obtain a microscopic operator $K^2_L$ which can be used to reproduce the observed $K_L$-band splitting in the even-$A$ nuclei with low-lying structure dominated by $S=0$ configurations. The algebraic form for this operator, its matrix elements and applications to different cases are discussed in the following sections.

3.4.1 Algebraic Expression for the $K^2_L$ Operator

In principle it is unnecessary to write down an explicit expression for the $K^2_L$ operator after having written down a form for $K^2$ because it is simply a special case ($S=0$) of the latter. As we will see however, it will prove useful to do so because one can then explicitly see in terms of matrix elements how and
why the rotor and SU(3) shell-model results are so similar. In terms of the
three rotational scalars $L^2$, $X_3^a$ and $X_4^a$, $\mathcal{R}_L^2$ is given as,

$$L^2 = \sum_\alpha L_\alpha L_\alpha = \sum_\alpha l_\alpha^2,$$

$$X_3^a = \sum_{\alpha, \beta} L_\alpha Q_{\alpha \beta} L_\beta = \sum_\alpha \lambda_\alpha l_\alpha^2, \quad (3.30)$$

$$X_4^a = \sum_{\alpha, \beta, \gamma} L_\alpha Q_{\alpha \beta} Q_{\beta \gamma} L_\gamma = \sum_\alpha \lambda_\alpha l_\alpha^2,$$

where $L_\alpha$ is the Cartesian component of the total orbital angular momentum,

$$L_\alpha = \sum_\alpha I_\alpha. \quad (3.31)$$

In terms of these rotational scalars, an expression for the $\mathcal{R}_L^2$ follows:

$$\mathcal{R}_L^2 = (\lambda_1 \lambda_2 L^2 + \lambda_3 X_3^a + X_4^a) / (2\lambda_3^2 + \lambda_1 \lambda_2), \quad (3.32)$$

where the $\lambda_i$'s are given in eq. (3.22).

Before continuing with our consideration of $\mathcal{R}_L^2$, we will first look at the
$X_3^a$ and $X_4^a$ operators that are factors in $\mathcal{R}_L^2$. As can be seen from eqs. (3.15)
and (3.30), these operators have the same structure as $Y_3^a$ and $Y_4^a$ and can be
obtained from them in the $S=0$ limit when $J=L$. The $X_3^a$ and $X_4^a$ operators were
first introduced by Racah (Rac 64). Three labels are required to completely
specify states within representations of SU(3). When SU(3) is reduced with
respect to SO(3), the angular momentum $L$ and its projection $M$ provide two of
these three labels. An additional label is needed to provide a resolution of
multiple occurrences of \( L \) in \((\lambda, \mu)\). Racah was the first to study this SU(3) \( \supset \) SO(3) multiplicity problem. His goal was to find a simple operator with rational eigenvalues that yields a complete and orthonormal labelling of basis states. He recognized that there are only two independent operators that can be used for this purpose, namely, the \( X_{3}^{a} \) and \( X_{4}^{a} \) introduced above. Unfortunately, as Racah and his student Sen (Sen 63) demonstrated, there is no linear combination of \( X_{3}^{a} \) and \( X_{4}^{a} \) that has simple rational eigenvalues. Others, in particular Bargmann and Moshinsky (BarMoh 60; BarMoh 61), extended the work of Racah on the search for an operator to give a physically meaningful resolution of SU(3) \( \supset \) SO(3) multiplicity problem. As pointed out previously, Elliott on the other hand, used a Hill-Wheeler projection technique to provide a simple but non-orthonormal resolution of the multiplicity. It is difficult to give a physical interpretation for \( X_{3}^{a} \) and \( X_{4}^{a} \), separately. Leschber, who used these operators throughout his work on a algebraic realization of rotor (\( S=0 \) case), studied the relationship of these operators to one another and the cancellation of their matrix elements the results for a special \( \chi \) in the linear form \( X_{3}^{a} + \chi X_{4}^{a} \) that turns out to be close to value required to a symmetric rotor: \( \chi = 1/\lambda_{3} \), see eq. (3.29).

### 3.4.2 Matrix Elements of the \( K_{L}^{2} \) Operator

Matrix elements of the \( X^{a} \)'s and therefore the \( K_{L}^{2} \) operator can be determined by setting \( S=0 \) in the expressions for the matrix elements of \( Y^{a} \)'s given in eqs. (3.26) and (3.27). However, due to the work of De Meyer and his co-workers (DeMVan 85), analytic results can be given for matrix element of
the $\mathcal{K}_L^2$ operator in a non-orthonormalized basis. Specifically, these authors have given analytic expressions for matrix elements of operators $O_f^\dagger$ and $Q_f^\dagger$ that are simply related to the $X^a$'s,

\begin{equation}
\left(3.33\right) \quad X_3^a = \frac{16}{36} O_f^\dagger ,
\end{equation}

\begin{equation}
\left(3.34\right) \quad X_3 = \frac{1}{72} (Q_f^\dagger + 36L^2 + 12L^4 - 16C_2L^2) ,
\end{equation}

where $L^2$, the square of the total angular momentum, and $C_2$ are the second order Casimir invariants of SO(3) and SU(3), respectively. If $\Omega$ and $\Lambda$ are matrices representing the operators $O_f^\dagger$ and $Q_f^\dagger$, respectively, then their matrix elements in the non-orthogonal Elliott basis are given for $\lambda \geq \mu$ by,

\begin{align}
\Omega_{K,K} &= \sqrt{6} (2\lambda+\mu+3)[L(L+1)-3K^2] , \\
\Omega_{K+2,K} &= -3[3(\mu-K)(\mu+K+2)(L+K+2)(L+K+1)(L-K)(L-K-1)/2]^{1/2} , \\
\Omega_{K-2,K} &= -3[3(\mu+K)(\mu-K+2)(L-K+2)(L-K+1)(L+K)(L+K-1)/2]^{1/2} , \quad (3.35)
\end{align}

and

\begin{align}
\Lambda_{K,K} &= 2[(2\lambda+\mu+3)^2 - 3(\mu^2-K^2+2\mu)]/[L(L+1)-3K^2] \\
-18K^2(K^2+1) + 6(5K^2-12)L(L+1)-12L^2(L+1)^2 , \\
\Lambda_{K+2,K} &= 6(2\lambda+\mu-3K)[(\mu-K)(\mu+K+2)(L+K+2)(L+K+1)(L-K)(L-K-1)]^{1/2} ,
\end{align}
\[ \Lambda_{K=2,K} = 6(2\lambda+\mu+3K)(\mu+K)(\mu-K+2)(L-K+2)(L-K+1) \times (L+K)(L+K-1)^{1/2}. \tag{3.36} \]

Results for \( \lambda < \mu \) can be obtained from these through the interchange \( \lambda \leftrightarrow \mu \).

Expressions (3.35) and (3.36) can be used in conjunction with eqs. (3.22), (3.32), (3.33) and (3.34) to arrive at the following matrix representation of \( \mathcal{R}_L^2 \) for the \( \lambda \geq \mu \) case:

\[
(\mathcal{R}_L^2)_{K,K} = \{(2/9)C_2-2\mu(\mu+2)/3+1/4+K^2/2\}|(L(L+1)-3K^2) \\
-(C_2/3+\mu(\mu+2)+7/4-K^2/2)[(\lambda+1)K^2]/[(\lambda+1)(\lambda+\mu+2)],
\]

\[
(\mathcal{R}_L^2)_{K-2,K} = -(K+1)[|\mu+1|^2-(K+1)^2]|f(L, K+1)|^{1/2}/(2K^2+1),
\]

\[
(\mathcal{R}_L^2)_{K+2,K} = (K-1)[|\mu-1|^2-(K-1)^2]|f(L, K-1)|^{1/2}/(2K+1), \tag{3.37}
\]

where \( C_2 \) is again the second order Casimir invariant of SU(3) and the function \( f(L, n) \) is given by \( f(L, n) = (L^2-n^2)(L^2-n^2+2L+1)/4 \). From this one can see that the representation of \( \mathcal{R}_L^2 \) in the Elliott basis is a tridiagonal, non-symmetric matrix. It can also be shown that for \( L < \min(\lambda, \mu) \), \( (\mathcal{R}_L^2)_{K,K} \rightarrow K^2 \) and \( (\mathcal{R}_L^2)_{K+2,K} \rightarrow 0 \) (DraWee 84a). However, it is important to know that while the \( L < \min(\lambda, \mu) \) condition is sufficient to guarantee agreement between the theories, it is an overly restrictive requirement. A somewhat less stringent and certainly more qualitative condition, but one that works extremely well, can be given; namely, for small \( L \) values in large \( (\lambda, \mu) \)
representations the $\mathcal{K}_L^2$ operator has very nearly the same eigenvalues as $I_3^2$ of the collective model. Examples that illustrate this are given in the next section.

### 3.4.3 Results for $^{24}\text{Mg}$ and $^{168}\text{Er}$

The simplest test of the theory is for the symmetric rotor, that is, hamiltonian (3.1) with $A_1=\alpha=A_2$ and $A_3=\alpha+\beta$,

$$H_R \rightarrow \alpha I_1^2 + \alpha I_2^2 + (\alpha + \beta) I_3^2 \rightarrow \alpha I^2 + \beta I_3^2 . \quad (3.38)$$

Further simplification can be done by setting $S=0$, $J=L$. In this case the expected shell-model hamiltonian [eq. (3.21)] is simply,

$$H_{SU3} \rightarrow H_0 + \alpha L^2 + \beta \mathcal{K}_L^2 \rightarrow H_0 + \hat{a}L^2 + \hat{b}X^4 + \hat{c}X^6 ;$$

$$\hat{a} = \alpha + \beta((\lambda-\mu)(\lambda+2\mu+3))/\delta ,$$

$$\hat{b} = 3\beta(2\lambda+\mu+3)/\delta ,$$

$$\hat{c} = +9\beta/\delta \quad \text{where} \quad \delta = 9((\lambda+1)(\lambda+\mu+2) . \quad (3.39)$$

The parameters $\alpha$ and $\beta$ can be determined from the excitation energies of the first two $L^\pi=2^+$ states of the system under consideration:
\[ E_{21} = 6\alpha \rightarrow \alpha = E_{21}/6 \]
\[ E_{22} = 6\alpha + 4\beta \rightarrow \beta = (E_{21} - E_{22})/4 \] (3.40)

Results for \(^{24}\text{Mg}\) and \(^{168}\text{Er}\) using this simple theory are shown in figs. (3.14) and (3.15), respectively. The SU(3) irreps selected for each were \((\lambda,\mu) = (8,4)\) and \((\lambda,\mu) = (30,8)\) as these are the representations with maximum deformation for four protons and four neutrons in the ds-shell and ten protons and ten neutrons in normal parity orbitals of the pseudo fp and gds-shells (DraWee 84a). The \(^{24}\text{Mg}\) and \(^{168}\text{Er}\) examples were chosen for this comparison because they have nearly prolate rotor spectra, they are representative nuclei for normal and pseudo shell-model applications of the theory, and they have large \(K_L\)-band splitting. Since the condition \(L << \min(\lambda,\mu)\) is sufficient to insure that the two theories yield identical results, differences that can be observed between the \(H_{SU3}\) and \(H_{ROT}\) spectra in figures (3.14) and (3.15) are due to the fact that this limit does not apply. In particular, since the \(L << \min(\lambda,\mu)\) condition is less well fulfilled for the \((\lambda,\mu) = (8,4)\) irrep than for the \((\lambda,\mu) = (30,8)\), differences in the results for \(H_{SU3}\) and \(H_{ROT}\) are greater for the \(^{24}\text{Mg}\) case than for \(^{168}\text{Er}\). Note, however, that even though the agreement is not perfect it extends well into the \(L > \min(\lambda,\mu)\) region.

Before quoting some results from a more sophisticated \(^{24}\text{Mg}\) calculation, consider figures (3.16) and (3.17) where eigenvalues of the \(K_L^2\) operator are plotted as a function of the total angular momentum \(L\). As above where \(K_L^2\) results are given for ds-shell and pseudo-SU(3) applications, here results for both the \((\lambda,\mu) = (8,4)\) and \((30,8)\) irreps of SU(3) and pseudo-SU(3)
Figure 3.14. Experimental (EXP) and theoretical (ROT and SU3 and SP3) spectra for $^{24}$Mg. The results labelled ROT are for a symmetric rotor Hamiltonian [eq. (3.38)] fit to the first two excited 2+ states of $^{24}$Mg ($E_{21} = 1.36859$ MeV and $E_{22} = 4.2385$ MeV). The one labelled SU3 is for the corresponding shell-model theory [eq. (3.39)] in the $(\lambda, \mu) = (8, 4)$ irrep which is the SU(3) representation having maximum deformation for four protons and four neutrons in the ds-shell. Note that for $L^\pi > 2^+$ in the $K^\pi = 2^+$ band the SU(3) energies fall below those of the rotor. This is due to the fact that the condition $L < \min(\lambda, \mu)$ for equivalence of the two theories is far from being satisfied. A much better fit to the experimental spectrum could be achieved by a direct and independent least-squares determination of the parameters of $H_R$ [eq. (3.1)] and $H_{SU3}$ [eq. (3.21)]. This was not done here as the purpose of the exercise was only to demonstrated the utility of the $K_L^2$ operator for generating $K_L$-band splitting. The results labelled SP3 are those of a symplectic shell-model calculation [eq. (3.41)] which took inter-shell mixing into account. In this case the theory also reproduces the E2 transition strengths without the use of an effective charge.
Figure 3.15. Experimental (EXP) and theoretical (ROT and SU3 and SP3) spectra for $^{168}$Er. The results labelled ROT are for a symmetric rotor Hamiltonian [eq. (3.38)] fit to the first two excited 2$^+$ states of $^{168}$Er ($E_{21} = 0.079800$ MeV and $E_{22} = 0.82111$ MeV). The one labelled SU3 is for the corresponding shell-model theory [eq. (3.39)] in the $(\lambda, \mu) = (30, 8)$ irrep which is the pseudo-SU(3) representation of maximum deformation for ten protons in the fp-shell and ten neutrons in the gds-shell of the pseudo oscillator. Note that in this case for $L^\pi > 4^+$ in the $K^\pi = 2^+$ band the SU(3) energies fall below those of the rotor. This is again due to the fact that the condition $L < \min(\lambda, \mu)$ for equivalence of the theories is far from being satisfied. The fact that in this case the agreement is better and extends to higher $L$ values than for $^{24}$Mg is because the dimensionality of the $(30, 8)$ irrep (5580) is more than an order of magnitude greater than that of the $(8, 4)$ irrep (315). Of course, a much better fit to the $^{168}$Er spectrum could be achieved by a direct and independent least-squares determination of the parameters of $H_R$ [eq. (3.1)] and $H_{SU3}$ [eq. (3.21)]. As for the $^{24}$Mg case, this was not done here as the purpose of this exercise was only to demonstrated the utility of the $R^L_K$ operator for generating $K_L$-band splitting. The results labelled SP3 are those of a symplectic shell-model calculation [eq. (3.41)] which took inter-shell mixing into account. In this case the theory again reproduces the E2 transition strengths without the use of an effective charge. The staggering between even and odd angular momentum values in the $K^\pi = 2^+$ band is a result of mixing of even $L$ members of the band with even $L$ states of the ground band. Note that the amount of this mixing increases with increasing $L$. For example, whereas for the $L^\pi = 2^+$ states it is less than 0.1%, for the $L^\pi = 4^+ (8^+)$ [12+] states it is about 0.5% (5%) [20%]. This mixing raises the energy of the even $L$ members of the $K^\pi = 2^+$ band relative to the odd $L$ members as the odd $L$ states have no partners to mix with in the $K^\pi = 0^+$ band.
Figure 3.16. Eigenvalues of the $\mathcal{K}_L^2$ operator [eq. (3.32)] in angular-momentum projected and orthonormalized basis states of the $\text{SU}(3) \supset \text{SO}(3)$ reduction for the leading $\text{SU}(3)$ representation of $^{24}\text{Mg}$, namely, $(\lambda, \mu) = (8, 4)$. Whereas for members of the $K^*_{L}=0^+$ band the eigenvalue of $\mathcal{K}_L^2$ is nearly zero (even for L values near the top of the band), for the $K^*_{L}\neq0^+$ bands there is a fall-off from the expected $K_L^2$ values. The fall-off increases with increasing L and is more pronounced the larger the $K_L$. The reason for this follows from the fact that SU(3) is a compact group with finite-dimensional irreps as compared with the symmetry group of the rotor, $T_5 \wedge \text{SO}(3)$, which is non-compact with infinite-dimensional representations.
Figure 3.17. Eigenvalues of the \( K_L^2 \) operator [eq. (3.32)] in angular-momentum projected and orthonormalized basis states of the SU(3) \( \supset \) SO(3) reduction for the leading pseudo SU(3) representation of the rare earth nucleus \(^{168}\text{Er}\), namely, \((\lambda,\mu) = (30,8)\). As seen in fig. (3.16) for the \(^{24}\text{Mg}\) case, for members of the \( K_L = 0^+ \) band the eigenvalue of \( K_L^2 \) is nearly zero, even for \( L \) values near the top of the band, whereas for the \( K_L \neq 0^+ \) bands there is a fall-off from the expected \( K_L^2 \) values. And the fall-off is again seen to increase with increasing \( L \), being more pronounced for larger \( K_L \) values. In the \(^{168}\text{Er}\) case, however, the \( L \)'s of interest to the low-lying structure more nearly satisfy the \( L \ll \min(\lambda,\mu) \) condition and, accordingly, the \( K_L \) quantum number is better defined.
are presented. From the plots it is clear that the $K_L^2$ operator, like $K_T^2$, does indeed generate $K_L$-band splitting, that is, it separates multiple occurrences of $L$ values within an irrep of SU(3) into distinct rotational bands. For all but the lowest spin members of each band, however, the $K_L^2$ eigenvalues are only approximately equal to $K^2 = 0, 2^2 = 4, 4^2 = 16$, etc. Note that the fall-off from the expected values increases with increasing $L$ and is more pronounced the larger the $K$. This is again a direct consequence of the fact that SU(3) is a compact group with finite dimensional irreps whereas the symmetry group of the rotor, $T_5 \times SO(3)$, is non-compact and has infinite dimensional representations. These $S=0$ examples show this as the fall-off occurs much sooner in the $(8,4)$ case than for the $(30,8)$ irrep. As for the $K_T^2$ cases, the differences go beyond that fact that the condition $L \ll \min(\lambda,\mu)$ is less well satisfied for the $(8,4)$ than for the $(30,8)$ irrep. In particular, it is because the dimensionality $d(\lambda,\mu) = (\lambda+\mu+2)(\lambda+1)(\mu+1)/2$ of the $(8,4)$ SU(3) irrep (315) is significantly less than that of the $(30,8)$ irrep (5580). This saturation effect manifests itself in other ways as well. In particular, for $^{24}$Mg it is well-known that in addition to the fact that the $L^\pi=8^+$ state falls below the expected $L(L+1)$ position for a rotor, the $8^+ \rightarrow 6^+ E2$ transition strength is less than about half the rotor value. Since this is in agreement with experiment, it serves as a confirmation of the shell-model as opposed to the rotor picture for the structure of $^{24}$Mg and, by extrapolation, for other deformed nuclei as well.

In figure (3.18) the diagonal matrix elements of the $K_L^2$ operator in angular momentum projected ($E_{LL}^{58}$) and orthonormalized basis states ($Ver_{68}$) are plotted as a function of $L$ for the $(\lambda,\mu)=(8,4)$ irrep. Similar results, but for the square root of diagonal matrix elements of the $K_L^2$ operator are shown
Figure 3.18. A plot of the diagonal matrix elements of the $K_L^2$ operator versus $L$ in angular momentum projected basis state of the SU(3) ⊇ SO(3) reduction for the leading SU(3) representation of $^{24}$Mg, namely, $(\lambda, \mu) = (8, 4)$. Note the similarity of these curves to those given in figure 3.16 for eigenvalues of the $K_L^2$ operator in the same SU(3) representation. The similarity is a direct result of the fact that the off-diagonal matrix elements of $K_L^2$ are small compared to the diagonal ones, see fig. (3.19).
for the (30,8) irrep in figure (3.19). The similarity of these results to the
eigenvalue curves given in figures (3.16) and (3.17) is an indication of the
relative size of the off-diagonal matrix elements in the angular momentum
projected basis. This is shown explicitly in figure (3.19) by means of error bars
for two different L values, namely, L=10 and 20. The fact that the error bars,
which indicate the relative size of the off-diagonal to diagonal matrix elements,
are larger for the L=20 case than L=10 is in agreement with the fact that the
condition L << min(λ,μ) is less true the larger the L value. The odd-even
staggering that is so pronounced for the K=2 curves in each figure is simply a
result of the orthonormalization. Specifically, the K=2, L=even states include
sufficient K=0 admixtures to guarantee orthogonality whereas there are no
K=0, L=odd states so in these case mixing is not required to gain an
orthonormal basis set. This applies to a lesser degree for the higher L values
as well. Though it is not obvious from these results, it is important to know
that the orthonormalization procedure preserves the tridiagonal character of the
\( \mathcal{K}_L^2 \) matrix. Note that the L=10 (12) state of the (λ,μ)=(8,4) irrep appears to
be more a part of the K=0 band than the K=2 (4) band. The highest L member
of each (λ,μ)=(30,8) band shows this same behavior. In general the maximum
L value of the Elliott bands can more appropriately be put into the ground-state
band, the next highest L in the first-excited band, etc. Results for spectra also
bear this out. This suggests that the Elliott rule (Ell 58) for assigning L values
to \( K_L \)-bands is flawed, in particular, the ground band series extends from the
\( \min(λ,μ) \) through to \( λ+μ \) and does not terminate at the \( \max(λ,μ) \) value, etc.
But this is only a minor matter of little consequence because in any particular
Figure 3.19. A plot of the square root of the diagonal matrix elements of the $K^2$ operator versus $L$ in angular momentum projected basis states of the SU(3) $\supset$ SO(3) reduction for the leading pseudo SU(3) representation of $^{168}$Er, namely, $(\lambda, \mu)=(30,8)$. The error bars given for the $L=10$ and $L=20$ cases indicate the relative size of the off-diagonal matrix elements. The odd-even staggering that is so pronounced for the $K_L=2$ curve is a result of the orthonormalization. Specifically, the $K_L=2$, $L$-even states include sufficient $K_L=0$ admixtures to guarantee orthogonality whereas for $K_L=2$, $L$-odd states mixing is not required to gain an orthonormal basis set because there are no $K_L=0$, $L$-odd states in the irrep. The same argument applies, but to a lesser degree, for members of the higher $K_L$ bands.
application the K label serves only to distinguish states and does not change the physics.

While these results suffice to illustrate that the $k^2_L$ operator yields $k_L$-band splitting within a shell-model framework, it is important to demonstrate the utility of the theory in carrying out large-scale shell-model calculations. Recently Draayer and co-workers calculated the excitation spectra and E2 transition rates for $^{24}\text{Mg}$ in the framework of the contracted symplectic model (BahDra 90; CasDra 89). These results are given in figure (3.14) under the heading SP3. The hamiltonian they used was simply,

$$H = H_0 - \frac{1}{2}Q^c \cdot Q^c + H_r,$$

where $H_r = aL^2 + bX^4 + cX^6$. (3.41)

The $Q^c$ in (3.41) is the collective quadrupole operator. As noted earlier, this operator has non-vanishing matrix elements between oscillator shells with $N' = N$ and $N' = N \pm 2$ quanta. Because of the off-diagonal couplings between major shells, the $Q^c \cdot Q^c$ interaction builds coherence into calculated eigenstates so the E2 rates reproduce observed values without an effective charge. The symmetry algebra of this hamiltonian is the non-compact symplectic group $\text{Sp}(3,\mathbb{R})$ which has the Elliott SU(3) symmetry as a maximal compact subgroup (RosRow 77; RosRow 79; RosRow 76). The residual interaction, $H_r$, is of the type introduced in (3.21) as the shell-model image of the rotor hamiltonian. Since within a major shell of the oscillator, $Q^c \cdot Q^c \rightarrow Q^a \cdot Q^a = 4C_2 \cdot 3L^2$, the function of $H_r$ is to reproduce the $k_L$-band splitting and adjust the effective moment-of-inertia of the system.
To see how this works, consider the four parameters $\chi$ and $a, b, c$ of the theory. The value of $\chi$ is fixed by the requirement on the theory to reproduce the $B(E2; 2^+ \rightarrow 0^+)$ transition strength. Typically this results in a $\chi$ that is close to the self-consistent value (Row 67). Since the main contribution of $Q^c \cdot Q^c$ to inter-shell dynamics is through its $Q^a \cdot Q^a$ part, it generates very little $K_L$-band splitting and contributes $3/2 \chi$ to the inertia parameter. This means that a good estimate for the $a$ of $H_r$ in (3.41) is simply $a = \hat{a} - 3\chi/2$. Similarly, for prolate spectra the values for $b$ and $c$ of $H_r$ should be approximately $\hat{b}$ and $\hat{c}$, respectively. And in particular, the ratio $b/c$ should be close to $-(2\lambda+\mu+3)/3$ which is the $\hat{b}/\hat{c}$ ratio. A least-squares fit to $^{24}$Mg data yielded the following values for the four parameters of the theory: $(\chi, a, b, c) = (0.0415, 0.14137, -0.042417, 0.0055368)$. The best-fit value for the $b/c$ ratio is therefore 7.661 which is to be compared with 7.667 for $\hat{b}/\hat{c} = -(2\lambda+\mu+3)/3$. Likewise, the best fit value for $a$, 0.14137, is within a factor of $2/3$ of the $\hat{a} - 3\chi/2$ estimate, 0.21393. Similar results hold for the $^{168}$Er case. These simple examples demonstrate the usefulness of both the $H_{\text{ROT}} \leftrightarrow H_{\text{SU3}}$ and $\mathcal{R}_L^2$ theories for determining the starting values for the parameters of symplectic shell-model analyses of nuclear structure.

For any particular nucleus the leading $\text{SU}(3)$ representation is known. This serves to fix the $\lambda_i$'s and therefore the $\mathcal{R}_L^2$ operator as a linear combination of three rotational scalars: $L^2, X_3^3 \sim (L \times Q^a \times L)^0$, see eq. (3.32). Although $L^2$ is a $(1+2)$-body operator, $X_3^3$ and $X_4^4$ have $3$-body and $(3+4)$-body parts, respectively. This means the $\mathcal{R}_L^2$ operator is not a traditional $(0+1+2)$-body shell-model interaction. Nevertheless, it is simple and it works. While this feature may explain why practitioners of shell-model theories have found it so
difficult to generate observed $K_L$-band splitting, it leaves us with another
problem, namely, understanding at a deeper level the microscopic origin of this
special $(0+1+2+3+4)$-body operator. From the way in which it was derived, it
is clear that $\mathcal{K}_L^2$ is very special. Though the $X^a$'s have 3-body and (3+4)-body
parts, they are far from general interactions of this type. Specifically, from the
derivation it is clear that in an intrinsic frame of reference they are simply
weighted sums of $(1+2)$-body operator forms. The appearance of the 3-body
and (3+4)-body parts is a reflection on our inability to identify within the
framework of a many-body theory a principal-axis frame of reference.

So far we have used the SU(3) image of the rotor hamiltonian and the
$\mathcal{K}_L^2$ operator as a residual interaction in a hamiltonian and applied it to the even
$A$ nuclei like $^{24}$Mg and $^{168}$Er. A hamiltonian using $\mathcal{K}_L^2$ is constructed and
applied to some odd $A$ nuclei in the next chapter because some ground work is
needed to formulate a rotor-plus-particle hamiltonian.
4.1. Introduction

The particle-plus-rotor model was proposed by Bohr and Mottelson (BohMot 53) to describe the interplay between particle degrees-of-freedom and the collective motion. They suggested taking a few of the so-called valence particles into account explicitly, treating them as though they move more or less independently in the deformed well of the core, and coupling them to a collective rotor representing the rest of the nucleons in a nucleus. This division into core and valence particles is not always unique. However, the unpaired nucleon in an odd-A nucleus can be considered to be a particle or hole attached to an even-even core. The Hamiltonian is generally divided into two parts: an intrinsic part \( H_{\text{intr}} \) and a collective part \( H_{\text{coll}} \). The \( H_{\text{intr}} \) Hamiltonian describes a valence particle or a subset of valence particles near the Fermi level, whereas \( H_{\text{coll}} \) describes the collective motion of the otherwise inert core. The total Hamiltonian is given as:

\[
H = H_{\text{intr}} + H_{\text{coll}}. \tag{4.1}
\]

If interactions between the valence particles are neglected, as is usually taken to be the case, the eigenvalues of \( H_{\text{intr}} \) are the single-particle energies of a particle in a deformed well (e.g., Nilsson energies, as describe in chapter 2).
The collective part $H_{\text{COLL}}$ describes the rotation of the core:

$$H_{\text{COLL}} = \sum_{i=1}^{3} \frac{R_i^2}{2I_i},$$  \hspace{1cm} (4.2)

where $R_i$ are the body-fixed components of the collective angular momentum of the core (fig. 2.3) and $1/2I_i$ are the inertia parameters which have already been introduced in section 3.1 (see table 3.1). If $j$ is the angular momentum of the valence particles (i.e., the sum over all single-particle angular momenta) then total angular momentum $I$ is given as:

$$I = R + j.$$ \hspace{1cm} (4.3)

Using eq. (4.3), $H_{\text{COLL}}$ can be rewritten as:

$$H_{\text{COLL}} = H_R + H_{\text{REC}} + H_{\text{COR}},$$  \hspace{1cm} (4.4)

where the rotor hamiltonian [see eq.(3.1)],

$$H_R = \sum_{i=1}^{3} \frac{I_i^2}{2I_i},$$ \hspace{1cm} (4.5)

acts only on the collective degrees-of-freedom. The recoil term,

$$H_{\text{REC}} = \sum_{i=1}^{3} \frac{\hat{p}_i^2}{2I_i},$$ \hspace{1cm} (4.6)
represents the reaction of the particle to the motion of the deformed field it sees. This part of the hamiltonian only acts on the coordinates of the valence particles; when there is more than a single valence nucleon the recoil term includes 2-body interactions. And finally, the coriolis term,

\[ H_{\text{COR}} = -\sum_{i=1}^{3} \frac{I_i \cdot \mathbf{j}_i}{I_i} , \]  

(4.7)

couples the rotor degrees-of-freedom to the degrees-of-freedom of the valence particles. This kinematic term is the only coupling between the particle and core degrees-of-freedom.

It can be easily shown that the components \( I_x' \), \( I_y' \), and \( I_z' \) of the total angular momentum operators in the laboratory system commute with the hamiltonian eq. (4.1). Although the rotational symmetry is generally violated in the intrinsic frame (for example, the Nilsson hamiltonian is not a rotational scalar), the model does conserve the total angular momentum of the total system. The phenomenological core maintains the rotational invariance.

The wave functions of the system can be written as:

\[ \psi_I = \sum_K C(I,K) \chi_K D_{MK} , \]

(4.8)

where \( \chi_K \) depends on the coordinates of the valence particles (e.g., bases states for the Nilsson hamiltonian, see section 2.3.) and the \( D_{MK} \) are Wigner D-functions which depend upon Euler angles. The \( C(I,K) \) are coefficients that come out of the diagonalization. A. Bohr (Boh 52) has discussed in detail the
transformation properties of these wave functions under rotations and the many simplifications resulting from these considerations. The simplest case, which includes only one valence particle and an axially symmetric core, is discussed in next section.

4.1.1. Symmetric Rotor

If the rotor has the 3-axis (or body-fixed z-axis) as a symmetry axis, i.e., $l_1 = l_2 = l$, there can be no collective rotation around that axis and the 3-component of $R$ has to vanish. From eq. (4.3) it follows immediately that $K$, the 3-component of total angular momentum $I$, has to be equal to $\Omega$, the 3-component of $j$ (fig. 2.3. and table 3.1):

$$K = \Omega.$$  \hfill (4.9)

In this case, using eq. (4.9), for the different terms of hamiltonian eq. (4.4), we obtain

$$H_R = \frac{I^2 - I_3^2}{2l},$$  \hfill (4.10)

$$H_{REC} = \frac{j_1^2 + j_2^2}{2l},$$  \hfill (4.11)

$$H_{COR} = \frac{l_1 j_1 + l_2 j_2}{l} = \frac{L_j + L_j^+}{2l}.$$  \hfill (4.12)
The $I_+$, etc., in eq. (4.12) are the usual raising and lowering operators. The single-particle eigenfunctions, $\chi_\Omega^\nu$, in the axially symmetric (e.g., the Nilsson Hamiltonian) case are given as:

$$\chi_k^\nu = \chi_\Omega^\nu = \sum_j C_j^\nu \chi_j^\Omega, \quad (4.13)$$

where the $\chi_j^\Omega$ are the bases vectors (for example, see section 2.3.) and the $C_j^\nu$ are coefficients found by diagonalizing the Hamiltonian.

Before presenting the SU(3) analogue of the Hamiltonian defined in eq. (4.1), it will be useful to consider the physical significance of each term in eqs. (4.10)-(4.12). This can be achieved by considering limits when only one of the terms dominants:

- **The strong coupling limit (deformation alignment):** The odd particle follows the motion of the even-$A$ core adiabatically. This limit is realized whenever the coupling to the deformation is much stronger than the perturbation of the single-particle motion by the Coriolis interaction.

- **The weak coupling limit (no alignment):** This limit is realized for very small deformations. In this case the odd particle essentially moves in a spherical shell-model potential that is only slightly disturbed by the deformation.

- **The decoupling limit (rotational alignment):** This limit is realized when the Coriolis force is so strong that the coupling to the deformation of the core can be neglected.

The recoil term acts only in the intrinsic coordinates and is normally dropped if the single-particle energies are adjusted to the experimental data, or simply
added to the single-particle hamiltonian $H_{\text{INTR}}$ if the single-particle levels are disturbed only slightly by the addition of this term.

So far we have not discussed the form of the intrinsic hamiltonian, $H_{\text{INTR}}$. For most research on deformed odd-$A$ nuclei, $H_{\text{INTR}}$ has been chosen to be the Nilsson hamiltonian, eq. (2.24). We will also make this choice. The complete hamiltonian for the case of a symmetric rotor in the strong coupling limit is then the following:

$$H = \frac{I^2 - I_3^2}{2I} + H_h - \hbar \omega_0(\delta) \left[ \beta r^2 Y_{20}(\theta',\phi') + 2\kappa l s + \mu l^2 \right], \quad (4.14)$$

where $H_h$, $\omega_0(\delta)$, $\beta$, $\kappa$, and $\mu$ have been defined in chapter 2 [eqs. (2.20), (2.21), and (2.25)]. In this strong coupling limit, the coriolis interaction is completely neglected. Taking it into account in first order perturbation theory, yields a contribution for $K = 1/2$ bands only.

The eigenvalues and the eigenvectors of the hamiltonian given in eq. (4.14) have been discussed in many standard text books, and therefore we will not discuss this case any further. We will instead introduce a hamiltonian analogues to the $H$ given in eq. (4.14), using SU(3) scalars and other 1-body and 2-body operators. This image of the $H$ given in eq. (4.14) will be diagonalized in the Elliott angular-momentum coupled, spin-projected basis.
4.2. SU(3) Model for Odd-A Nuclei

A model built on the SU(3) algebra that is suitable for an analysis of odd-mass nuclei is proposed in what follows.

4.2.1. The Hamiltonian

The hamiltonian given in eq. (4.14) is a suitable choice for studying deformed nuclei that display axially symmetry. A shell-model hamiltonian that is analogous to this can be written as:

\[ H_{SU3} = H_o + A_J J^2 + A_K \mathcal{R}_3^2 - \frac{1}{2} \chi Q^a Q^a + C \sum_i l_i s_i + D \sum_i l_i^2. \]  

In eq. (4.16), \( H_o \) is the harmonic oscillator hamiltonian, \( J \) and \( I \) are used interchangeably, and the \( \mathcal{R}_3^2 \) operator is the SU(3) image of the \( 1^2 \) operator:

\[ \mathcal{R}_3 = (\lambda_1 \lambda_2 J^2 + \lambda_3 Y_3^f + Y_3^d) / (2 \lambda_3^2 + \lambda_1 \lambda_2), \]  

where the \( \lambda_i \)'s are given in eq. (3.22) and the \( Y^a \) operators are defined in eqs. (3.24) and (3.25). The \( \mathcal{R}_3^2 \) operator has been shown to reproduce the \( K_j \)-band splitting in odd-mass nuclei (NaqDra 92a). The \( Q^a \) in eq. (4.16) is the algebraic quadrupole operator. As discussed in chapter 3, the collective quadrupole operator \( Q^c \) has non-vanishing matrix elements between oscillator shells with \( N' = N \pm 2 \) quanta (like the term \( r^2 Y_{20} \) in (4.14)), it has been replaced by
algebraic quadrupole operator (Ell 58) since within a major shell of the oscillator \( Q^c \rightarrow Q^a \). In the 1-body interactions \( l_i, s_i \) and \( l_i^2, l_i \) and \( s_i \) are respectively the single-particle orbital angular momentum and spin and the sum is over the valence particles.

4.2.2. Bases Space

The symmetry group of the valence space in which the hamiltonian given in eq. (4.15) acts is \( U(4d) \) where, as discussed earlier in chapters 2 and 3, \( d = (N+1)(N+2)/2 \) is the spatial degeneracy of \( N \)-th oscillator shell and the factor 4 denotes the spin-isospin degrees-of-freedom. Of course, when the protons and neutron fill different shells as in heavy nuclei, the space-spin-isospin symmetry group \( U(4d) \) should be replaced by the proton-neutron direct product structure \( U(2d_\alpha) \otimes U(2d_\nu) \), where \( d_\alpha = (N+1)(N_\alpha + 2)/2 \) with \( \alpha = (\pi, \nu) \). However, for light nuclei where both protons and neutron occupy the same oscillator shell we will use the scheme shown in fig. 2.4. The basis states used for diagonalization of the hamiltonian have been used in chapter 3 and are given as follows:

\[
|m[f]\alpha(\lambda, \mu)\kappa L;|f]\beta STM_T ; JM_J \rangle = |\gamma(\lambda, \mu)\kappa LS ; JM_J \rangle, \tag{4.17}
\]

where the labels have been defined in eq. (3.29).

While the symmetries used in the above classification scheme are exact for some of the interactions in the hamiltonian, eq. (4.15), they are broken by
other. The first four interactions namely, $H_0$, $J^2$, $R_d^2$ and $Q^a \cdot Q^a$ do not couple irreps with different $(\lambda \mu)$ and therefore preserve the $U(1)$, $U(4)$ and $SU(3)$ symmetries. Within the same $SU(3)$ irrep the $R_d^2$ operator mixes states with different $L$ values (breaking the $SO(3)$ symmetry) but $Q^a \cdot Q^a$ preserves $SO(3)$ in addition to other symmetries as it does not couple the states with different $L$ values. The 1-body $\sum_i l_i$ term breaks the SU(3) symmetry and mixes different SU(3) irreps within the same spatial representation [f] whereas the 1-body $\sum_i l_i \cdot s_i$ interaction couples states with different spatial and spin symmetries. The extent to which the U(1) and SU(3) symmetries are preserved or broken depends on the relative strengths of these operators and this aspect will be discussed later in some details. In the next section we give the expression for the matrix elements of the hamiltonian given in eq. (4.15).

4.2.3. Matrix Elements

Expressions for the matrix elements of some of the interactions in the hamiltonian (4.15) have already been given in chapter 3. The $H_0$, $J^2$ and $Q^a \cdot Q^a$ parts of $H$ are diagonal in these bases (4.17) and have eigenvalues $N\omega$, $J(J+1)$, and $4C_2-3L(L+1)$, respectively. $C_2$ in this expression, as defined earlier, is the Casimir invariant of SU(3) group and has the eigenvalue $\lambda^2 + \mu^2 + \lambda \mu + 3\lambda + 3\mu$. The matrix elements of $R_d^2$ operator can be obtained using eqs. (3.26)-(3.28).

The matrix elements of the 1-body operators $\sum_i l_i$ and $\sum_i l_i \cdot s_i$ can be found by first transforming them into irreducible tensors $T^{(\lambda\mu\nu)\lambda L\ell J L_j T_e}$ and then using an expression for the reduced matrix element of these irreducible tensors.
operators. These operators are decomposed into these irreducible tensors as follows:

\[
\sum_{i} l_i^2 = \sum_{l(\lambda_\mu_\omega)} (-1)^N 2l(l + 1)(2l + 1)^{1/2} \langle (N0)l; (0N)ll(l_\mu_\omega) \kappa_\omega L_\omega = 0 \rangle \\
\times T^{(\lambda_\mu_\omega)\kappa_\omega L_\omega = S_\omega J_\omega = T_\omega = 0},
\]  

(4.18)

\[
\sum_{i} l_i s_i = \sum_{l(\lambda_\mu_\omega)} (-1)^{N+1} [l(l + 1)(2l + 1)]^{1/2} \langle (N0)l; (0N)ll(l_\mu_\omega) \kappa_\omega L_\omega = 1 \rangle \\
\times T^{(\lambda_\mu_\omega)\kappa_\omega L_\omega = 1, S_\omega = 1, J_\omega = T_\omega = 0},
\]  

(4.19)

\[
T^{(\lambda_\mu_\omega)\kappa_\omega L_\omega S_\omega J_\omega T_\omega = [a^+a]^{(\lambda_\mu_\omega)} } \kappa_\omega L_\omega S_\omega J_\omega T_\omega,
\]  

(4.20)

where \( a^+ \) and \( a \) are creation and annihilation operators. Details regarding the structure of \( T^{(\lambda_\mu_\omega)\kappa_\omega L_\omega S_\omega J_\omega T_\omega} \) are given in Appendices B and C. The double barred coefficient is an SU(3) ⊃ SO(3) isoscalar usually known as an SU(3) ⊃ SO(3) Wigner coefficient (DraAki 73; Ver 68) for the orthonormal basis \( l(\lambda_\mu)\kappa L M_L > \)

where the Elliott label \( K \) has been replaced by the label \( \kappa \) introduced by Vergados (Ver 68). A computer program for evaluating these isoscalars is available (AkiDra 73). For the N=2 shell, in particular, eqs. (4.18) and (4.19) have the form:

\[
\sum_{i} l_i^2 = 10\sqrt{6} T^{(00)\kappa_\omega = S_\omega = J_\omega = T_\omega = 0} + 2\sqrt{30} T^{(22)\kappa_\omega = S_\omega = J_\omega = T_\omega = 0},
\]  

(4.21)

\[
\sum_{i} l_i s_i = -\sqrt{30} T^{(11)\kappa_\omega = S_\omega = 1, J_\omega = T_\omega = 0}.
\]  

(4.22)
Matrix elements of the irreducible tensors $T^{(\lambda,\mu_o)}_{\kappa L_o S_o J_o T_o}$ are given in terms of triple barred reduced matrix elements as follows:

$$
\langle \psi | T^{(\lambda,\mu_o)}_{\kappa L_o S_o J_o T_o} | \psi' \rangle = \langle T'M_{T'}T_oM_{T_o} | T'M_T \rangle \langle J'M',J_oM_o | JM \rangle (4.23)
$$

$$
\times \chi \left\{ \begin{array}{c} L' \ S' \ J' \\ L_0 \ S_0 \ J_o \end{array} \right\} \sum_p \langle (\lambda'\mu')_{\kappa' L'} \; ; \; (\lambda_o\mu_o)_{\kappa_o L_o} \| (\lambda\mu)_{\kappa L} \rangle_p 
$$

$$
\times \langle m|f\alpha(\lambda,\mu),\beta(ST) \ || \ || T^{(\lambda,\mu_o)}_{S,T_o} || \ || m'|f'|\alpha'(\lambda',\mu'),\beta'(S'T') \rangle_p ,
$$

where the $\langle \ldots | \ldots \rangle$ are the Clebsch-Gordan coefficients of $SO(3)$, $\chi$ is a Jahn-Hope coefficients, and the triple-barred quantities are $SU(3)$ reduced matrix elements (see appendix B). Computer programs for evaluating them are available. Using eqs. (4.18), (4.19), and (4.23) the matrix elements of spin-orbit and orbit-orbit interactions in hamiltonian (4.15) can be evaluated.

4.3. Application of SU(3) Model to Light Nuclei.

Once the expressions for the matrix elements of different interactions in the hamiltonian (4.15) are known, we can find its matrix representation and can diagonalize it to get its eigenvalues. This has been done for two cases: $^{21}$Ne and $^{23}$Na, and are reported in what follows.
4.3.1. Full Space (ds)\(^5\) Results for \(^{21}\)Ne

To test the potential usefulness of the hamiltonian (4.15) in carrying out detailed shell-model calculations, it was diagonalized in the full (ds)\(^5\) \(T=\frac{1}{2}\) space. The constants C and D were fixed at the values that are required to reproduce the observed splitting of the \(d_{5/2}, s_{1/2}\) and \(d_{3/2}\) levels in \(^{17}\)O, namely, -2.03 and 0.194 Mev, respectively. The strength \(\chi\) of the quadrupole-quadrupole interaction and \(A_J\) and \(A_K\) were allowed to vary with a least-squares fitting procedure employed to obtain a best overall fit to the observed experimental spectrum. The results are shown on the far right as Theory 2 in figure 4.1. The results labeled Theory 1 shown on the left in the figure are for a full ds shell-model calculation that used a so-called realistic interaction, that is, a renormalized 2-body form fit to the experimental spectra and E2 transition rate data of the light ds-shell nuclei (HofBet 89). The experimental spectrum in the center was taken from the Table of Isotopes (LedShi 78). Best fit values for the three parameters \(\chi\), \(A_J\), and \(A_K\) were found to be 0.1187, which compares favorably with the value required to reproduce the observed moment of inertia of the ground state rotational band in \(^{20}\)Ne using the same hamiltonian but with \(A_J\) and \(A_K\) set to zero, -0.02632, and -0.4250 Mev, respectively. The calculations showed that the ground \(K_J = \frac{3}{2}\) and first excited \(K_J = \frac{1}{2}\) bands derive predominantly from the \(L = 1, K_L = 1\) state \((K_J = K_L \pm \frac{1}{2})\) projected out of the irreps \([f](\lambda\lambda) = [41](81)\) of SU(6) and SU(3). Because of this, and the fact that the \(K_J = \frac{3}{2}\) bandhead lies below the \(K_J = \frac{1}{2}\) bandhead, the sign of \(A_J\) in the hamiltonian is negative. The \(K_J = \frac{5}{2}\) excited bandhead at 3.73 Mev is a mixture of a \(K_J = \frac{5}{2}\) bandhead projected out of the \([41](62)\) irrep, a
Figure 4.1. Excitation spectra for $^{21}\text{Ne}$. The spectrum on the right labelled Theory 2 is for the present case, using the Hamiltonian given in (4.15), while the one on the left labelled Theory 1 is for a full ds-shell model calculation that used a so-called realistic ds-shell interaction, that is, a renormalized 2-body form with 63 independent matrix elements fit to the experimental spectra and E2 transition rate data of the light ds-shell nuclei. To get the ground $K_J = \frac{3}{2}$ band to lie below the first excited $K_J = \frac{1}{2}$ band requires the sign of the constant $A_K$ multiplying the $R_2^2$ operator in (4.15) to be negative. A complete analysis of the calculated eigenstates for Hamiltonian (4.15) is given in Table 4.1.
Table 4.1. Analysis of calculated eigenstates for $^{21}$Ne in terms of their SU(6) $\{[\ell]\}$ and SU(3) $\{\mu\}$ irreducible parts.

<table>
<thead>
<tr>
<th>$<a href="%5Cmu">\ell</a> \backslash J$</th>
<th>3/2$_1$</th>
<th>5/2$_1$</th>
<th>7/2$_1$</th>
<th>9/2$_1$</th>
<th>11/2$_1$</th>
<th>1/2$_1$</th>
<th>5/2$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[41] (81)</td>
<td>77.5</td>
<td>75.4</td>
<td>70.8</td>
<td>61.8</td>
<td>55.3</td>
<td>64.9</td>
<td>53.6</td>
</tr>
<tr>
<td>(62)</td>
<td>5.0</td>
<td>5.4</td>
<td>6.3</td>
<td>4.3</td>
<td>4.6</td>
<td>17.3</td>
<td>20.9</td>
</tr>
<tr>
<td>(43)</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>(51)</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>Rest</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>Total</td>
<td>82.6</td>
<td>80.9</td>
<td>77.2</td>
<td>66.2</td>
<td>60.0</td>
<td>82.7$^#$</td>
<td>75.0$^#$</td>
</tr>
<tr>
<td>[32] (62)</td>
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<td>10.1</td>
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<td>20.4</td>
<td>27.3</td>
<td>10.0</td>
<td>14.0</td>
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<tr>
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<td>0.8</td>
<td>1.3</td>
<td>2.0</td>
<td>4.2</td>
<td>1.6</td>
<td>3.0</td>
</tr>
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<td>0.3</td>
<td>0.4</td>
</tr>
<tr>
<td>(32)</td>
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<td>•</td>
<td>•</td>
<td>•</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>(24)</td>
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<td>•</td>
<td>0.1</td>
<td>•</td>
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<td></td>
</tr>
<tr>
<td>Rest</td>
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<td></td>
<td></td>
<td>0.1</td>
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</tr>
<tr>
<td>Total</td>
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<td>11.1$^#$</td>
<td>15.3</td>
<td>22.6</td>
<td>31.8</td>
<td>12.0</td>
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</tr>
<tr>
<td>(43)</td>
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<td>0.7</td>
<td>1.1</td>
<td>2.6</td>
<td>4.6</td>
</tr>
<tr>
<td>(51)</td>
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<td>0.2</td>
<td>0.3</td>
<td>0.1</td>
<td>0.5</td>
<td>0.7</td>
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<tr>
<td>Rest</td>
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<td>0.1</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>6.3$^#$</td>
<td>7.0</td>
<td>6.2$^#$</td>
<td>9.0$^#$</td>
<td>5.4</td>
<td>4.7</td>
<td>6.3</td>
</tr>
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<td>1.1</td>
<td>2.1</td>
<td>2.3</td>
<td>0.1</td>
<td>0.2</td>
</tr>
<tr>
<td>(24)</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td>0.1</td>
<td>0.4</td>
<td>0.3</td>
<td>0.6</td>
</tr>
<tr>
<td>(32)</td>
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<td>•</td>
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<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Rest</td>
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<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Total</td>
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<td>1.0</td>
<td>1.2</td>
<td>2.2</td>
<td>2.8</td>
<td>0.5</td>
<td>1.0</td>
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<tr>
<td>[21111] (32)</td>
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<td>•</td>
<td>0.2</td>
<td>•</td>
<td>•</td>
<td>0.1</td>
</tr>
<tr>
<td>Rest</td>
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<td>•</td>
<td>•</td>
<td>•</td>
<td>•</td>
<td></td>
</tr>
<tr>
<td>Total</td>
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<td>•</td>
<td>0.2</td>
<td>•</td>
<td>•</td>
<td>0.1</td>
</tr>
<tr>
<td>[111111]</td>
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<td>•</td>
<td>A</td>
<td>A</td>
<td>A</td>
<td>•</td>
<td></td>
</tr>
</tbody>
</table>

* Less than 0.05
$^\#$ Total does not match due to rounding
A Absent
second $\frac{5}{2}$ state from the (81) irrep of SU(3), and a $K_J = \frac{5}{2}$ band projected out of the [32](62) irrep. A full analysis of the calculated eigenstates is given in table 4.1. One can see from table 4.1 that while the $J^\pi = 3/2^+$ ground band is dominated (77.5%) by the $[f^-(\lambda,\mu)] = [41](81)$ symmetry, the percentage decreases as one moves up the band to states of higher spin. The first excited $J^\pi = 1/2^+$ bandhead state is likewise dominated (64.9%) by the [41](81) symmetry but the $J^\pi = 5/2^+$ bandhead state shows considerably more [41](62) strength. The SU(6) mixing which is caused by the spin-orbit interaction, though not large (~20%), is important for obtaining reasonable agreement with the excitation spectrum.

4.3.2. Truncated (ds)$^7$ Results for $^{23}$Na

The Hamiltonian (4.15) was also diagonalized in the truncated (ds)$^7$, $T=1/2$ space. Only three spatial symmetries [43], [421] and [331] were used. In this case, however, the coefficients C and D were also allowed to vary along with the strength $\chi$ of quadrupole-quadrupole interaction and the parameters $A_J$ and $A_K$ to obtain a best overall fit to the observed experimental spectrum by a least-squares fitting procedure. The results are labeled as Theory in fig. 4.2. The experimental spectrum labeled Experiment was taken from the Table of Isotopes (LedShi 78). The best-fit values for C and D were found to be -2.71 and 0.190 Mev, respectively, which are very close to the values required to reproduce the observed splitting of the levels in $^{17}$O, i.e., -2.03 and 0.194 Mev. The values of $\chi$, $A_J$ and $A_K$ were found to be 0.1808, -0.0805, and -0.3854 Mev, respectively. The analysis of the calculated eigenstates shows that the
Figure 4.2. Excitation spectra for $^{23}\text{Na}$. The spectrum on the right labelled Theory is for the present case, using the hamiltonian given in (4.15), while the one on the left labelled Experiment is taken from the Table of Isotopes.
Table 4.2. Analysis of calculated eigenstates for $^{23}$Na in terms of their SU(6) \( \{ [f] \} \) and SU(3) \( \{ (\lambda \mu) \} \) irreducible parts.

<table>
<thead>
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<th>([f](\lambda \mu) ) ( \backslash J )</th>
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ground $K_J=3/2$ and first excited $K_J=1/2$ bands derive predominantly from the \(L=1, K_L=1\) states \((K_J=K_L\pm 1/2)\) projected out of the irreps \([f](\lambda \mu )=[43](83)\) of U(6) and SU(3). The sign of \(A_J\) in the hamiltonian is negative because the \(K_J=3/2\) bandhead lies below the \(K_J=1/2\) bandhead. Although the agreement for the ground \(K_J=3/2\) band is not very good, the excited \(K_J=1/2\) band matches with experiment fairly well. One of the reasons for the disagreement may be the use of a truncated model space. A full analysis of the calculated eigenstates is given in table 4.2.

The successful application and importance of the SU(3) model for light nuclei can be explained by noticing the dominance of the quadrupole-quadrupole interaction, \(Q \cdot Q\), over the 1-body \(I \cdot s\) and \(I^2\) terms as well as over all other 2-body interactions (Ell 58; Har 68). Even though the spin-orbit interaction is strong, yrast states of odd-A nuclei like \(^{21}\text{Ne}\), as seen above, and even-A nuclei such as \(^{20}\text{Ne}\) and \(^{24}\text{Mg}\), are typically 60-80% pure leading SU(3) representations. To understand this one need only recognize that the \(Q \cdot Q\) operator conserves the spatial symmetry and has eigenvalues \(<Q \cdot Q > = 4C_2 - 3L(L+1)\) where \(C_2\) is the SU(3) Casimir invariant. Since the expectation value of \(Q \cdot Q\) is proportional to the square of the deformation, it subdivides each spatial irrep \([f]\) into \((\lambda \mu )\) irreps of SU(3) with the least deformed of these lying highest and most deformed lowest. By how much each spatial irrep \([f]\) of U(d) and then the \((\lambda \mu )\) irreps of SU(3) are separated depends upon the relative strengths of symmetry preserving \(Q \cdot Q\) interaction and symmetry breaking terms such as \(I \cdot s\). The available model space also plays an important role because the action of symmetry preserving and symmetry breaking interactions depend upon weather or not the space favors strongly deformed configurations.
Light nuclei in the ds-shell have leading irreps with large deformation so \(Q\cdot Q\) is dominant over all other symmetry breaking interactions and yrast states have relatively good \(|f\rangle\) and \((\lambda\mu)\) quantum labels. If the space is restricted to a subshell of the ds shell this situation may be different and symmetry breaking interactions can overpower \(Q\cdot Q\). From the success of the SU(3) model in the ds-shell it is clear that the many-particle dynamics can promote quadrupole collectivity over single particle and other non-collective effects.
CHAPTER 5
CONCLUSION

In this concluding chapter the results of our work will be summarized and some possible follow-up research projects will be suggested. The objective of this thesis project, as has been mentioned many times, was to bridge the gap between the collective (geometrical) and single-particle (shell model) interpretations of nuclear structure for odd-mass systems. Early work on this subject was done by pioneers such as Nilsson, Elliott and many others. Also, Draayer and Leschber established a shell-model realization of a quantum rotor that was successfully used to describe the rotational motion in even-mass nuclei such as $^{24}\text{Mg}$ from a shell-model perspective. The purpose of this research was to extend that work, as suggested by Leschber in his thesis, to the particle-plus-rotor model so that it can be applied to a shell-model description of rotational motion in odd-mass nuclei as well. In the particle-plus-rotor model the nucleus is considered to be a rotating core with the odd nucleon coupled to it.

We started our work by including the spin degree-of-freedom into Leschber's algebraic realization of the quantum rotor. This was done by introducing three rotational invariants, namely, $J^2$, $Y_1 = \frac{1}{6}\sqrt{30}|J\times Q\times J|^9$, and $Y_4 = -\frac{1}{18}\sqrt{3}|(J\times Q)^1\times (Q\times J)^1|^0$. The shell-model image of a rotor hamiltonian with spin is a simple linear combination of these three scalars. The equivalence of the invariants $\text{Tr}[(Q^c)^2]$ and $\text{Tr}[(Q^c)^3]$, of the symmetry group of rotor and
SU(3) Casimir invariants, $C_2$ and $C_3$ was used to establish a mapping between the inertia parameters $A_1$, $A_2$ and $A_3$ of rotor hamiltonian and coefficients $a$, $b$, and $c$ of its SU(3) image [see eqs. (3.1) and (3.21)]. Known values of $\lambda$ and $\mu$ for the leading irreps of deformed nuclei were used to fix the values of the coefficients $a$, $b$, and $c$. Expressions for matrix elements of the $Y_3^a$ and $Y_4^a$ operators were given in terms of SU(2) Racah coefficients and reduced SU(3) $\supset SO(3)$ coupling coefficients. They are therefore calculable because computer codes for the evaluation of these coefficients are readily available. The eigenvalues of the quantum rotor for different rotor geometries (prolate, oblate, and the most asymmetric case) were compared with those of its SU(3) image for the leading normal SU(3) irrep of the odd-mass nucleus $^{25}$Mg, and leading pseudo SU(3) irreps of $^{165}$Er and $^{159}$Dy. The eigenvalues produced by the two hamiltonians were in good agreement which is an indication of the success of the mapping.

An observed characteristic feature of strongly deformed even-mass and odd-mass nuclei, namely the energy splitting of KL-bands ($S=0$) and KJ-bands ($S\neq0$), respectively, was also studied by introducing $K_1^L$ and $K_2^L$ operators. The expression for the $K_1^L$ operator was obtained from the SU(3) image of the rotor hamiltonian by selecting the inertia parameters so that only the $I_3^2$ term survived, that is, $A_1=A_2=0$, and $A_3\neq0$. Eigenvalues of the $K_2^L$ operator were evaluated for the leading SU(3) irreps of the odd-mass normal SU(3) nucleus $^{25}$Mg and the odd-mass pseudo-SU(3) nuclei $^{165}$Er and $^{159}$Dy. These were found to be in good agreement with the corresponding collective model results. The $K_1^L$ operator, which can be obtained as a special limit ($S \to 0$) of the $K_2^L$ operator, was also obtained from the operators $X_3^a$ and $X_4^a$ that were used by
Leschber in his work. The eigenvalues of the $\mathcal{K}_L^2$ operator were evaluated for the leading normal-SU(3) irrep of $^{24}\text{Mg}$ and the leading pseudo-SU(3) irrep of $^{168}\text{Er}$. The SU(3) were found to be in good agreement with the collective model description of K-band splitting.

While the results produced by the $\mathcal{K}_L^2$ and $\mathcal{K}_J^2$ operators explain why the practitioners of shell model theories have found it so difficult to generate the observed $K_L$-band and $K_J$-band splitting, they leave us with another problem, namely, understanding of the microscopic origin of these $(0+1+2+3+4)$-body operators. The $\mathcal{K}_L^2$ and $\mathcal{K}_J^2$ operators are different than a normal shell-model interaction because they include 3-body and 4-body interactions in addition to the usual $(0+1+2)$-body parts. However, since the combination of these higher-order interaction terms is dictated by the quantum rotor to shell-model mapping constraint, a very specific linear combination enters into the construction of $\mathcal{K}_L^2$ and $\mathcal{K}_J^2$. An interesting question that remains unexplored and hence unanswered is whether or not there exists a $(0+1+2)$-body operator form that achieves the $K_L$ and $K_J$-band splitting in an equally simple manner.

At this point we want to emphasize that since the collective and shell-model schemes are fundamentally different, the relation between the two hamiltonians has the character of a mapping rather than an exact mathematical equivalence. The rotor picture describes the rotation phenomena without any consideration of intrinsic structure of the nucleus, whereas the SU(3) $\Rightarrow$ SO(3) algebra is a shell-model scheme which employes the fact that the nucleus is built from discrete particles. The finiteness of the SU(3) irrep spaces as compared to those of the rotor is a consequence of this difference. However, the results of this research support the notion of the coexistence of rotational
and intrinsic parts in an SU(3) description of the dynamics. The SU(3) wavefunctions can be thought of as composed of a rotational part that depends upon the rotational degrees-of-freedom, i.e., the three Euler angles, and an intrinsic part which is a function of the remaining degrees-of-freedom. The equivalence of the eigenvalues by the rotor hamiltonian and its SU(3) image and the results produced by the $R^2_l$ and $R^2_o$ suggest that the SU(3) hamiltonian acts only on the collective part of these wavefunctions. To involve the intrinsic degrees-of-freedom as well as the collective rotational parts, interactions which probe non-rotational phenomena such as $\sum_i l_i s_i$ were added to the rotor hamiltonian.

An SU(3) analogue of the particle-plus-rotor hamiltonian that uses the Nilsson hamiltonian as the intrinsic part was constructed:

$$ H = H_0 + A_J J^2 + A_K R^2_l - \frac{1}{2} \chi Q^a Q^a + C \sum_i l_i s_i + D \sum_i l_i^2 $$  \hspace{1cm} (5.1)

where the interactions $J^2$, $R^2_l$ and $Q^a Q^a$ act on the rotational component of the wavefunctions while the others ($\sum_i l_i s_i$ and $\sum_i l_i^2$) probe in addition the intrinsic degrees-of-freedom. This hamiltonian (5.1) was diagonalized in the full $(ds)^5 T=1/2$ space in order to reproduce the experimental spectrum of odd-mass nucleus $^{21}$Ne. The constants C and D were fixed at -2.03 and 0.194 Mev, respectively, the values that are required to reproduce the observed splitting of the single-particle levels in the $^{17}$O spectrum. The three parameters $\chi$, $A_J$, and $A_K$ were varied with a least square fitting procedure to obtain a best fit to the observed experimental spectrum. The value for $\chi$ was found to be in agreement with that which is needed to reproduce the experimentally observed spectrum.
of $^{20}\text{Ne}$. A full analysis of the eigenstates showed that the mixing of SU(6) irreps by the spin-orbit term only was not large but is needed to get a good fit to the experimental results.

The Hamiltonian was also diagonalized in the truncated $(ds)^7 S=1/2$ space to reproduce the experimental spectrum of another odd-mass nucleus, $^{23}\text{Na}$. The parameters were again allowed to vary with the least square procedure to get a best fit to experimental data. The results were found to be in good agreement with the experiment. In both the above cases the $(\lambda\mu)$ of the leading SU(3) irreps namely, $(\lambda\mu) = (81)$ and $(83)$ for $^{21}\text{Ne}$ and $^{23}\text{Na}$, respectively, were used to fix the coefficients of $J^2$, $Y_3^6$ and $Y_4^\pi$ terms in $K_3^\pi$ operator. These values correspond to different moments of inertia (other than $A_1=A_2=0$, and $A_3=0$) for the secondary irreps which, however, does not affect our calculations very much because first of all the $K_3^\pi$ operator acts only within a single irrep, and secondly, contributions from non-leading irreps to members of the yrast band is typically 60-80%.

Although the SU(3) Hamiltonian works well when applied to light mass nuclei, it is not a suitable choice in the case of heavy nuclei, but as discussed in the text, the pseudo SU(3) scheme can be applied successfully in the latter case. SU(3) is the symmetry group of harmonic oscillator and in the heavy nuclei the strength of the spin-orbit interaction needed for shell closure at magic numbers is so large that it destroys the underlying SU(3) symmetry. The levels with highest j value in an oscillator shell are pushed down and penetrate into the shell below. The levels that remain can be relabelled as orbitals of a pseudo-oscillator shell with one less quanta plus a unique parity intruder from the shell above. Another feature of heavy nuclei is that the valence neutrons
and protons may be filling different shells. These differences must to be taken into consideration before the extension of the SU(3) hamiltonian to heavy deformed nuclei can be realized. It has been shown by Draayer (DraNaq 90) that a transformation to pseudo-orbital and pseudo-spin angular momentum operators leads to a hamiltonian with a much smaller spin-orbit interaction strength and one that for deformed nuclei favors the pseudo-SU(3) coupling scheme. The unique parity or intruder level from the shell above is not taken into account explicitly, but J. Escher, a member of the nuclear theory group at LSU, is investigating this matter further and it is anticipated that the results of her research will represent a step forward towards the successful extension of the SU(3) model to the study of heavy deformed nuclei.

In this work the spin degree-of-freedom, which enters explicitly for odd-mass nuclei, was taken into account by incorporating it as a simple extension of Leschber's realization of quantum rotor for spin zero: the angular momentum $L$ of the even-mass spin zero quantum rotor was extended to total angular momentum $I$ of an odd-mass rotor with non-zero spin by simply adding in the spin degree-of-freedom, $I = L + S$. This picture is suitable for cases when the spatial and spin degrees-of-freedom are strongly coupled, as for the light nuclei of the ds-shell. However, in some rare earth and actinide nuclei the spin degree-of-freedom appears to be weakly coupled to the rotational motion. This observation is consistent with the pseudo-spin and pseudo-SU(3) concepts. In the latter case one can use different realization of the rotational motion. C. Bahri, another member of nuclear theory group at LSU, is working on a spin-rotor model in which the intrinsic spin is weakly coupled to the angular momentum. Adapting it in an interpretation of the pseudo-SU(3) coupling
scheme, means replacing the spin-rotor part of the hamiltonian with its pseudo-SU(3) counterpart rather than the quantum-rotor by its SU(3) counterpart as was done in our work.

A further extension of our scheme can be achieved by considering excitations into other shells. This can be accomplished through the symplectic model, \( \text{Sp}(3,\mathbb{R}) \) which is the dynamical symmetry group of the harmonic oscillator. This model allows one to include couplings generated by the real quadrupole-quadrupole interaction, \( Q \cdot Q \) and not just \( Q^a \cdot Q^a \), to the \( N+2n \) and \( N-2n \) shells \((n=1, 2, ...)\) in contrast to the SU(3) model which is restricted to only one active shell \((n=0)\).

This work has focused on rotational motion in the odd-mass nuclei, however, there are other modes like vibrations that have not even been described. We realize that even though rotational motion is an important mode, it is only one in complex systems which show many others. We must admit that in spite of good progress, our knowledge and understanding of the nucleus is still quite limited and many question, including some raised in this work, are left unexplored and unanswered. Many open research opportunities remain; as a corollary to Murphy's law states: "Every solution breeds new problems."
BIBLIOGRAPHY

AkiDra 73  Y. Akiyama and J. P. Draayer, Computer Physics Communications. 5 (1973) 405-415.


BarMoh 60  V. Bargmann and M. Moshinsky, Nucl. Phys.18 (1960) 697.

BarMoh 61  V. Bargmann and M. Moshinsky, Nucl. Phys. 23 (1961) 177.


BorHei 26 M. Born, W. Heisenberg et al., Zeit. Phys. 35 (1926) 557.

BorJor 25 M. Born and P. Jordan, Z. Physik. 34 (1925) 858.

Cas 31   H. B. G. Casimir, Rotation of a Rigid body in Quantum Mechanics. La Hague, J. B. Wolters 1931


Ell 66  J. P. Elliott, The International school of Physics "Enrico Fermi". (1966)


EscBah 91  J. Escher, C. Bahri et al., Submitted for publication.


Har 68  M. Harvey, Advances in Physics. 1 (1968) 67-182.

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<td>Hei 32a</td>
<td>W. Heisenberg, Z. PhysiK. 77 (1932) 1.</td>
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<td>Hei 32b</td>
<td>W. Heisenberg, Z. Physik. 78 (1932) 156.</td>
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<td>Ivanenko, Nature. 129 (1932) 798.</td>
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<td>O. Klein, Zeit. Phys. 29 (1929) 60.</td>
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<td>KleSom 97</td>
<td>F. Klein and A. Sommerfeld, Theorie des Kreisels. Leipzig, Teubner 1897-1910</td>
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<td>LedShi 78</td>
<td>C. M. Lederer and V. S. Shirley, Table of Isotopes. New York, Wiley 1978</td>
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Rac 64  G. Racah, Group theoretical concepts and methods in elementary particle physics. New York, Gordon and Breach 1964


Row 67  D. J. Rowe, Physical Review. 162 (No. 4) (1967) 162-871.


APPENDIX A
LIE GROUPS AND LIE ALGEBRA

A set of continuous transformations with an infinite number of elements where every element can be characterized in terms of \( r \) parameters defines a Lie group. For example, the SU(2) group can be characterized in terms of the direction of the rotation axis and the angle of rotation about that axis. The group of rotations in three dimensions, SO(3), is another example. In this case the group elements are usually parameterized in terms of three Euler angles. For every \( r \) parameter Lie group there exists a set of \( r \) operators which generate the corresponding infinitesimal transformations. These generators satisfy the following commutation relations:

\[
[ X_{\alpha}, X_{\beta} ] = c^{\gamma}_{\alpha\beta} X_{\gamma}, \tag{A.1}
\]

where \( c^{\gamma}_{\alpha\beta} \) are structure constants. The structure constants actually identify the group and determine most of its properties. The set of operators that satisfy the commutation relations (A.1) are said to form a Lie algebra. The angular momentum operators \( L_x, L_y, \) and \( L_z \) which generate infinitesimal rotations about the \( x, y, \) and \( z \) axes, respectively, are a familiar example of group generators. Their commutation relations are well-known \( ([L_\alpha, L_\beta] = i\epsilon_{\alpha\beta\gamma} L_\gamma; \) \((\alpha\beta\gamma)\) cyclic\) and of the (A.1) type. These three operators are the generators of SO(3) and form a Lie algebra. Other Lie group and the associated Lie algebras can be considered to be generalizations of the familiar angular momentum case.
Every finite transformation $U$ or element of the group can be given in terms of the $r$ generators \{${X}_i; i=1,2,...,r$\} and $r$ parameters \{$\alpha_i; i=1,2,...,r$\} by:

$$U(\alpha_1, \alpha_2, ..., \alpha_r) = \exp\{\sum_{i=1}^{r} \alpha_i{X}_i\} \quad (A.2)$$

Since most properties of a group are determined by its structure constants and its generators, much can be learned about a group by studying its Lie algebra.

A function of the generators $C = f({X}_i)$, which commutes with all the generators is called a Casimir invariant:

$$[C, {X}_i] = 0, \quad i=1, 2, ..., r \quad (A.3)$$

As an example, one can again use the group $SO(3)$ where $L^2 = L_x^2 + L_y^2 + L_z^2$ is a function of the generators that commutes with all the generators. It is the only Casimir invariant of $SO(3)$. The number of independent Casimir invariants that can be formed is equal to the rank of the group. A function of either generator $X_i$ and non-generator forms $Y_j$ or a combination, $S(G,N) = f(X_i, Y_j)$ that commutes with all the generators of the group is called a group scalar. For example, $L^2$ is a scalar for $U(1)$ generated by $L_z$, but is a function of the non-generators $L_x$ and $L_y$ along with the generator $L_z$. A Casimir invariant is a scalar but a scalar is not necessarily a Casimir invariant.

The relevance of a symmetry to a particular problem depends upon the commutation properties of its generators with the system's Hamiltonian. If the Hamiltonian is formed from combinations of a group's Casimir invariants, simple analytic results can be given for its eigenvalues and its eigenvectors are basis states of the group's irreducible representations. On the other hand, if the Hamiltonian involves more than just Casimir invariants but still only group scalars, the eigenvalues may no longer be simple but the Hamiltonian matrix
will be block-diagonal within irreducible representations of the group and each
eigenvector will be degenerate with degeneracy equal to the dimensionality of
the group irrep. (In the angular momentum case, this is the \((2L+1)\) rotational
degeneracy which follows because the Hamiltonian is a rotational scalar.)
Another important case is when the Hamiltonian is made up of only group
generators, but in more than just the form of Casimir invariants. In this case
the dynamics is defined solely within irreducible representations of the group
— there are no matrix elements coupling different irreps nor are there matrix
elements coupling different occurrences of the same irrep. The irrep's
degeneracy is lifted, but the irrep labels remain good quantum numbers.
\((H = aL^2 + L_z)\) is a simple \(SO(3)\) example.) The triaxial quantum rotor is an
example of the last two symmetry types: it is built of generators of \(T_5 \wedge SO(3)\)
and therefore only couples basis states within irreps of that group and at the
same time it is a rotational scalar so it displays the \((2L+1)\) degeneracy of
\(SO(3)\). In general, a group is guaranteed to reveal an important symmetry if the
generators of its Lie algebra satisfy simple commutation relations with the
Hamiltonian.
Matrix elements of operators introduced in the text are expressed in terms of SU(3) reduced matrix elements (RME) and SU(3) Clebsch-Gordan coefficients. Even product operators are defined in terms of the SU(3) RME's of the factor operators. For example, the RME of $Y_4 = [(J \times Q)^1 \times (Q \times J)^1]^0$ is given in terms of the RME's of the $Q$ and $J$ operators. Some of the relations used in obtaining these expressions are given in what follows.

B.1. Reduced Matrix Element Relations

In some cases the SU(3) RME relation is just a generalization of the corresponding SU(2) RME result. These simple relations will be given first. The SU(2) RME of an operator $O$ with SU(2) (spherical) tensor character $J_0$, $M_0$ is given as:

$$\langle JM | O^{J_0 M_0} | J'M' \rangle = \frac{(-1)^{2J}}{\sqrt{2J+1}} \langle J'M', J_0 M_0 | JM \rangle \langle j | O^j | J \rangle.$$  (B.1)

Another important relation is the expression for the RME of a product tensor operator in terms of the RME's of its composite parts:
where an SU(2) $U$-coefficient has been used instead of a $6j$ coefficient,

$$U(J''J_2J_1 \mid J''J_3) = (-1)^{J''+J_2+J_1} \sqrt{(2J''+1)(2J_3+1)} \begin{pmatrix} J' & J_2 & J'' \\ J_1 & J_3 & J \end{pmatrix}.$$  (B.3)

The expression corresponding to (B.1) for SU(3) RME's is given as:

$$(\lambda, \mu)_{\kappa \ell M} \bigg| O^{(\lambda_0 \mu_0)_{\kappa_0 L_0 M_0}} \bigg| (\lambda' \mu')_{\kappa' L' M'} = \langle L'M', L_0 M_0 \mid \ell M \rangle$$  (B.4)

$$\times \sum_{\rho} \langle (\lambda' \mu')_{\kappa' L'}; (\lambda_0 \mu_0)_{\kappa_0 L_0} \parallel (\lambda \mu)_{\kappa L} \rangle \langle (\lambda \mu) \parallel | O^{(\lambda_0 \mu_0)} \rangle \parallel | (\lambda' \mu')_{\rho} \rangle.$$

where $(\lambda_0 \mu_0)_{\kappa_0 L_0 M_0}$ is the SU(3) tensor character of the operator $O$. The SU(3) tensor character of the operator $Q^a$, for example, is $(\lambda_0 \mu_0)_{\kappa_0 L_0} = (11)_{12}$. The coefficients $\langle (\lambda' \mu')_{\kappa' L'}; (\lambda_0 \mu_0)_{\kappa_0 L_0} \parallel (\lambda \mu)_{\kappa L} \rangle_{\rho}$ are SU(3) isoscalar factors which are SU(3) coupling coefficients analogous to SU(2) Clebsch-Gordan coefficients. From (B.1) and (B.4) we can get the relation,

$$(\lambda, \mu)_{\kappa L} \bigg| O^{(\lambda_0 \mu_0)_{\kappa_0 L_0}} \bigg| (\lambda' \mu')_{\kappa' L'} = \sqrt{2L + 1} \times$$  (B.5)

$$\sum_{\rho} \langle (\lambda' \mu')_{\kappa' L'}; (\lambda_0 \mu_0)_{\kappa_0 L_0} \parallel (\lambda \mu)_{\kappa L} \rangle_{\rho} \times \langle (\lambda \mu) \parallel | O^{(\lambda_0 \mu_0)} \rangle \parallel | (\lambda' \mu')_{\rho} \rangle.$$

The SU(3) expression for the RME of a product operator in terms of the composite operators is a generalization of (B.2) and is given as:
\[
\langle \lambda, \mu \rangle \left[ \left[ O^{(\lambda_1 \mu_1)} \times O^{(\lambda_2 \mu_2)} \right]^{(\lambda_3 \mu_3)p} \right] \left[ \langle \lambda', \mu' \rangle \right]^{p'} = \sum_{\rho_1, \rho_1, \rho'} \left\{ \begin{array}{c}
(00) (\lambda_1 \mu_1) (\lambda_1 \mu_1) \\
(\lambda_2 \mu_2) (00) (\lambda_2 \mu_2) \\
(\lambda_2 \mu_2) (\lambda_1 \mu_1) (\lambda_3 \mu_3) \rho' 
\end{array} \right\}
\times U((\lambda', \mu')(\lambda_2 \mu_2)(\lambda_1 \mu_1); (\lambda'', \mu'') \rho_2 \rho_1 (\lambda_3 \mu_3) \rho' \rho'') \quad (B.6)
\]

\[
\times \langle \lambda, \mu \rangle \left[ \left[ O^{(\lambda_1 \mu_1)} \right] \left[ \langle \lambda'', \mu'' \rangle \right]_{\rho_1} \langle \lambda'', \mu'' \rangle \left[ \left[ O^{(\lambda_2 \mu_2)} \right] \left[ \langle \lambda', \mu' \rangle \right]_{\rho_1} \langle \lambda', \mu' \rangle \right]_{\rho'} 
\]

where the following relation has been employed for the isoscalar factor

\[
\langle (\lambda_1 \mu_1) \alpha_1, (\lambda_2 \mu_2) \alpha_2 \mid (\lambda_3 \mu_3) \alpha_3 \rangle_{\rho} = \sum_{\rho'} \left\{ \begin{array}{c}
(00) (\lambda_1 \mu_1) (\lambda_1 \mu_1) \\
(\lambda_2 \mu_2) (00) (\lambda_2 \mu_2) \\
(\lambda_2 \mu_2) (\lambda_1 \mu_1) (\lambda_3 \mu_3) \rho' 
\end{array} \right\}
\times \langle (\lambda_2 \mu_2) \alpha_2, (\lambda_1 \mu_1) \alpha_1 \mid (\lambda_3 \mu_3) \alpha_3 \rangle_{\rho'}
\]

\[= \sum_{\rho'} Z((\lambda_1 \mu_1)(00)(\lambda_3 \mu_3)(\lambda_2 \mu_2); (\lambda_1 \mu_1) 1 \rho (\lambda_2 \mu_2) 1 \rho') \langle (\lambda_2 \mu_2) \alpha_2, (\lambda_1 \mu_1) \alpha_1 \mid (\lambda_3 \mu_3) \alpha_3 \rangle_{\rho'} \quad (B.7)
\]

involving a 9-(\lambda \mu) coefficient and a Z coefficient (Mil 78). Note that in the case of multiplicity free coupling the 9-(\lambda \mu) coefficient acquires the simple unitary value \((-1)^{\lambda_1+\mu_1+\lambda_2+\mu_2-\lambda_3-\mu_3}\).

\subsection*{B.2. SU(3) Tensor Matrix Elements}

In this subsection an expression is presented for the matrix elements of a one-body fermion tensor operator \(O^{(\lambda \mu)}_{kLS,JM,TM}\) between valence-shell
basis states. These are required to carry out calculations in a shell-model space adapted to the space-spin-isospin SU(3)⊗SU(4) symmetry. For a given total angular momentum J and total isospin T, a complete set of basis states in such a symmetry scheme is given by

$$|\Psi\rangle = |m[f] \alpha(\lambda\mu) \kappa L, \beta(ST);JM_{J},M_{T}\rangle,$$

(B.8)

where m is the number of active particles in a major oscillator shell N, [f] labels the spatial symmetry of the wavefunction (DraLeb 89), α and β respectively label the multiplicity of the SU(3) (λμ) and spin-isospin (S,T) irreps occurring for the [f] symmetry (DraPur 68; Rac 64), and κ labels the multiplicity of orbital angular momentum states L. The fermion operator O is defined as:

$$O^{(\lambda\mu) \kappa L S;JM_{J},M_{T}} = [a_{(N0)lmn,lmn}^{\dagger}a_{(N0)lmn,lmn}^{\alpha(\lambda\mu) \kappa L S;JM_{J},M_{T}} ,$$

(B.9)

where $a_{(N0)lmn,lmn}^{\dagger}$ and $a_{(N0)lmn,lmn}$ are the single-particle annihilation and creation operators that annihilate or create a particle in a state with quantum numbers (N0)lmn. Within the (B.8) basis, matrix elements of the one-body fermion tensor (B.9) are given by:

$$\langle \Psi_1 | O^{(\lambda\mu) \kappa L S;JM_{J},M_{T}} | \Psi_2 \rangle = \langle TM_{T2},TM_{T1}| TM_{T},\langle J_{2}M_{2},JM_{J}J_{1}M_{1} \rangle$$

$$\times \chi_{L_{2} \rightarrow L_{1},S_{2} \rightarrow S_{1},J_{2} \rightarrow J_{1}} \sum_{\rho} \langle \lambda_{2} \mu_{2},\kappa_{2}L_{2};(\lambda_{1}\mu_{1}) \kappa L \parallel (\lambda_{1}\mu_{1}) \kappa_{1} L_{1}\rangle_{\rho}$$

(B.10)
where $\langle -,-,1 \rangle$'s are standard Clebsch-Gordan coefficients and enter in the expression as a result of reduction of $JM$ and $TM_T$ to $J$ and $T$, respectively [see (B.1)]. The Jahn-Hope $\chi$-coefficient arises because of the standard reduction of the JT RME into a product of orbital and spin dependent parts (DraAki 73). The triple-bar reduced matrix element, which is reduced with respect to both SU(3) and spin-isospin, has been referred to in the text as the SU(3) reduced matrix element. Since the remaining factors in (B.10) are only associated with geometrical symmetry, it is clear that the triple-bar matrix element contains the physical dependence that dictates the amount of coupling between different $(\lambda\mu)ST$ irreps in the model space.
APPENDIX C
SECOND QUANTIZATION AND ONE-BODY OPERATORS

Second quantization is a very useful formulation for handling the many-body problem. In this formulation an m-particle basis state is represented as:

\[ | n_1 n_2 ... n_i ... n_d > = a_{n_1}^+ a_{n_2}^+ ... a_{n_i}^+ ... a_{n_d}^+ | > \]  \hspace{1cm} (C.1)

where \( d \) is the total number of levels (equal to \( 2(N+1)(N+2) \) for protons and neutrons in the \( N \)-th shell of the oscillator) and \( n_i \) is 1 if the \( i \)-th level is occupied and 0 if it is not occupied. The symbol \( \nu_k \) represents the complete set of spatial, spin, and isospin quantum numbers \( \{ N, l, \frac{1}{2}, j, m_j, \tau, m_\tau \} \) of the \( k \)-th occupied single-particle state. The fermion creation operators \( a_{n_i}^+ \) act on the vacuum \( | > \) containing no particles to create a single-particle state with quantum numbers \( \nu \).

A one-body operator only involves the degrees of freedom of a single particle when acting on a many-particle state. It can be represented as

\[ F = \sum_{i=1}^{m} f_i \]  \hspace{1cm} (C.2)

where \( f_i \) acts on \( i \)-th particle and the sum is over all particles. (The sum over all particles insures that \( F \) does not change the permutation symmetry of states to which it is applied.) The second quantized form for this \( F \) is given by
\[ F = \sum_{v,v'}^d <v \mid f \mid v'> a_v^+ a_{v'} \]  \hspace{1cm} (C.3)

where \( <v \mid f \mid v'> \) is the matrix element of the one-body operator \( f \) between single-particle states with quantum numbers \( v \) and \( v' \). This result (C.3) is the starting point for determining a tensor decomposition for one-body operators, as is shown in what follows.

A procedure for calculating matrix elements of irreducible SU(3) tensor operators \( T^{(\lambda \mu)kLST} \) between the SU(3) \( \supset \) SO(3) basis states used in the text is given in Appendix B. Evaluating matrix elements of a one-body operator \( F \) is therefore straightforward if it can be decomposed as a linear combination of SU(3) tensor operators:

\[ F = \sum_{\alpha} C(\alpha) T^\alpha, \]  \hspace{1cm} (C.4)

where \( \alpha = (\lambda \mu)kLST \) runs over the complete set of tensor labels and the \( C(\alpha) \) are \( F \) dependent constants which must be determined for each one-body operator under consideration. This tensor decomposition for the one-body interaction operators \( I^2 \) and \( I \cdot s \) will be given next.

Consider the orbit-orbit interaction term first. It can be written in second quantized form as

\[ \sum_{i=1}^A l_i^2 = \sum_{v,v'} <v \mid l_i^2 \mid v'> a_v^+ a_{v'}, \]  \hspace{1cm} (C.5)

where \( l \mid v > \) are the allowed single-particle states
where \(<-,-\rangle\) are Clebsch-Gordan coefficients and \(N\) is the oscillator quantum number. The matrix elements of \(I^2\) in (C.5) are \(l(l+1)\) so one finds

\[
\sum_{i=1}^{A} l_i^2 = \sum_{\nu} l(l+1) a_{\nu}^+ a_{\nu}
\]

\[
= \sum_{N \mu n \nu} l(l+1) a_{N(1/2)jM_n,1/2m_n}^+ a_{N(1/2)jM_n,1/2m_n}^ \n
= \sum_{Nlj} \sqrt{2(2j+1)} l(l+1) \sum_{LS} U \left( \begin{array}{c} l+1/2 j \\ l+1/2 j \\ L S 0 \end{array} \right) \left( \begin{array}{c} l+1/2 j \\ l+1/2 j \\ L S 0 \end{array} \right) \n \]

\[
\times (-1)^{N} \langle (N0)l;(0N)lll(\lambda\mu)\kappa\lambda|a^+ \times a^\dagger(\lambda\mu)\kappa(\lambda\mu)\kappa(\lambda\mu)\kappa|l(l+1)=0,T=Mr=0 \rangle
\]  

(C.7)

where the definition of a spherical tensor is used in the second step. The SU(3) \(\supset SO(3)\) isoscalar factor \((-;--;l--;\) enters because of the coupling of the SU(3) representations \((N0)\) of \(a^+\) and \((0N)\) \(a\). Using the result

\[
U \left( \begin{array}{c} l+1/2 j \\ l+1/2 j \\ L S 0 \end{array} \right) = (2j+1)(2L+1) \left( \begin{array}{c} l+1/2 j \\ l+1/2 j \\ L S 0 \end{array} \right)
\]
\[
\begin{align*}
&= (-1)^{l+1/2+j+1} \sqrt{(2j+1)(2L+1)} \begin{pmatrix}
  l & 1/2 & j \\
  1/2 & l & L
\end{pmatrix},
\end{align*}
\]

and the relation
\[
\sum_j (-1)^{j+1/2} \sqrt{(2j+1)(2l+1)} \begin{pmatrix}
  1 & 1/2 & j \\
  1/2 & l & L
\end{pmatrix} = \delta_{L,0} \sqrt{2(1/2+1)} (2l+1)
\]

the final expression for the orbit-orbit interaction can be written as:
\[
\sum_{i=1}^A l_i^2 = \sum_{N(\lambda \mu \ell \xi)} (-1)^N 2l(l+1) \sqrt{2l+1} \langle (N0)\ell; (0N)\ell\ell|\ell(\lambda \mu)\kappa L=0 \rangle
\times (a^* a)^{\lambda \mu \kappa (L=1,S=1)J=0,M_J=0;T=0,M_T=0}.
\] (C.8)

It follows from this result there is a non-zero contribution for \((\lambda, \mu) = (0,0)\) and \((2,2)\) only.

Starting from the single-particle matrix elements of the I-s interaction \(\langle [j(j+1)-l(l+1)-3/4]/2 \rangle\) and following a similar procedure the expression for the decomposition of one-body spin-orbit interaction can also be determined. The final result is given by
\[
\sum_{i=1}^A l_i^2 = \sum_{N(\lambda \mu \ell \xi)} (-1)^{N+1} \sqrt{l(l+1)(2l+1)} \langle (N0)\ell; (0N)\ell\ell|\ell(\lambda \mu)\kappa L=1 \rangle
\times (a^* a)^{\lambda \mu \kappa (L=1,S=1)J=0,M_J=0;T=0,M_T=0}.
\] (C.9)
In this case there is a non-zero contribution only for \((\lambda, \mu) = (1, 1)\). The more general operators \((n_j)\) which count the number of particles in the \(j\)-th orbital involve the higher rank SU(3) tensors as well: \((\lambda, \mu) = (3, 3), (4, 4), ..., (N, N)\). The fact that these higher rank tensor do not enter for the orbit-orbit and spin-orbit interactions is an interesting result in its own right — it leads to the notion of a shell-independent pseudo-spin transformation.
D.1. Evaluating and Diagonalizing the Hamiltonian

Title of program: HUSNHAM

Computer: IBM 3090/600J

Operating System: MVS/XA

Programming language used: FORTRAN

Peripherals used: None

Number of lines in program: 1785

Nature of the physical Problem:

Low-lying energy levels of well-deformed, odd-mass nuclei can be described by the SU(3) shell-model hamiltonian (NaqDra 92) given as:

\[ H_{SU3} = H_0 + A_J J^2 + A_K \mathcal{K}_J^2 - \frac{1}{2} \mathbf{Q}^2 \mathbf{Q}^2 + C \sum_i I_i \cdot s_i + D \sum_i I_i^2. \]  \hspace{1cm} (D.1)

where the operator \( \mathcal{K}_J^2 \) is a linear combination of three rotational scalars: \( J^2 \), \( Y_3 = [(J \times Q^a) \times J]^0 \) and \( Y_4 = [(J \times Q^a)^1 \times (J \times Q^a)^1]^0 \) (NaqDra 92). A more general hamiltonian \( H'_{SU3} \), formed by adding the \( L^2 \) and Majorana interactions to \( H_{SU3} \) and taking \( J^2 \), \( Y_3 \) and \( Y_4 \) to be independent operators, can be written as:
\[ H_{SU3} = H_0 + A J^2 + A_L L^2 + A_M M + B_3 Y_3^3 + B_4 Y_4^3 - \frac{1}{2} \chi Q^a Q^a \]
\[ + C \sum_i l_i s_i + D \sum_i l_i^2. \]  

(D.2)

The program HUSNHAM calculates matrix representations of \( H_{SU3} \) (and therefore of \( H_{SU3} \)) for specified values of the total angular momentum using angular-momentum-projected (Ell 58), spin-coupled, and orthonormalized bases states (Ver 68). These matrix representations of \( H_{SU3} \) are diagonalized and a specified number of their eigenvalues and eigenvectors displayed. Multiple values of the total angular momentum \( J \) and the parameters \( \chi \) and \( C \) can be chosen in a single run. The user is required to specify the total spin \( S \) and isospin \( T \), give the bases states, and provide the SU(3) reduced matrix elements of the various operators that enter in (D.2), see Appendix B.
Program description:
This program constructs and diagonalizes the hamiltonian

\[ H = \hbar w H_0 - 0.5 \chi Q(a) Q(a) + \frac{A_m}{2} M + C_1 l(i) \cdot s(i) + D_1 l(i) \cdot l(i) + A_1 L^2 + A_j J^2 + B_y Y_3A + C_y Y_4A \]

where

- \( H_0 \) = isotropic harmonic oscillator hamiltonian
- \( Q(a) Q(a) \) = algebraic quadrupole-quadrupole interaction
- \( M \) = Majorana space symmetry operator
- \( l(i) \cdot s(i) \) = one-body spin-orbit interaction
- \( l(i) \cdot l(i) \) = one-body orbit-orbit interaction
- \( L^2 \) = total orbital angular momentum operator
- \( J^2 \) = total angular momentum operator
- \( Y_3A \) = K-band splitting operator \((J \times Q) \cdot J\)
- \( Y_4A \)

 External subprograms required.

- BLOCKS : routine for loading in factorials.
- IODATA : routine for reading in SU(3) rmeas.
- INPUT : routine to read in hamiltonian parameters, etcetera.
- HAMINT : routine to generate various hamiltonian interactions
- HAMATRIX : routine to construct and diagonalize hamiltonian matrix
- OUTPUTBS : routine to write out basis states
- OUTPUTEN : routine to write out eigenstate information, etcetera.
- PACKSU3B : routine to generate basis state labels in packed form.

@PROCESS DC(ENERGY, RMEDAT)

PROGRAM HUSNHAM
IMPLICIT REAL*8 (A-H, O-Z)
CHARACTER*2 DIAGONALIZE, YES/'Y/', NO/'N'/

IFILE1 : Unit number for input file of irrep labels.
IFILE2 : Unit number for input file of SU(3) rmeas.
IFILESTART : Starting unit number for different sets of 2J hamiltonian interaction matrices.
PARAMETER (IFILE1=3, IFILE2=8, IFILESTART=10)

NUMINT : total number of separate interactions in hamiltonian
IDIMHAM : dimension of hamiltonian matrix, etcetera.
IDIMMEIG : max number of eigenvectors to be retained
IDIMJT : dimension of \((J, T)\) label arrays
IDIMPAR : dimension of \(C\) and \(J2X\) arrays
PARAMETER (NUMINT=9, IDIMHAM=999, IDIMMEIG=20, IDIMPAR=10, IDIMJT=10)

HAM : hamiltonian matrix
EIVAL : eigenvalue array
EIVEC : eigenvector array
COMMON/ENERGY/ HAM(IDIMHAM, IDIMHAM), EIVAL(IDIMHAM), & EIVEC(IDIMHAM, IDIMHAM)

C : parameter strength for l.s spin-orbit interaction.
CHI : parameter strength for Q(a),Q(a) interaction.
STRENGTH : array for strengths of various interactions
DIMENSION C(IDIMPAR), CHI(IDIMPAR), STRENGTH(NUMINT)

I2JX : array for 2J values input
I2TX : isospin values for desired output states
LABEL : Array for packed labels of basis states.
DIMENSION I2TX(IDIMJT), I2JX(IDIMJT), LABEL(3, IDIMHAM)

IBTREDIM : dimension for SU(3) rme binary tree.
IRMTRREDIM : dimension for SU(3) rme array
PARAMETER(IBTREDIM=100000, IBTREDIM=12*IRMTRREDIM)

IBTREE : Binary tree array of labels for SU(3) rmes
RMTRZE : Array for SU(3) rmes of tensor operators
COMMON/RUEDAT/ RMTRZE(IRMTRREDIM), IBTREE(-9:IBTREDIM)

Startup and input.

Read in factorials for SU(3) routines.
CALL BLOCKS

Read Raske's RMEs in coded form.
File 8 is the output of Raske's RMELOOK.
CALL IODATA(1, 1, IFILE2, NUMI, NUMF)
READ(IFILE2) INDEX, ICOUNT
READ(IFILE2) (IBTREE(I), I=-9, INDEX)
READ(IFILE2) (RMTRZE(I), I=1, ICOUNT)

Read in parameter values, etcetera.
CALL INPUT(DIAGONALIZE, NETA, NPAR, NJ, I2JX, NT, I2TX, NC, & CHI, NC, C, STRENGTH, NL, NG, NLV, NGV, IFILE1)

Construct Hamiltonian for (J,T) values input.

DO 1000 IX=1, NJ ! Loop for possible 2J values.
       J2=I2JX(IX)
DO 1000 IY=1, NT ! Loop for possible 2T values.
       ITT=I2TX(IY)
       IFILE=IFILESTART + J2

Generate basis for given (J,T).
CALL PACKS03B(J2, IFILE1, NETA, NS, IDIMHAM, LABEL, *1000)
Calculate matrices of various hamiltonian interactions.
CALL HAMINT(IFILE, J2, NETA, NS, IDIMHAM, LABEL)
Write out the basis to screen and file.
CALL OUTPUTBS(NETA, NS, LABEL)
C Construct and diagonalize hamiltonian, output results, if desired.

IF (DIAGONALIZE .EQ. YES) THEN
  DO 900, JC=1, NC ! Loop for different C values
    STRENGTH(4)=C(JC)
    DO 800, INX=1, NCHI ! Loop for different chi values
      STRENGTH(2)=-0.5D0*CHI(INX)
      Construct and diagonalize hamiltonian.
      CALL HAMATRIX(J2, IFILE, NS, NUMINT, STRENGTH, 60) ! debug
      Write out eigenvalues, etcetera.
      CALL OUTPUTEN(NS, NL, NG, NLV, NGV, IFILE)
  800  CONTINUE ! Chi parameter loop
  900  CONTINUE ! C parameter loop
END IF

1000 CONTINUE ! (J, T) loop
STOP
END

SUBROUTINE INPUT(DIAGONALIZE, NETA, NPAR, NJ, I2JX, NT, I2TX, NCHI, &
                 CHI, NC, C, STRENGTH, NL, NG, NLV, NGV, IFILE)

Program Description
Subprogram to read input information for HUSNHAM program.

Parameters:
DIAGONALIZE : yes/no flag with regard to diagonalizing matrix
NETA : number of oscillator quanta for shell, e.g. 2 for ds-shell
NPAR : number of particles in valance shell.
I2JX(NJ) : NJ values of 2J ang. mom. values.
I2TX(NJ) : NT values of 2T isospin values.
CHI(NCHI) : NCHI values of chi parameter values for Q.Q
C(NC) : NC values of C parameter values for spin-orbit
STRENGTH : strength values of interactions.
NL, NG : NLth to NGth eigenvalue to be printed.
NLV, NGV : NLVth to NGVth eigenvector to be printed.
IFILE : unit number for input file of irrep labels.

READIN : subprogram to check for yes or no answer

IMPLICIT REAL*8(A-H,O-Z)
CHARACTER*2 DIAGONALIZE

DIMENSION I2JX(*), I2TX(*), C(*), CHI(*), STRENGTH(*)

Read label information from file.
READ (IFILE, *) NETA ! oscillator q.n
READ (IFILE, *) NPAR ! # of particles

WRITE(6, '(A)') ' Diagonalize matrix?'
CALL READIN(DIAGONALIZE, *10)
Read in ang. mom. 2J and spin 2S values desired.
WRITE(6,'(A)') ' Enter total number of 2J values to be input:'
READ(5,*), NJ
WRITE(6,'(A)') ' Enter 2J values:
READ(5,*), (I2JX(I), I=1,NJ)
WRITE(6,'(A)') ' Enter total number of 2T values to be input:
READ(5,*), NT
WRITE(6,'(A)') ' Enter 2T values:
READ(5,*), (I2TX(I), I=1,NT)

Read in hamiltonian parameter values.
H = hw*HO + 0.5*CHI*Q.Q + AM*M + C*1(I).s(I) + D*1(I).1(I) + A1*L**2 + Aj*J**2 + By*Y3A + Cy*Y3A
WRITE(6,'(A)') ' Enter total number of CHI values to be input:
READ(5,*), NCHI
WRITE(6,'(A)') ' Enter chi values:
READ(5,*), (CHI(I), I=1,NCHI)
WRITE(6,'(A,A)') ' CHI', CHI(I), I=1,NCHI
WRITE(6,'(A,A)') ' Enter hw, AM, Al, and D coefficients:
READ (5, *) HW, AM, Al, D
WRITE(6,'(4(A, 1PD11.4,2X))') ' HW=',HW, ' AM=',AM, ' Al=',Al, ' D=',D
WRITE(6,'(A, A)') ' Enter A, By, and Cy rotor coefficients:
READ (5, *) Aj, BY, CY
WRITE(6,'(4(A,1PD11.4,2X))') ' Aj=',Aj,' BY=',BY,' CY=',CY
STRENGTH(1)=HW
STRENGTH(3)=AM
STRENGTH(5)=D
STRENGTH(6)=BY
STRENGTH(7)=CY
STRENGTH(8)=Al
STRENGTH(9)=Aj
WRITE(6,'(A)') ' Enter total number of l.s coeffs to be input:
READ(5,*), NC
WRITE(6,'(A)') ' Enter l.s coeffs:
READ(5,*), (C(IC), IC=1,NC)
WRITE(6,'(A)') ' C', C(IC), IC=1,NC
WRITE(6,'(A)') ' Enter lower and upper number of eigvals to print:
WRITE(6,'(A)') ' (Zero for all):'
READ(5,*), ML, NG
WRITE(6,'(A)') ' Enter lower and upper number of eigvector components to print:
WRITE(6,'(A)') ' (Zero for all):'
READ(5,*), NLV,NGV
RETURN
END

SUBROUTINE HAMINT(IFILE,J2,NE,T,MATDIM,IDIMLAB,LBL)

Program Description:
Subprogram to generate matrix elements of various interactions in hamiltonian.

-----------------------------------------------------------------------
IMPLICIT REAL*8(A-H,O-Z)

DIMENSION LABEL(3,IDIMLAB)

CALL H0(NETA,MATDIM)
INTERACT=1
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,MATDIM,MATDIM)

CALL QQA(MATDIM,LABEL)
INTERACT=2
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,MATDIM,MATDIM)

CALL MAJORANA(MATDIM,LABEL)
INTERACT=3
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,MATDIM,MATDIM)

CALL SPINORB(NETA, NTERM, MATDIM, LABEL)
INTERACT=4
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,NTERM,NTERM)

CALL ORBORB(NETA, NTERM, MATDIM, LABEL)
INTERACT=5
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,NTERM,NTERM)

IF(J2 .NE. 0) THEN
   CALL Y3A(NTERM,MATDIM,LABEL)
ELSE
   NTERM=0
END IF
INTERACT=6
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,NTERM,NTERM)

IF(J2 .NE. 0) THEN
   CALL Y4A(NTERM,MATDIM,LABEL)
ELSE
   NTERM=0
END IF
INTERACT=7
WRITE(IFILE) J2, INTERACT, MATDIM
CALL IODATA(0,0,IFILE,NTERM,NTERM)

CALL LSQUARE(MATDIM,LABEL)
INTERACT=8
WRITE (IFILE) J2, INTERACT, MATDIM
CALL IODATA(0, 0, IFILE, MATDIM, MATDIM)
C
REWRIND (IFILE)
RETURN
END
SUBROUTINE HO (NETA, MATDIM)
C
Prgram Description
Construct the matrix for the harmonic oscillator hamiltonian HO.
C
Parameters:
NETA : number of single-particle quanta for shell,
e.g. 2 for ds-shell.
MATDIM : dimension of matrix to be constructed.
C
IMPLICIT REAL*8 (A-H, O-Z)
C
IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER (IDIMIM = 100000, IDIMFM = 100000)
C
IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)
C
Statement function to pack matrix indices.
INDEX(I, J, MATDIM) = I + ((2*MATDIM-J)*(J-1))/2 ! J .LE. I (ES SL)
INDEX(I, J, MATDIM) = J + I*(I-1)/2 ! J .LE. I (IM SL)
C
DO I=1, MATDIM
  IM(I) = INDEX(I, I, MATDIM)
  FM(I) = DFLOAT (NETA) + 1.5 DO
END DO
RETURN
END
SUBROUTINE QAQA (MATDIM, LABEL)
C
Prgram Description
Construct the matrix for the algebraic quadrupole-quadrupole interaction.
C
Parameters
MATDIM : dimension of matrix to be constructed.
LABEL : input array of packed basis states.
C
IMPLICIT REAL*8 (A-H, O-Z)
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IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)

IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)

DIMENSION LABEL(3,*)

Statement function to pack matrix indices.
INDEX(I,J,MATDIM)=I + ((2*MATDIM-J)*(J-1))/2 ! J .LE. I (ESSL)
INDEX(I,J,MATDIM)=J + I*(I-1)/2 ! J .LE. I (IMSL)

SU(3) quadratic Casimir operator.
SU3CAS(LA,MU)=DFLOAT((LA+MU+3)*(LA+MU) - LA*MU)

DO I=1,MATDIM
   CALL UNPKSU3B(I,LABEL,NFAR,IALPHA,LM,MU,K,L,IP0,IP1,IP2,
                  IBETA,I2S,I2T,I2J)
   VALUE=4.0*SU3CAS(LM,MU) - 3.0*DFLOAT(L*(L+1))
   IM(I)=INDEX(I,I,MATDIM)
   FM(I)=VALUE
END DO
RETURN
END

PROCESS DC (MEDATA)

SUBROUTINE LSQUARE (MATDIM, LABEL)

Program Description
Construct the matrix for the L^2 - L*(L+1) interaction.

Parameters:
MATDIM : dimension of matrix to be constructed.
LABEL : input array of packed basis states.

IMPLICIT REAL*8 (A-H, O-Z)

IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)

IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)

DIMENSION LABEL(3,*)

Statement function to pack matrix indices.
INDEX(I,J,MATDIM)=I + ((2*MATDIM-J)*(J-1))/2 ! J .LE. I (ESSL)
INDEX(I,J,MATDIM)=J + I*(I-1)/2 ! J .LE. I (IMSL)

DO I=1,MATDIM
   CALL UNPKSU3B(I,LABEL,NFAR,IALPHA,LM,MU,K,L,IP0,IP1,IP2,
                  IBETA,I2S,I2T,I2J)
VALUE=DFLOAT(L*(L+1))
IM(I)=INDEX(I, I, MATDIM)
FM(I)=VALUE
END DO
RETURN
END
SUBROUTINE MAJORANA(MATDIM, LABEL)
   C Program Description
   Construct the matrix for the space symmetry Majorana interaction.
   C Parameters:
   MATDIM : dimension of matrix to be constructed.
   LABEL : input array of packed basis states.
   C
   IMPLICIT REAL*8(A-H, O-Z)
   C
   IDIMIM : dimension for array IM
   IDIMFM : dimension for array FM
   PARAMETER(IDIMIM=100000, IDIMFM=100000)
   C
   IM : array for packed matrix indices
   FM : array for non-zero values of matrix
   COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)
   C
   DIMENSION LABEL(3,

   Statement function to pack matrix indices.
   INDEX(I, J, MATDIM)=I + ((2*MATDIM-J)*(J-1))/2  ! J .LE. I (ESSL)
   INDEX(I, J, MATDIM)=J + I*(I-1)/2  ! J .LE. I (IMSL)
   C
   DO I=1, MATDIM
      CALL UNFKSU3B(I, LABEL, NPAR, IALPHA, LM, MU, K, L, IP0, IP1, IP2, &
                     IBETA, I2S, I2T, I2J)
      LVALUE=IP0*(IP0+8) + IP1*(IP1+4) + IP2*IP2  ! Twice P, P', P''
      IM(I)=INDEX(I, I, MATDIM)
      FM(I)=0.12500*DFLOAT(LVALUE) ! SU(4) Casimir only.
   END DO
RETURN
END
SUBROUTINE SPINORB(META, NTERM, MATDIM, LABEL)
   C Program Description
   Subprogram to calculate matrix elements for spin-orbit interaction l(i).s(i).
   C
   Parameters:
   META : number of single-particle quanta for shell,
   e.g. 2 for ds-shell.
NTERM : number of non-zero m.e.s on output
MATDIM: dimension of matrix to be constructed
LABEL : input array of packed basis state labels

Subprograms
DJHR3 : routine to compute SU(2) Jahn-Hope coefficients.
ERROR : exit routine with error message
TREEV2 : binary tree routine for retrieving SU(3) rmes.
UNPKSU3B : routine to unpack labels for basis states.
YU3R3W : routine to compute SU(3) > SO(3) Wigner coefficients.

IMPLICIT REAL*8 (A-H,O-Z)

TOLERANCE : tolerance limit for retraining non-zero m.e. values
NUMTENS : maximum number possible for SU(3) tensors in a shell
NSU3 : dimension of wigner array
PARAMETER(TOLERANCE=1.D-14,NSU3=9,NUMTENS=5)

COEFF : array for SU(3) tensor expansion coefficients
LAM : array for (LAM, LAM) SU(3) tensor label
LABTENS: Array of packed tensor operator labels.
LABOPR : Array of packed operator labels to retrieve rmes.
WIGNER : SU(3) Wigner array
DIMENSION COEFF(NUMTENS), LAM(NUMTENS), LABTENS(NUMTENS), & LABOPR(8), WIGNER(NSU3,NSU3,NSU3,NSU3)

IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)

IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)

IBTREDIM : dimension for SU(3) rme binary tree.
IRMTREDIM : dimension for SU(3) rme array
PARAMETER(IRMTREDIM=100000, IBTREDIM=12*IRMTREDIM)

IBTREE : Binary tree array of labels for SU(3) rmes
RMTree : Array for SU(3) rmes of tensor operators
COMMON/RMDEDAT/ RMTree(IRMTREDIM), IBTREE(-9:IBTREDIM)

DIMENSION LABEL(3, *)

Statement functions.

Statement function to pack matrix indices.
INDEX(I,J,MATDIM)=I + ((2*MATDIM-J)*(J-1))/2 ! J .LE. I (ESSL)
INDEX(I,J,MATDIM)=J + I*(I-1)/2 ! J .LE. I (IMSL)

Packing function for SU(3) rmes. (8, 8, 8)
IPACK4(I1, I2, I3, I4)=
& IOR(I4, ISHFT(IOR(I3, ISHFT(IOR(I2, ISHFT(I1, 8)), 8)), 8))

Packing function for SU(3) rmes. (7, 5, 5, 5, 5)
IPACK6(I1, I2, I3, I4, I5, I6)=IOR(I6, ISHFT(IOR(I5, ISHFT(IOR(I4, & ISHFT(IOR(I3, ISHFT(IOR(I2, ISHFT(I1, 5)), 5)), 5)), 5)), 5))
Determine possible tensors and coefficient values.

LSPMIN=0
IF (BTEST(NETA,0)) LSPMIN=1
NTENSOR=0
DO IETA=1,NETA,2 ! Range of possible tensors.
   NTENSOR=NTENSOR + 1
   LAM(NTENSOR)=IETA
   COEFF(NTENSOR)=0.DO
   LAMTENS(NTENSOR)=IPACK4(IETA, IETA, 2, 0) ! (IETA, IETA) tensor
   DO 2,LSP=LSPMIN,NETA,2 ! Range of single-particle ang. mom.
      2 CONTINUE
      IF (BTEST(NETA+1, 0)) COEFF(NTENSOR)=-COEFF(NTENSOR)
   END DO

Construct matrix.

Pack operator information for different tensors.
LABOPR(6)=IPACK4(NETA, 0, 1, 1) ! fermion creation operator
LABOPR(7)=IPACK4(0, NETA, 1, 1) ! fermion annihilation operator

Calculate spin-orbit m.e. <IL?1.s?ZR>
Run through bra states.
NTERM=0
DO IL=1,MATDIM

Unpack basis state labels.
CALL UNFKSU3B(IL, LABEL, NPAR, IALPHAL, LML, MUL, KL, LL, 
   IP0L, IP1L, IP2L, IBETAL, I2SL, I2TL, I2J)

Pack basis info for retrieval of m.e.
LABOPR(1)=IPACK4(NPAR, IP0L, IP1L, IP2L+128) ! # particles & SU(4)
LABOPR(2)=IPACK4(LML, MUL, I2SL, I2TL) ! SU(3) & 2(S,T) label

Run through the ket states (lower triangle).
DO IR=1,IL

Unpack basis state labels.
CALL UNFKSU3B(IR, LABEL, NPAR, XALPHAR, LMR, MUR, KR, LR, 
   IP0R, IP1R, IP2R, IBETAR, I2SR, I2TR, I2J)

Pack basis info for retrieval of m.e.
LABOPR(3)=IPACK4(NPAR, IP0R, IP1R, IP2R+128) ! # particles & SU(4)
LABOPR(4)=IPACK4(LMR, MUR, I2SR, I2TR) ! SU(3) & 2(S,T) label

DHBOPR=DJHR3(2*LR, I2SR, I2J, 2, 2, 0, 2*IL, I2SL, I2J)
VALUE=0.DO
DO 50, NTENS=1, NTENSOR
   CALL YU3R3M(LMR, MUR, LAM(NTENS), LAM(NTENS), LML, MUL, LR, 1, 
      LL, KOMAX, K1MAX, K2MAX, K3MAX, WIGNER, *50)
   LABOPR(5)=LABTENS(NTENS)
   50 CONTINUE
DO 40,K0=1,K0MAX ! Rho multiplicity.
C Pack multiplicity labels for operator, left, and right sta
LABOPR(8)—IPACK6(K0,1,BETAL,BETAR,ALPHAL,ALPHAR)
C
C Call Pree <(ML,NUL) ’SL,TL??T(LAM,LAM)1,0??(LNR,MUR) SR, TR>K
RME=0.D0
CALL TREEV2(0,LABOPR,IBTREE,*10,*70,*40)
10 INDX=IBTREE(-5)+IBTREE(-6)
RME=RMTREE(IBTREE(INDX))
20 IF (RME .NE. 0.D0) THEN
C Add T(IETA,ETA,1,0) tensor contribution
VALUE=VALUE + COEFF(NTENS)*DJHOPE*WIGNER(K0,KR,1,KL)*RME
END IF
40 CONTINUE
50 CONTINUE
60 IF (ABS(VALUE) .GT. TOLERANCE) THEN
NTERM=NTERM+1
IM(NTERM)=INDEX(IL,IR,MATDIM)
FM(NTERM)=VALUE
END IF
END DO
END DO
RETURN
70 CALL ERROR('SPINORB: Overflow of IBTREE.‘)
END
@PROCESS DC(MEDATA, RMEDAT)
SUBROUTINE ORBORB(NETA,NTERM,MATDIM,LABEL)
C Program Description
C Subprogram to calculate matrix elements for orbit-orbit
C interaction l(i) .l(i).
C
C Parameters
C NETA : number of single-particle quanta for shell,
C e.g. 2 for 2s-shell.
C NTERM : number of non-zero m.e.s on output
C MATDIM : dimension of matrix to be constructed
C LABEL : input array of packed basis state labels
C
C Subprograms
C DJHR3 : routine to compute SU(2) Jahn-Hope coefficients.
C ERROR : exit routine with error message
C TREEV2 : binary tree routine for retrieving SU(3) rmes.
C UNPKSU3B : routine to unpack labels for basis states.
C YU3R3W : routine to compute SU(3) > SO(3) Wigner coefficients.
C
C IMPLICIT REAL*S(A-H,O-Z)
C
C TOLERANCE : tolerance limit for retraining non-zero m.e. values
C NUMTENS : maximum number possible for SU(3) tensors in a shell
C NSU3 : dimension of wigner array
C PARAMETER(TOLERANCE=1.D-14,NSU3=9,NUMTENS=5)
COEFF : array for SU(3) tensor expansion coefficients
LAM : array for (LAM,LAM) SU(3) tensor label
LABTENS: Array to pack tensor operator labels.
LABOPR : Array of packed operator labels to retrieve rmes.
WIGNER : SU(3) Wigner array
DIMENSION COEFF(NUMTENS), LAM(NUMTENS), LABTENS(NUMTENS),
        LABOPR(8), WIGNER(NSU3,NSU3,NSU3)

IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER (IDIMIM=100000, IDIMFM=100000)
IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)

IBTREDIM : dimension for SU(3) rms binary tree.
IRMREDIM : dimension for SU(3) rme array
PARAMETER (IRMREDIM=100000, IBTREDIM=12*IRMREDIM)
IBTREE : Binary tree array of labels for SU(3) rmes
RMTREE : Array for SU(3) rmes of tensor operators
COMMON/REMDAT/ RMTREE(IRMREDIM), IBTREE(-9:IBTREDIM)

DIMENSION LABEL(3,*)

Statement function.
Statement function to pack matrix indices.
INDEX(I,J,MATDIM)=I + ((2*MATDIM-J)*(J-1))/2 ! J LE I (ESSL)
INDEX(I,J,MATDIM)=J + I*(I-1)/2 ! J LE I (IMSL)
Packing function for SU(3) rmes. (8,8,8,8)
IPACK4(I1,I2,I3,I4)=
 & IOR(I4,ISHFT(IOR(I3,ISHFT(IOR(I2,ISHFT(I1,8)),8)),8))
Packing function for SU(3) rmes. (7,5,5,5,5)
IPACK6(I1,I2,I3,I4,I5,I6)=JOR(I6,ISHFT(IOR(I5,ISHFT(IOR(I4,
 & ISHFT(IOR(I3,ISHFT(IOR(I2,ISHFT(I1,5)),5)),5)),5)),5))

Determine possible tensors and coefficient values.
LSPMIN=0
IF (BTEST (NETA, 0) ) LSPMIN=1
NTENSOR=0
DO IETA=0,NETA,2 ! Range of possible tensors.
   NTENSOR=NTENSOR+1
   LAM(NTENSOR)=IETA
   COEFF(NTENSOR)=0.0D0
   LABTENS(NTENSOR)=IPACK4(IETA,IETA,0,0) ! (IETA,IETA) tensor
   DO 2, LSP=LSPMIN,NETA,2 ! Range of single-particle ang. mom.
      CALL YU3R3W(NETA,0,0,NETA,IETA,IETA,LSP,LSP,
      & 0,KOMAX,KMAX,K2MAX,K3MAX,WIGNER,*2)
      DLFACT=DLFLOT(2*LSP*(LSP+1)) *DSQRT(DFLOAT(2*LSP+1))
      COEFF(NTENSOR)=COEFF(NTENSOR) + DLFACT*WIGNER(1,1,1,1)
   2 CONTINUE
   IF (BTEST (NETA, 0) ) COEFF(NTENSOR)=-COEFF(NTENSOR)
END DO
Construct matrix.

Pack operator information for different tensors.
LABOPR(6) = IPACK4(NETA, 0, 1, 1) ! fermion creation operator
LABOPR(7) = IPACK4(0, NETA, 1, 1) ! fermion annihilation operator

Calculate orbit-orbit m.e. <IL?1.1?IR>

Run through bra states.
NTERM = 0
DO IL = 1, MATDIM

Unpack basis state labels.
CALL UNPKSU3B(IL, LABEL, NFAR, IALPHAL, LML, MUL, KL, LL,
   IPOL, IPIL, IP2L, IBEtal, I2SL, I2TL, I2J)

Pack basis info for retrieval of rme.
LABOPR(1) = IPACK4(NPAR, IPOL, IPIL, IP2L + 128) ! # particles & SU(4)
LABOPR(2) = IPACK4(LML, MUL, I2SL, I2TL) ! SU(3) & 2(S,T) labels

Run through the ket states (lower triangle).
DO IR = 1, IL

Unpack basis state labels.
CALL UNPKSU3B(IR, LABEL, NFAR, IALPHAR, LMR, MUR, KR, LR,
   IP0R, IP1R, IP2R, IBEtAR, I2SR, I2TR, I2J)

Pack basis info for retrieval of rme.
LABOPR(3) = IPACK4(NPAR, IP0R, IP1R, IP2R + 128) ! # particles & SU(4)
LABOPR(4) = IPACK4(LMR, MUR, I2SR, I2TR) ! SU(3) & 2(S,T) labels

Generate matrix elements of T(0, 0, 0, 0) tensor
VALUE = 0.0
DO 50, NTENS = 1, NTENSOR
   CALL Y3R3W(LMR, MUR, LAM(NTENS), LAM(NTENS), LML, MUL, LR, 0,
      IPOL, IPIL, IP2L, IBEtal, I2SL, I2TL, I2J)
   LABOPR(5) = LABTENS(NTENS)
   DO 40, KO = 1, KOMAX ! Rho multiplicity.
      CALL TREEV2(0, LABOPR, IBTREE, *10, *130, *40)
   10 INDEX = IBTREE(-5) + IBTREE(-6)
   RME = RMTREE(IBTREE(INDEX))
   IF (RME .NE. 0.00) THEN
      Add T(LAM, LAM, 0, 0) tensor contribution.
      VALUE = VALUE + COEFF(NTENS) * WIGNER(KO, KR, 1, KL) * RME
   END IF
   CONTINUE
   END DO
   CONTINUE
   IF (ABS(VALUE) .GT. TOLERANCE) THEN
      NTERN = NTERN + 1
      IM(NTERN) = INDEX(IL, IR, MATDIM)
      FM(NTERN) = VALUE
   END IF
END DO
END DO
RETURN

CALL ERROR(' ORBORB: Overflow of IBTREE. ')
SUBROUTINE Y3A (NTERM, MATDIM, LABEL)

Program Description
Construct the matrix for the Y3A operator. This operator is used to account for the splitting of rotational K-bands and is the \((JxQ).J\) operator.

Parameters:
- **NTERM**: number of non-zero matrix elements on output
- **MATDIM**: dimension of matrix to be constructed
- **LABEL**: input array of packed basis state labels

Subprograms:
- **ERROR**: exit routine with error message
- **RMEJQJ**: routine for RMEs of \((JxQ).J\) operator.

Reference: B. Naqvi and J.P. Draayer, KJ-band paper.

Note: Subprogram assumes that multiple \(K\) states for an SU(3) irrep occur successively in basis.

IMPLICIT REAL*8(A-H, O-Z)
DATA KUAX, KRMAX /0, 0/
LOGICAL LOG1, LOG2, LOG3

TOLERANCE : tolerance limit for retraining non-zero m.e. values
NSU3 : dimension of array for Wigner coefficient.
PARAMETER (TOLERANCE=1.D-14, NSU3=9)

RME : array for RMEs of \((JxQ).J\) operator.
DIMENSION RME(NSU3, NSU3), LABEL(3, *)

IMDIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER (IMDIM=100000, IDIMFM=100000)

IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON /MEDATA/ FM(IDIMFM), IM(IDIMIM)

Statement functions.

Statement function to pack matrix indices.
INDEX (I, J, MATDIM) = I + ((2*MATDIM-J)*(J-1))/2 ! J .LE. I (ESSL)
INDEX (I, J, MATDIM) = J + I*(I-1)/2 ! J .LE. I (IMSL)

Multiplicity function for \(L\) states in SU(3) irrep \((LM, MU)\).
MULT (LM, MU, L) = MAX0 (0, (LM+MU+2-L)/2) - MAX0 (0, (LM+1-L)/2) -
& MAX0(0,(MU+1-L)/2)
C --------------------------------------------------------------------------------------------------------
C Construct matrix.
C --------------------------------------------------------------------------------------------------------

CONST=DSQRT(10.DO)/6.DO
NTERM=0
IL=1
DO WHILE(IL .LE. MATDIM)
C Unpack basis state labels.
CALL UNFKSU3B(IL,LABEL,NPAR,IALPHAL,LML,MUL,KL,LL,ILPOL,IPIL,IP2L,IBETAL,I2SL,I2TL,I2J)
KLMAX=MULTR3(LML,MUL,LL)
IR=1
DO WHILE(IR .LE. IL)
C Unpack basis state labels.
CALL UNPXSU3B(IR,LABEL,NPAR,IALPHAR,LMR,MUR,KR,LR,IFOR,IF1R,IP2R,IBETAR,I2SR,X2TR,12J)
KRMAX=MULTR3(LMR,MUR,LR)
C Calculate matrix element only if K, L, & S different.
LOG1=IALPHAL.EQ.IALPHAR .AND. LML.EQ.LMR .AND. MUL.EQ.MUR
LOG2=IP0L.EQ.IP0R .AND. IP1L.EQ.IP1R .AND. IP2L.EQ.IP2R
LOG3=IBETAL.EQ.IBETAR .AND. I2SL.EQ.I2SR
IF(LOG1 .AND. LOG2 .AND. LOG3) THEN
IF(KL.EQ.I .AND. KL.EQ.KR) THEN ! Matrix for range of K label
C Generate (JxQ).J rme.
CALL RMEJQJ(LML,MUL,I2SL,KLMAX,LL,12J,KRMAX,LR,12J,RME,*30)
DO 20 MR=1,KRMAX
DO 20 ML=1,KLMAX
VALUE=CONST*RME(ML,MR)
IF(ABS(VALUE) .GT. TOLERANCE) THEN
ILEFT=IL+ML-1
IRITE=IR+MR-1
IF(IRITE .LE. ILEFT) THEN
NTERM=NTERM+1
IM(NTERM)=INDEX(ILEFT,IRITE,MATDIM)
FM(NTERM)=VALUE
END IF
END IF
20 CONTINUE
ELSE
WRITE(6,*) ' KLMAX=',KLMAX,' KRMAX=',KRMAX
WRITE(6,*) ' IL=',IL,' KL=',KL,' IR=',IR,' KR=',KR
CALL ERROR(' Y3A: Multiple K states do not occur '//
'successively in basis.')
END IF ! KL if construct
END IF ! LOG if construct
30 IR=IR + KRMAX
END DO ! IR loop
IL=IL + KLMAX
END DO ! IL loop
RETURN
END
$PROCESS DC(MEDATA)
SUBROUTINE Y4A(NTERM, MATDIM, LABEL)

Program Description
Construct the matrix for the Y4A operator. This operator is
used to account for the splitting of rotational K-bands
and is the (Jx)(QJ) operator.

Parameters:
NTERM : number of non-zero matrix elements on output
MATDIM: dimension of matrix to be constructed
LABEL : input array of packed basis state labels

Subprograms:
ERROR : exit routine with error message
RMIJQQJ: routine for RMEs of (JxQ). (QxJ) operator.

Reference: H. Naqvi and J.P. Draayer, KJ-band paper.

Note: Subprogram assumes that multiple K states for an SU(3)
irrep occur successively in basis.

IMPLICIT REAL*8(A-H,0-Z)
DATA KLMAX, KRMAX/0,0/
LOGICAL LOG1, LOG2, LOG3
TOLERANCE : tolerance limit for retraining non-zero m.e. values
NSU3 : dimension of array for Wigner coefficients.
PARAMETER(TOLERANCE=1.D-14, NSU3=9)
DIMENSION RME(NSU3,NSU3), LABEL(3, *)
IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)
DIMENSION IM(IDIMIM), FM(IDIMFM)

Statement functions.
Statement function to pack matrix indices.
INDEX(I,J,MATDIM)=I + ((2*MATDIM-J)*(J-1))/2  ! ESSL
INDEX(I,J,MATDIM)=J + I*(I-1)/2  ! IMSL

Multiplicity function for L states in SU(3) irrep (LM, MU).
MULT(LM, MU, L)=MAX0(0, (LM+MU+2-L)/2) - MAX0(0, (LM+1-L)/2) - 
& MAX0(0, (MU+1-L)/2)
Construct matrix.

```
CONST=-5.DO/18.DO
NTERM=0
IL=1
DO WHILE(IL .LE. MATDIM)

C Unpack basis state labels.
CALL UNPKSU3B(IL, LABEL, NPAR, IALPHAL, LML, MUL, KL, LL,
& IPOL, IP1L, IP2L, IBETAL, I2SL, I2TL, I2J)
IR=1
KLMAX=MULT(LML, MUL, LL)
DO WHILE(IR .LE. IL)

C Unpack basis state labels.
CALL UNPKSU3B(IR, LABEL, NPAR, IALPHAR, LMR, MUR, KR, LR,
& IPOR, IP1R, IP2R, IBETAR, I2SR, I2TR, I2J)
KRMAX=MULT(LMR, MUR, LR)

C Calculate matrix element only if K, L, & S different.
LOG1=IALPHAL.EQ.IALPHAR .AND. LML.EQ.LMR .AND. MUL.EQ.MUR
LOG2=IPOL.EQ.IPOR .AND. IP1L.EQ.IP1R .AND. IP2L.EQ.IP2R
LOG3=IBETAL.EQ.IBETAR .AND. I2SL.EQ.I2SR
IF (LOG1 .AND. LOG2 .AND. LOG3) THEN
  IF (KL.EQ.1 .AND. KR.EQ.1) THEN ! Matrix for range of K label
    IF(KL.EQ.1 .AND. KR.EQ.1) THEN ! Matrix for range of K label
      IF(KL.EQ.1 .AND. KR.EQ.1) THEN ! Matrix for range of K label
        CALL RMEJQQJ(LML, MUL, I2SL, KLMAX, LL, I2J, KRMAX, LR, I2J,
        & RME,*30)
      DO 20, MR-1, KRMAX
        DO 20, ML-1, KLMAX
          VALUE=RME(ML,MR)
          IF(ABS(VALUE) .GT. TOLERANCE) THEN
            ILEFT=IL+ML-1
            IRITE=IR+MR-1
            IF(IRITE .LE. ILEFT) THEN
              NTERM=NTERM+1
              IN(NTERM)=INDEX(ILEFT, IRITE, MATDIM)
              FM(NTERM)=CONST*VALUE
            END IF
          END IF
        END DO
      END DO
      ELSE
        CALL ERROR(' Y4A: Multiple K states do not occur '/
        & 'successively in basis.')
        END IF ! KL if construct
    END IF ! LOG if construct
  END IF ! LOG if construct
END IF ! LOG if construct
20 CONTINUE
ELSE
  CALL ERROR(' Y4A: Multiple K states do not occur '/
  & 'successively in basis.')
  END IF ! KL if construct
END IF ! LOG if construct
30 IR=IR + KRMAX
END DO ! IR loop
IL=IL + KLMAX
END DO ! IL loop
RETURN
END
SUBROUTINE RMEJQQJ(LM, MU, IS, KLMAX, LL, JR, RN, RME, *)
```
Program Description
This program calculates the reduced matrix element of the operator
'(JxQ).J' in the basis | (Lm, Mu) S KL L J >.

-------------------------------------------------------------
Parameters:
(Lm, Mu) = (Lambda, Mu) = SU3 irrep label.
IS = 2*spin of left and right states
KL(KR) = The multiplicity label of the orbital angular momentum
LL(LR) = 2*the orbital angular momentum of left(right) state. Must be even integer.
JL(JR) = 2*the total angular momentum of left(right) state. Must be even(odd) integer if IS is even(odd). Only JL=JR is the allowed coupling.
RME = array of reduced matrix elements (Output)

-------------------------------------------------------------
IMPLICIT REAL*8(A-H,0-Z)

PARAMETER(NSU3=9)

DIMENSION WIGNER(NSU3,NSU3,NSU3,NSU3),RME(KLMAX,KRMAX)

IF(JL .NE. JR) RETURN 1

FAC1 = DFLOAT(JL*(JL+2)*(JL+1)/2.0) ! Extra 2 spherical norm
FAC2 = DSQRT(DFLOAT(3*((LM+MU+3)*(LM+MU)-LM*MU)*(2*LL+1)))

IF(MU .NE. 0) FAC2 = -FAC2

Find Racah Coefficients.
RAC = DRR3(JL,2,JL,2,JR,4)*DRR3(IS,JL,2*LL,4,2*LR,JR)

IF(RAC .NE. 0.0D0) THEN

Find the SU3 Wigner coefficient.
CALL YU3R3W(LM,MU,1,1,IM,MU,LR,2,LL,KOX,KRMAX,KOX,KLMAX,WIGNER,*30)

Calculate (JxQ).J matrix element
DO 10,MR=1,KRMAX
  DO 10,ML=1,KLMAX
    RME(ML,MR) = FAC1*FAC2*RAC*WIGNER(1,MR,1,ML)
  10 CONTINUE
ELSE
  RETURN 1
END IF
(LM,MU) = (lambda, MU) = SU3 irrep label
IS* = 2*spin of left and right states (spin is a good Q.N)
KL(KR) = The multiplicity label of the orbital angular momentum
LL(LR) of the left(right) state. (NOT the value of 'K')
JL(JR) = Orbital angular momentum of left(right) state.
JL(JR) = Twice total angular momentum of left(right) state. Must be
an even(odd) integer if IS is even(odd).
RME = array of reduced matrix elements (output)

Comments:
1) Does not check for the existence of the given left and right
   states in the given (LM, MU)
2) Does not check the existence of J's for the given S and L's.
3) Does not check for the allowed coupling between LL & LR
   and JL & JR.

IMPLICIT REAL*8(A-H, O-Z)
NSU3 : dimension of array for Wigner coefficient.
PARAMETER(NSU3=9)
WIGNER : array for Wigner coefficient.
DIMENSION WIGNER1(NSU3,NSU3,NSU3,NSU3), RME(KLMAX,KRMAX),
         & WIGNER2(NSU3,NSU3,NSU3,NSU3)

IF(JL .NE. JR) RETURN 1
DO 10, KR=1, KRMAX
DO 10, KL=1, KLMAX
   RME(KL,KR)=0. DO
10 CONTINUE

Find factors depending only on the given J value
FAC1=3.0*DFLOAT(JL*(JL+2)*(JL+1)) ! Extra 12 spherical norm
FAC2=DSQRT(DFLOAT(2*LL+1)*DFLOAT((LM+MU+3)*LM+MU) - LM*MU)

Find intermediate J values for J-sum
JPMAX=JL+4
JPMIN=IBABS(JL-4)

Find factors depending on the intermediate J value
FAC3=DFLOAT(JF+1)*DRR3(2, JL, 4, JP, JL, 2)**2
FACTOR=FAC1*FAC2*FAC3

Find the intermediate L values for L-sum
IF(FACTOR .NE. 0.0) THEN
   LPMAX=(JP+IS)/2
   LPMIN=IBABS(JP-IS)/2

Find remaining Racah Coefficients.
FAC4=DSQRT(DFLOAT(2*LP+1))*DRR3(IS, JP, 2*LL, 4, 2*LP, JL)
& DRR3(IS, JP, 2*LR, 4, 2*LP, JL)

Determine phase.
IF(BTEST(LL+LP+1, 0)) FAC4=-FAC4

Find the SU(3) Wigner coefficients.
CALL YU3R3H(LM, MU, 1, 1, LM, MU, LR, 2, LP, KOX, KRMAX, KOX,
& KMAX, WIGNER1, *50)
CALL YU3R3W(LM, MU, 1, 1, LM, MU, LP, 2, LL, KQX, KPMAX, KOX, &
   KLMAX, WIGNER2, *50)
DO 30, KR=1, KPMAX
DO 30, KL=1, KLMAX
C Do loop for K-sum
SUM=0.DO
DO 20, KP=1, KPMAX
C Find the rme of (JxQ).(JxQ)
SUM=SUM + WIGNER1(1, KR, 1, KP)*WIGNER2(1, KP, 1, KL)
20 CONTINUE
RME(KL, KR)=RME(KL, KR) + FACTOR*FAC4*SUM
30 CONTINUE
50 CONTINUE
END IF ! FACTOR if construct.
100 CONTINUE
RETURN
END

SUBROUTINE OUTPUTBS(NETA, NS, LABEL)
C -----------------------------------------------------------
C
C Program Description
C This program is used to write the basis on screen.
C
C -----------------------------------------------------------

C Parameters:
C NETA: Number of Oscillator quanta for the shell.
C NS: Number of basis states.
C Label: Input array of packed basis states.
C
C -----------------------------------------------------------

IMPLICIT REAL*8(A-H,O-Z)
LOGICAL ALLEIGVAL, ALLEIGVEC
C
IFUN : array for U(N) labels,
IFU4 : array for U(4) labels
IPU4 : array for SU(4) labels
LABEL : Array for packed labels of basis states.
DIMENSION IFUN(36), IFU4(4), IPU4(3), LABEL(3, *)

C Write out the basis to screen.
WRITE(6,*) ' Oscillator shell NETA = ', NETA
WRITE(6,*) ' Number of basis states= ', NS
WRITE(6, '(1X,20(1H*),A,20(1H*))') ' BASIS'
   T55, '2P1', T59, '2P2', T65, '2J')

DO 10, IL=1, NS
   CALL UNPKSU3B(IL, LABEL, NP4R, IALPHA, LM, MU, K, L, IP0, IP1, IP2, &
      IBEItA, IT2S, IT2T, IT2J)
   IFU4(1)=IP0
   IFU4(2)=IP1
   IFU4(3)=IP2
   CALL FPFLIP(1, NP4R, NETA, IFUN, IFU4, IPU4)
10 CONTINUE
WRITE(6,5) IL,NPAR, (IFUN(IUN),IUN=1,6), IALPHA, LM, MU, K, L,
   IBETA, T28, T2T, IP0, IP1, IP2, I2J
5 FORMAT(6(13,12,T6,12,T34,12,T39,12,T44,12,T48,12,T52,12,T56,12,
   T60,12,T65,12))
10 CONTINUE
RETURN
END

PROCESS DC(ENERGY, MDATA)

SUBROUTINE HAMATRIX(J2, IFILE, MATDIM, NUMINT, STRENGTH, IFILEX)

C ---------------------------------------------------------------------
C C Program Description
C Subprogram to construct the hamiltonian matrix
C
C H = A0*HO - 0.5*CHI*Q(a),Q(a) + C*1(i).s(i) + D gentimes l(i).l(i)
C + A1*L**2 + Aj*J**2 + By*Y3A + Cy*Y4A
C
diagonalize it, and then output the eigensolutions.
C ---------------------------------------------------------------------
C Parameters:
C J2 : twice total angular momentum of matrix being constructed.
C IFILE : unit number of file of input matrix elements
C MATDIM : dimension of matrix
C NUMINT : number of interactions making up hamiltonian
C STRENGTH : array for strength of each of the interaction terms
C IFILEX : output file of matrix for debugging
C ---------------------------------------------------------------------
C IMPLICIT REAL*8(A-H,0-Z)
C
C IDIMIM : dimension for array IM
C IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)
C
C IM : array for packed matrix indices
C FM : array for non-zero values of matrix
COMMON/MDATA/ FM(IDIMFM), IM(IDIMIM)
C
C IDIMHAM: dimension for hamiltonian matrix HAM
PARAMETER(IDIMHAM=999)
C
C HAM : hamiltonian matrix
C EIVAL : eigenvalue array
C EIVEC : eigenvector array
COMMON/ENERGY/ HAM(IDIMHAM, IDIMHAM), EIVAL(IDIMHAM),
& EIVEC(IDIMHAM, IDIMHAM)
C
C DIMENSION STRENGTH(*)
C
C Zero hamiltonian matrix.
DO 5, IR=1, MATDIM
   DO 5, IL=1, MATDIM
      HAM(IL, IR)=0.00
5 CONTINUE

C DO INT=1, NUMINT-1
READ (IFILE) J2, INTRACT, MATDIM
IF (INTRACT .NE. INT)
& CALL ERROR (' HAMATRIX: Interaction numbers do not match. ')
CALL IODATA (1, 0, IFILE, NTERMS, NTERMS)
C
DO 10, ITERM = 1, NTERMS
   INDEX = IM (ITEM)
   I = NINT (SQRT (2.0*INDEX))
   J = INDEX - I*(I-1)/2
   HAM (I, J) = HAM (I, J) + STRENGTH (INT) * FM (ITEM)
10 CONTINUE
END DO
C
C Add J**2 term.
DO 20, I = 1, MATDIM
   HAM (I, I) = HAM (I, I) + STRENGTH (NUMINT) * DFLOAT (J2*(J2+2)) / 4.0
20 CONTINUE
C
DO 30, IR = 1, MATDIM
   DO 30, IL = 1, IR
      HAM (IL, IR) = HAM (IR, IL)
30 CONTINUE
C
CALL OUTPUT (MATDIM, IFILEX) ! debug
C
C Diagonalize hamiltonian matrix.
C EVEC(J, I) is the j'th component of the i'th eigenvector.
CALL DEVCSF (MATDIM, HAM, IDIMHAM, EIVAL, EIVEC, IDIMHAM)
CALL NORMALI (MATDIM) ! Normalize eigenvectors.
RETURN
END
C
C PROGRAM DC(ENERGY)
SUBROUTINE NORMALI (NDIMVEC)
C
C Program Description
This program normalizes the column vectors contained in the given matrix.
C
C Parameters:
NDIMVEC: dimension of the vector to be normalised.
C
C IMPLICIT REAL*8 (A-H, O-Z)
C
IDIMHAM : dimension of hamiltonian matrix, etcetera.
PARAMETER (IDIMHAM = 999)
C
HAM : hamiltonian matrix
EIVAL : eigenvalue array
EIVEC : eigenvector array
COMMON/ENERGY/ HAM (IDIMHAM, IDIMHAM), EIVAL (IDIMHAM),
& EIVEC (IDIMHAM, IDIMHAM)
C
DO 20 ISTATE = 1, NDIMVEC ! run through eigenstates
SUMSQ = 0.0
DO 10 ICOMP = 1, NDIMVEC ! run through components
SUBROUTINE OUTPUTEN(NS, NL, NG, NLV, NGV, IFILE)

C Program Description
Subprogram to write out eigenstate information.

PARAMETER(IDIMHAM=999)
PARAMETER(ENERGY)
COMMON/ENERGY/ HAM (IDIMHAM, IDIMHAM) , EIVAL (IDIMHAM), EIVEC (IDIMHAM, IDIMHAM)

IF (NL .EQ. 0 .AND. NG .EQ. 0) THEN
   NGREAT = NS
ELSE
   NGREAT = MIN0(NS, NG)
END IF
IF (NLV .EQ. 0 .AND. NGV .EQ. 0) THEN
   NGVEC = NS
ELSE
   NGVEC = MIN0(NS, NGV)
END IF
WRITE(6, *(1X,20(1H*),A,20(1H*))) ' EIGENSTATES '
IF (NLV .LE. NGV) THEN
   DO 10, I=1, NGREAT
      WRITE(6, 2) EIVAL(I)
      WRITE(6, 3) EIVEC(I)
      WRITE(6, 4) (EIVEC(J, I), J=1, NGVEC)
   10 CONTINUE
ELSE
   DO 20, I=1, NGREAT
      WRITE(6, 2) EIVAL(I)
      WRITE(6, 3) EIVEC(I)
      WRITE(6, 4) (EIVEC(J, I), J=1, NGVEC)
   20 CONTINUE
SUBROUTINE IODATA(IOTYPE, IOTREE, IOFILE, NUMI, NUMF)

Program Description
Subprogram to read in, or write out, a paired set of very large integer and real arrays in fixed byte sets in unformatted form.

Parameters:
IOTYPE: switch to determine if read or write operation
  = 0 for write, otherwise read operation
IOTREE: switch to determine if array is for SU(3) rmes or matrix elements
  = 0 for matrix elements, otherwise SU(3) rmes
IOFILE: unit number for input or output file.
NUMI : number of non-zero elements in integer array
NUMF : number of non-zero elements in real array

IMPLICIT REAL*8 (A-H,O-Z)

IBTREDIM : dimension for SU(3) rme binary tree.
IRMTREDIM : dimension for SU(3) rme array
PARAMETER(IRMTREDIM=100000, IBTREDIM=12*IRMTREDIM)

IBTREE : Binary tree array of labels for SU(3) rmes
RMTREE : Array for SU(3) rmes of tensor operators
COMMON/RMEDAT/ RMTREE(IRMTREDIM),IBTREE(-9:IBTREDIM)

IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)

IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)

SU(3) rme case
IF(IOTREE .NE. 0) THEN
  IF (IOTYPE.EQ.0) THEN
    WRITE(IOFILE)NUMI,NUMF
    WRITE(IOFILE)(IBTREE(I), I=-9,0)
  ELSE
    READ(IOFILE)NUMI,NUMF
    READ(IOFILE)(IBTREE(I), I=-9,0)
  ENDIF
ENDIF

SPLIT: LRECL=1724 & BLKSIZE=32760 --> 430 4 BYTE SETS PER RECORD
(Buffer size is 32760 so split into 19 records with
4 bytes per record plus 4 bytes per block overhead:
19*(1720+4)+4=32760 for optimum buffer utilization)
NRUN=NUMI
NREC=NRUN/430
NBEG=1
NEND=430
C IO FULL BLOCKS, INTEGER ARRAY
IF (NREC.NE.0) THEN
  DO 10 NR=1,NREC
    IF (IOTYPE.EQ.0) THEN
      WRITE(IOFILE)(IBTREE(N),N-NBZG,HBND)
    ELSE
      READ(IOFILE)(IBTREE(N),N-NBEG,NEND)
    ENDIF
    NBEG=NEND+1
  ENDIF
  NEND=NEND+430
10
C IO RESIDUAL
IF (NBEG.LE.NRUN) THEN
  IF (IOTYPE.EQ.0) THEN
    WRITE(IOFILE)(IBTREE(N),N-NBEG,NRUN)
  ELSE
    READ(IOFILE)(IBTREE(N),N-NBEG,NRUN)
  ENDIF
ENDIF

SPLIT: LRECL=1724 & BLKSIZE=32760 --> 215 8 BYTE SETS PER RECORD
BUFFER SIZE IS 32760 SO SPLIT INTO 19 RECORDS WITH
4 BYTES PER RECORD PLUS 4 BYTES PER BLOCK OVERHEAD:
19*(1720+4)+4=32760 FOR OPTIMUM BUFFER UTILIZATION)
NRUN=NRUN
NREC=NRUN/215
NBEG=1
NEND=215
C IO FULL BLOCKS, REAL ARRAY
DO 20 NR=1,NREC
  IF (IOTYPE.EQ.0) THEN
    WRITE(IOFILE)(RMTREE(N),N-NBZG,NEND)
  ELSE
    READ(IOFILE)(RMTREE(N),N-NBEG,NEND)
  ENDIF
  NBEG=NEND+1
20
NEND=NEND+215
C IO RESIDUAL
IF (NBEG.LE.NRUN) THEN
  IF (IOTYPE.EQ.0) THEN
    WRITE(IOFILE)(RMTREE(N),N-NBEG,NRUN)
  ELSE
    READ(IOFILE)(RMTREE(N),N-NBEG,NRUN)
  ENDIF
ENDIF
ELSE
  Matrix element case
  IF (IOTYPE.EQ.0) THEN
    WRITE(IOFILE)NUMI,NUMF
  ELSE
    READ(IOFILE)NUMI,NUMF
  ENDIF
ENDIF

SPLIT: LRECL=1724 & BLKSIZE=32760 --> 430 4 BYTE SETS PER RECORD
BUFFER SIZE IS 32760 SO SPLIT INTO 19 RECORDS WITH
4 BYTES PER RECORD PLUS 4 BYTES PER BLOCK OVERHEAD:
19*(1720+4)+4=32760 FOR OPTIMUM BUFFER UTILIZATION)
NRUN=NRUN
NREC=NRUN/430
NBEG=1
NEND=430

C IO FULL BLOCKS, INTEGER ARRAY
IF (NREC .NE. 0) THEN
   DO 30 NR=1,NREC
      IF (IOTYPE.EQ.0) THEN
         WRITE(IOFILE) (IM(N),N=NBE, NEND)
      ELSE
         READ(IOFILE) (IM(N),N=NBE, NEND)
      ENDIF
      NBEG=NBE+1
   30 NEND=NEND+430
ENDIF

C IO RESIDUAL
IF (NBEG.LE.NRUN) THEN
   IF (IOTYPE.EQ.0) THEN
      WRITE(IOFILE) (IM(N),N=NBE, NRU)
   ELSE
      READ(IOFILE) (IM(N),N=NBE, NRU)
   ENDIF
ENDIF

C SPLIT: LRECL=1724 & BLKSIZE=32760 --> 215 8 BYTE SETS PER RECORD
C (BUFFER SIZE IS 32760 SO SPLIT INTO 19 RECORDS WITH
C 4 BYTES PER RECORD PLUS 4 BYTES PER BLOCK OVERHEAD:
C 19*(1720+4)+4=32760 FOR OPTIMUM BUFFER UTILIZATION)
NRU=NUMF
NREC=NRU/215
NBEG=1
NEND=215

C IO FULL BLOCKS, REAL ARRAY
DO 40 NR=1,NREC
   IF (IOTYPE.EQ.0) THEN
      WRITE(IOFILE) (FM(N),N=NBE, NEND)
   ELSE
      READ(IOFILE) (FM(N),N=NBE, NEND)
   ENDIF
   NBEG=NBE+1
40 NEND=NEND+215

C IO RESIDUAL
IF (NBEG.LE.NRUN) THEN
   IF (IOTYPE.EQ.0) THEN
      WRITE(IOFILE) (FM(N),N=NBE, NRU)
   ELSE
      READ(IOFILE) (FM(N),N=NBE, NRU)
   ENDIF
ENDIF
END IF
RETURN
END

SUBROUTINE OUTPUT(NS,IFILE)
C------------------------------------------------------------------
C Program Description
C This program writes the hamiltonian matrix on the output file.
C------------------------------------------------------------------
Parameters:
NS: Dimension of the hamiltonian matrix
IFILE: Number assigned to the output file.

IMPLICIT REAL*8 (A-E, O-Z)
IDIMHAM : dimension of hamiltonian matrix, etcetera.
PARAMETER (IDIMHAM=999)
HAM : hamiltonian matrix
EIVAL : eigenvalue array
EIVEC : eigenvector array
COMMON/ENERGY/ HAM (IDIMHAM, IDIMHAM), EIVAL (IDIMHAM),
& EIVEC (IDIMHAM, IDIMHAM)

DO IL=1, NS
  DO IR=1, NS
    IF (HAM (IL, IR) .NE. 0.0) WRITE (IFILE, *) IL, IR, HAM (IL, IR)
  END DO
END DO
RETURN

SUBROUTINE PACKSU3B (I2J, IFILE, NETA, NSTATES, IDIM, LABEL, *)
Program Description:
Program to generate SU(3)xSU(2)xSU(2) basis states for an oscillator shell N,

|n (f) ALPHA(LM, MU)KL, (P0, P1, P2)BETA ST; J>,
The information in the spatial permutation label (f) is equivalently carried in the SU(4) irrep labels, at least for coding purposes.
The labels are packed as follows:
(n, P0, P1, P2) -> (8, 8, 8, 8)
(LM, MU, 2S, 2T) -> (8, 8, 8, 8)
(ALPHA, BETA, K, L, 2J) -> (4, 4, 8, 8, 8)

Parameters.
I2J : twice the total angular momentum (input)
IFILE : unit number for input file of SU(3)xSU(2)xSU(2) irrep labels (input)
NETA : number of oscillator quanta for shell, (input)
NSTATES : total number of basis states (output)
IDIM : dimension of LABEL in calling program (output)
LABEL (3, IDIM) : array where the packed labels are stored (output)
RETURN 1 : no states for input I2J.

DIMENSION LABEL (3, IDIM)
Packing function for four labels (8, 8, 8, 8)
IPACK4(I1, I2, I3, I4)=IOR(I4, ISHFT(IOR(I3, ISHFT(IOR(I2, 
  ISHFT(I1, 8)), 8)), 8)), 8))

C Packing function for five labels (4,4,8,8,8)
IPACK5(I1, I2, I3, I4, I5)=IOR(I5, ISHFT(IOR(I4, ISHFT(IOR(I3, 
  I5, ISHFT(IOR(I2, I5, 8)), 8)), 8)), 8), 8))

C Multiplicity function for L states in SU(3) irrep (LM, MU).
MULT(LM, MU, L)=MAXO(0, (LM+MU+2-L)/2) - MAXO(0, (LM+1-L)/2) -  
& MAXO(0, (MU+1-L)/2)

C Read in header information of irrep label file.
REWIND(IFILE) ! rewind input file
READ(IFILE,*) META ! oscillator q.n.
READ(IFILE,*) NPAR ! no. of particles
READ(IFILE, '(I3,/)' ) NIRREPS

C Generate basis states.
NSTATES=0
DO IRREP=1, NIRREPS
  READ(IFILE,*) IFSPACE, IALPHAMX, LM, MU, IBETAMX, I2S, I2T, IP0, 
  & IP1, IP2
  LMAX=MINT(MU+LM, (I2J+I2S)/2)
  LMIN=ABS(I2J-I2S)/2
  DO L=LMIN, LMAX ! Ang. mom. L values.
    KAPMAX=MULT(MU, LM, L)
    IF(KAPMAX .NE. 0) THEN
      DO 10, 1ALPHA=1, IALPHAMX ! Alpha multiplicity
        DO 10, 1BETA=1, IBETAMX ! Beta multiplicity
          DO 10, 1KAPPA=1, KAPMAX ! L multiplicity
            Pack labels into LABEL.
            NSTATES=NSTATES + 1
            LABEL(1,NSTATES)=IPACK4(NPAR, IP0, IP1, IP2+128)
            LABEL(2,NSTATES)=IPACK4(LM, MU, I2S, I2T)
            LABEL(3,NSTATES)=IPACK5(IALPHA, IBETA, KAPPA, L, I2J)
 10    CONTINUE
      END IF
    END DO
  END DO
IF(NSTATES .EQ. 0) RETURN 1
IF(NSTATES .GT. IDIM) & CALL ERROR(' PACKSU3B: LABEL array overflow. ')
RETURN

END

SUBROUTINE UNFKSU3B(I, LABEL, NPAR, IALPHA, LM, MU, K, L, 
  & IP0, IP1, IP2, IBETA, I2S, I2T, I2J)

C Program Description:
C Subprogram to unpack the packed labels of SU(3)xSU(2)xSU(2) basis 
C states coupled to total angular momentum (J=L+S) for an oscillator 
C shell N:
C |W (f) ALPHA(LM, MU)KL, (P0,P1,P2)BETA ST; J>
C The information in the spatial permutation label (f) is 
C equivalently carried in the SU(4) irrep labels, at least for 
C coding purposes.
C The labels are packed as follows:
C (N,P0,P1,P2) -> (8,8,8,8)
(LM, MU, 2S, 2T) -> (8, 8, 8, 8)
(ALPHA, BETA, K, L, 2J) -> (4, 4, 8, 8)

Parameters:
I : Running index of basis state (input)
LABEL(3,*) : array where the packed labels are stored (input)
NPAR : number of active particles (output)
IALPHA : multiplicity label for (LM, MU) SU(3) irrep (output)
LM, MU : SU(3) irrep labels (output)
K : angular momentum L multiplicity label (output)
L : orbital angular momentum (output)
IP0, IP1, IP2 : SU(4) irrep labels (output)
IBETA : multiplicity label of (S, T) in SU(4) irrep (output)
I2S, I2T : twice spin and isospin (2S, 2T) (output)
I2J : twice the total angular momentum (output)

DIMENSION LABEL(3, *)

IUNPK(I, J, K) = IAND(ISHFT(I, J), K)
DATA NBIT4, NBIT8, ZF, ZFF/ ! Hexadecimal

LB1 = LABEL(1, I)
LB2 = LABEL(2, I)
LB3 = LABEL(3, I)
NPAR = IUNPK(LB1, -24, NBIT8)
IP0 = IUNPK(LB1, -16, NBIT8)
IP1 = IUNPK(LB1, -8, NBIT8)
IP2 = IUNPK(LB1, 0, NBIT8) - 128
LM = IUNPK(LB2, -24, NBIT8)
MU = IUNPK(LB2, -16, NBIT8)
I2S = IUNPK(LB2, -8, NBIT8)
I2T = IUNPK(LB2, 0, NBIT8)
IALPHA = IUNPK(LB3, -28, NBIT4)
IBETA = IUNPK(LB3, -24, NBIT4)
K = IUNPK(LB3, -16, NBIT8)
L = IUNPK(LB3, -8, NBIT8)
I2J = IUNPK(LB3, 0, NBIT8)
RETURN
END

SUBROUTINE FPFLIP (ICODE, NPAR, IETA, IFUN, IFU4, IFU4)

Program Description:
Program to change U(omega) f irrep label to SU(4) 2(p) labels
or vice-versa. For example, U(6) to SU(4), etcetera.

Parameters:
ICODE : switch to determine f to P or P to f change.
   = 0 for f to P change, non-zero for p to f.
NPAR : number of particles in oscillator shell.
IETA : oscillator shell number, e.g. 2 for ds-shell.
IFUN : spatial symmetry irrep f.
DIMENSION IFUN(36), IFU4(4), IPU4(3)
JMAX=(IITA+1)*(IETA+2)/2
K=0
IF (ICODE .EQ. 0) THEN
  DO 10, I=1, 4
    K=K+1
    IFU4(I)=0
    DO 10, J=1,JMAX
      IF (IFUN(J) .GE. K) IFU4(I)=IFU4(I) + 1
      IFU4(1)=IFU4(1) + IFU4(2) - IFU4(3) - IFU4(4)
      IFU4(2)=IFU4(1) - IFU4(2) + IFU4(3) - IFU4(4)
      IFU4(3)=IFU4(1) - IFU4(2) - IFU4(3) + IFU4(4)
    ELSE
      IFU4(1)=(NPAR +IFU4(1) +IFU4(2) +IFU4(3))/4
      IFU4(2)=IFU4(1) - (IFU4(2) + IFU4(3))/2
      IFU4(3)=IFU4(1) - (IFU4(1) + IFU4(3))/2
      IFU4(4)=IFU4(1) - (IFU4(1) + IFU4(2))/2
    DO 20, I=1, JMAX
      K=K+1
      IFUN(I)=0
      DO 20, J=1, 4
        IF (IFUN(J) .GE. K) IFUN(I)=IFUN(I) + 1
      END IF
      RETURN
END

FUNCTION DJHR3 (J1T, J2T, J3T, J4T, J5T, J6T, J7T, J8T, J9T)
-----------------------------------------------------------------
JAHN-HEIFE COEFFICIENTS FOR R3--TRIANGLE RELATIONS CHECKED IN DELTA
REFERENCES--ANGULAR MOMENTUM IN QUANTUM MECHANICS, A.R. EDMONDS,
PRINCETON
---------------------------------------------------------------
IMPLICIT REAL*8(D)
DJHR3=0.D0
IITMIN=MAX0(IABS(J1T-J9T), IABS(J2T-J6T), IABS(J4T-J8T))+1
IITMAX=MINO(J1T+J9T, J2T+J6T, J4T+J8T)+1
IF (IITMIN.GT. IITMAX) RETURN
DO 10 IIT=IITMIN, IITMAX, 2
  IIT=IIT-1
10 DJHR3=DRR3(J1T, J9T, J4T, J8T, IT, J7T) * 
   DRR3(J2T, J6T, JBT, J4T, IT, J5T) * DRR3(J1T, J9T, J2T, J6T, IT, J3T)
DJHR3=DSQRT(DFLOAT((J3T+1) * (J6T+1) * (J7T+1) * (J8T+1))) * DJHR3
RETURN
END

FUNCTION MULTR3(LM, MU, L)
C
C This function computes the maximum possible multiplicity
C of angular momentum states L for a given SU(3) irreducible
C representation (LM, MU).
C A119 (1968) 577-590, equation following (19).
C
MULTR3=MAX0(0, (LM+MU+2-L)/2) - MAX0(0, (LM+1-L)/2) -
  1 MAX0(0, (MU+1-L)/2)
SUBROUTINE READIN(ANS, *)

Subprogram to limit response to Yes or No answer.

PARAMETER(LOOPMAX=25)
CHARACTER*2 ANS, YES, YEA, NO, NOP
LOGICAL OK
SAVE LOOP
DATA YES/'Y'/, YEA/'y'/, NO/'N'/, NOP/'n'/

OK=.FALSE.
READ(5, '(A)', END=10) ANS
IF(ANS .EQ. YEA) THEN
   ANS = YES
   OK=.TRUE.
ELSE IF (ANS .EQ. NOP) THEN
   ANS = NO
   OK=.TRUE.
ELSE IF (ANS .EQ. YES) THEN
   OK=.TRUE.
ELSE IF (ANS .EQ. NO) THEN
   OK=.TRUE.
END IF
IF(.NOT. OK) THEN
   WRITE(6, '(A)') ' **Use Y (y) for yes and N (n) for no!'
   LOOP=LOOP + 1
   IF(LOOP .LT. LOOPMAX) THEN
      RETURN
   ELSE
      STOP 'READIN: enough attempts!'
   END IF
END IF

RETURN
END

C
SUBROUTINE ERROR(LITER)

Exit program because of gross error.

CHARACTER*(*) LITER
WRITE(6, '(A,A)') ' ***** ATTENTION ', LITER
STOP
END
D.2. Least Squares Fitting of Hamiltonian Parameters

Title of program: PGDSHL

Computer: IBM 3090/600J

Operating System: MVS/XA

Programming language used: FORTRAN

Peripherals used: None

Number of lines in program: 827

Nature of the physical Problem:

The parameters of a theory are usually varied to get a best overall fit to experimental data. In the present case this is accomplished by using HAL, a general shell-model package that determines best (least-squares) fit values for the parameters of the theory by comparing calculated eigenenergies and transition rates to input experimental data. The routine PGDSHL in HAL (called as Option 6) does this for the $H'_{SU3}$ hamiltonian given in (D.2). The program HUSNHAM (see Section D.1.) is used to calculate matrix representations of the interactions in $H'_{SU3}$ which are then used as input to PGDSHL. Starting values for the parameters are provided by the user who also specifies which of the coefficients are to be kept fixed and which are to be varied by specifying an associated set of parameters called NFRPAR. The program PGDSHL diagonalizes the matrix, matches the eigenvalues to the experimental data, calculates the squares of differences, uses the values of the coefficients given by the first iteration to start the second iteration and so on. The user may choose among the various $H'_{SU3}$ hamiltonians by specifying a value for the parameter NCASE as follows:
NCASE = 1 \rightarrow H_o \text{ only}

= 2 \rightarrow H_o + Q^a Q^a

= 3 \rightarrow H_o + Q^a Q^a + M + \sum_i l_i s_i + \sum_i l_i^2

= 4 \rightarrow H_o + Q^a Q^a + M + \sum_i l_i s_i + \sum_i l_i^2 + J^2 + Y_3^3 + Y_4^4

= 5 \rightarrow H_o + Q^a Q^a + M + \sum_i l_i s_i + \sum_i l_i^2 + J^2 + Y_3^3 + Y_4^4 + L^2

The ratio of the coefficients of \(Y_3^3\) and \(Y_4^4\) can be fixed to the value required to form the \(\mathcal{K}_F^2\) operator (NaqDra 92) by choosing a negative value for the \(Y_4^4\) NFRPAR parameter.
Program Description:
OPTION #6 OF THE "HAL" SHELL MODEL PACKAGE

Parameters:
NUMFRB : number of problem (used to label output)
VALRED : values of variables in reduced set for least squares
VALCAL : calculated values of observables for least squares fit
NUMOBS : number of observable values
NUMRED : number of parameter values in reduced set

SUBROUTINE PGDSHL(NUMFRB, VALRED, VALCAL, NUMOBS, NUMRED)
IMPLICIT REAL*8(E, F, H, R, W, X)
LOGICAL LSLLOPER/.FALSE./, KJOPER/.FALSE./
NMATRX : Maximum dimension of hamiltonian matrices for any given
angular momentum J sub-block.
NBE2MX : Maximum number of non-zero matrix elements for Q
operator between any two angular momentum states.
PARAMETER(NMATRX=999, NBE2MX=110000)
COMMON/BKCON/ITYPE, ITIME, ITNRO, IPRNT, EIGVAL(20), EIGVEC(NMATRX, 20) ! Eigensolutions
DIMENSION VALPAR(11), VALRED(*), VALCAL(*), NFRPAR(11)
DIMENSION LABEL(3, NMATRX), JTWICX(10)
DATA JDEL, JMIN, JMAX, NEASK, NVASK/1, 4*0/, RATIOLLS/0.DO/
DATA XPI/3.1415926535897932D0/

Executed on first iteration only ...
IF(ITIME .EQ. 0) THEN
   CALL INPUT (NCASE, NPARM, LM, MU, NEASK, NVASK, NFRNT, NCOMP,
&    LSLLOPER, RATIOLLS, KJOPER, VALPAR, NFRPAR, NPREAL, NNREAL,
&    METAP, METAN, NVALP, NVALN, NJ, NISO, JTWICE)

Determine total quanta, nucleons, protons, and neutrons.
CALL NQANTA(QTOTP, NSTOP, NPSEUDO, NNSEUDO, METAP, METAN,
&    NVALP, NVALN)

Determine actual number of particles and quanta
NTOT=NPREAL+NNREAL
CALL NQFIND(NPREAL, NNREAL, QTOT)

Reduce parameter set to include nonzero values only
CALL ZAPPAR(0, NPREAL, NFRPAR, VALPAR, NUMRED, VALRED)

Output input information to screen.
CALL OUTINPUT(NCASE, KJOPER, VALPAR, NFRPAR, NPARM, NTOT, NTP, NETAP, NETAN, NVALP, NVALN, QTOTP, QTOT, NJ, NISO, JTWICE)

ITIME = ITIME + 1
IF (ITRNO .NE. 0) RETURN ! Least squares termination?
END IF

C

Commence parameter variations for hamiltonian.

C

IF (IPRNT .EQ. 1) WRITE (6, 5) NUMRPRB ! final results can be printed
5 FORMAT (' Details for Problem Number ', 3X, I3)
CALL ZAPPAR (1, NPARM, NFRPAR, VALPAR, NUMRED, VALRED) ! reduce number of param
C

DO 20, JDOUBLE = 1, NJ ! Possible ang mom states.
   J2 = JTWICE (JDOUBLE)
C

NEVAL = NEASK
NVECT = NVASK
C

Construct and diagonalize hamiltonian for parameter values.
CALL DSHENG (VALPAR, J2, LM, MU, NCASE, LSLLOPER, RATIOLLS, KJOPER, NEVAL, NVECT, NPARM, NDIM)
C

Output energies and eigenvectors to log file
CALL OUTEIG (IPRNT, NFRNT, NCOMP, J2, JMIN, NETAP, NDIM, NEVAL, NVECT, LABEL, NMATRX)
C

IF (ITRNO .NE. 0) THEN
   DO 10, N = 1, NEVAL
      GOSEEK = SNGL (EIGVAL (N))
      CALL GETCAL (1, J2, N, J2, N, GOSEEK, VALCAL)
10 CONTINUE
END IF
20 CONTINUE

ITIME = ITIME + 1
RETURN
END
SUBROUTINE INPUT (NCASE, NPARM, LM, MU, NEASK, NVASK, NFRNT, NCOMP, & LSLLOPER, RATIOLLS, KJOPER, VALPAR, NFRPAR, NPREAL, NNREAL, & NETAP, NETAN, NVALP, NVALN, NJ, NISO, JTWICE)

C

Program Description:
Routine to read in input values for PGDSHL calling routine.
All the routine arguments are explained in the comments preceeding the corresponding read statements.

C

CHARACTER RECORD=80
LOGICAL LSLLOPER, KJOPER
DIMENSION VALPAR(*), NFRPAR(*), JTWICE(*)
C

MODEL SPECIFICATION
NCASE = Version of the ds-shell hamiltonian (1, 2, 3, 4, 5)
= 1 -- H.O. only
= 2 --> H.O. + Q.Q (algb)
= 3 --> H.O. + Q.Q (algb) + M + 1(i).s(i) + 1(i).1(i)
= 4 --> H.O. + Q.Q (algb) + M + 1(i).s(i) + 1(i).1(i)
   + J.J + Y3A + Y4A
5 -> H.O. + Q.Q (algb) + M + l(i).s(i) + l(i).l(i) + J.J + Y3A + Y4A + L.L

NPARM = number of model parameters (e.g. 8 for case 4)
LM,MU = leading SU(3) irrep labels for nucleus

READ(5, '(A)') RECORD ! Skip record.

READ(5,*) NCASE, NPARM, LM, MU

MODEL PARAMETERS
Input parameters of the theory ...
VALPAR(*)

1 -> DMB  h-bar-omega value (boson excitation)
2 -> QQ  q.q interaction strength
3 -> M  Majorana interaction strength
4 -> l(i).s(i) strength of one-body spin-orbit force
5 -> l(i).l(i) strength of one-body orbit-orbit force
6 -> J.J  strength of J**2 interaction
7 -> Y3A  strength of JQQJ interaction
8 -> Y4A  strength of JQQQJ interaction
9 -> L.L  strength of L**2 interaction

Notes:
In case of Spin S=0 care must be taken in choosing parameters
6 and 9 since J = L in this case.

NFRPAR(*)=0 means parameter (*) is frozen

Notes:
1) If the spin-orbit and orbit-orbit interactions are to be
   kept in the same ratio then choose NFRPAR(5) = negative. This
   will freeze l(i).l(i) strength.
2) If KJSQ operator option is desired then choose a negative
   value for NFRPAR(8). This will fix the strengths of J**2, Y3A
   and Y4A suitable for KJSQ operator. Y4A strength will be
   frozen

READ(5, '(A)') RECORD ! Skip record.
READ(5,*) (VALPAR(N),N=1,NPARM)
READ(5, '(A)') RECORD ! Skip record.
READ(5,*) (NFRPAR(N),N=1,NPARM)
IF(NFRPAR(5) .LT. 0) THEN
   LSLLOPER=.TRUE.
   NFRPAR(5)=0
   RATIOLL=VALPAR(5)/VALPAR(4)
END IF
IF(NFRPAR(8) .LT. 0) THEN
   KJSQ=.TRUE.
   NFRPAR(8)=0
   VALPAR(8)=0.0D0
END IF
NUCLEAR PHYSICS

NPREAL = actual number of protons
NNREAL = actual number of neutrons
    ... NTOT=NPREAL+NNREAL --> NTOT iff real shell application
NETAP = proton shell number
NETAN = neutron shell number
    ... used to determine oscillator strength parameter
NVALP = number of valence protons
NVALN = number of valence neutrons
    ... NTOT=CORES+NVALP+NVALN --> NTOT iff real shell only

READ(5, '(A)') RECORD ! Skip record.
READ(5, *) NPREAL, NNREAL, NETAP, NETAN, NVALP, NVALN

ANGULAR MOMENTUM & ISOSPIN VALUES
NJ = number of angular momentum values to be input
NISO = twice total isospin of the nucleus (negative if n,p formalism)
JTWICE = twice minimum angular momentum values
READ(5, '(A)') RECORD ! Skip record.
READ(5, *) NJ, NISO
READ(5, '(A)') RECORD ! Skip record.
READ(5, *) (JTWICE(I), I=1,NJ)

RETURN
END

SUBROUTINE OUTINPUT(NCASE, KJOPER, VALPAR, NFRPAN, NPARM, NTOT, NTOTP,
& NETAP, NETAN, NVALP, NVALN, QTOTP, QTOT, NJ, NISO, JTWICE)

Program Description:
Routine to write out input values for PGSHEL calling routine.
All the routine arguments are explained in the formats
following the corresponding write statements.

LOGICAL KJOPER
DIMENSION VALPAR(*), NFRPAN(*), JTWICE(*)

WRITE(6,10) NCASE
10 FORMAT('0',8X,'... Model used = ',I2)
IF(NCASE .LE. 3) THEN
    WRITE(6,20) (VALPAR(N), NFRPAN(N), N=1, NPARM)
ELSE
    WRITE(6,20) (VALPAR(N), NFRPAN(N), N=1, 5)
END IF
20 FORMAT('0 Results are for the following case: ',
A 14X,'Status*/'
B'0 H-Bar-Omega: ',1PE12.5X,' DNB ',I10/
C' Q-Q Interaction: ',1PE12.5X,' Qa.Qa ',I10/
D' Majorana Interaction: ',1PE12.5X,' M ',I10/
E' Spin-orbit force: ',1PE12.5X,' l(1).s(1) ',I10/
F' Orbit-orbit force: ',1PE12.5X,' l(1).l(1) ',I10)
IF(NCASE .GT. 3) THEN
    IF(KJOPER) THEN
        WRITE(6,22) (VALPAR(N), NFRPAN(N), N=6, 7)
22 FORMAT(
B' KJ interaction: ',1PE12.5X, ' KJ ',I10)
ELSE
WRITE (6, 24) (VALPAR(N), NFRPAR(N), N=6, 8)
24 FORMAT (a
B' Y3A interaction: ', 1PE12.5, 5X, ' JQJ ', I10/
C' Y4A interaction: ', 1PE12.5, 5X, ' JQQJ ', I10)

IF (NCASE.EQ.5) WRITE (6, 25) VALPAR(9), NFRPAR(9)
25 FORMAT (a
END IF
END IF
WRITE (6, 26)
26 FORMAT (a
*Status = 0 --> frozen ... fixed input', /
A ' = 1 --> initial value ... nils')

IF (NTOT.EQ. NTOTP) THEN
WRITE (6, 30)
30 FORMAT (a
' *****************************■ (  /
1 ***** Actual not Pseudo *****', /
2 ***************************************************************************)
ELSE
WRITE (6, 40)
40 FORMAT (a
' *****************************■ (  /
1 ***** Pseudo not Actual *****', /
2 ***************************************************************************)
ENDIF

WRITE (6, 50) NETAP, NETAN
50 FORMAT (a
' Proton shell = ', I3, 3X, 'Neutron shell = ', I3)
WRITE (6, 60) NTOTP
60 FORMAT (a
' Number of nucleons being considered = ', I4)
WRITE (6, 70) NVALN, NVALP
70 FORMAT (a
' Valence space: Neutrons = ',
& I3, 2X, 'Protons = ', I3)
IF (QTOTP.EQ. QTOT) THEN
WRITE (6, 80) QTOTP
80 FORMAT (a
Harmonic Oscillator Eigenvalue = ', 2F8.1)
ELSE
WRITE (6, 80) QTOTP, QTOT
ENDIF
80 FORMAT (a
Total isospin of the nuclear system 2T= ', I3)
C
IF (NISO.GE. 0) WRITE (6, 90) NISO
90 FORMAT (a
Total number of nucleons in system = ', I3)
C
IF (NTOTP.NE. NTOT) WRITE (6, 100) NTOT
100 FORMAT (a
Results from 2xJ 6(I3), 2X, 'next ...')/
RETURN
END

$PROCESS DC(ENGR)
SUBROUTINE OUTEIG (IPRINT, NPRINT, NCOMP, J2, JMIN, NETAP, NDIM,
& NVAL, NVECT, LABEL, LADOIM)
C
C Program Description:
C Routine to write out eigensolutions for PGDSHL calling routine.
C
Parameters:

IPRNT : control variable specifying final results may be printed
= 1 to print, otherwise suppress printing

NFRNT : control for whether or not eigenvectors are printed
= 1 to print, otherwise suppress printing

J2 : total angular momentum of matrix subblock diagonalized

JMIN : twice angular momentum value of ground state

NETAP : number of single-particle oscillator quanta for proton shell

NDIM : dimension of diagonalized matrix

NEVAL : number of eigenvalues obtained from diagonalization

NVECT : number of eigenvectors retained from diagonalization

LABEL : packed basis state labels

Subprograms:

PACKSU3B : routine to generate basis state labels in packed form

UNPKSU3B : routine to unpack basis state labels

IMPLICIT REAL*8(E, F, R, W, X)

NTESTDIM: maximum number of eigenstates for which details desired

IFILEIRR : unit number for input file of SU(3)xSU(4) irrep labels

JTILESTART : starting unit number for different sets of 2J eigenvectors.

PARAMETER(NTESTDIM=50, IFILEIRR=7, JTILESTART=40)

TEST : controls which eigenstates are written out in detail

LOGICAL TEST(NTESTDIM)/NTESTDIM=.FALSE./

NMATRIX : Maximum dimension of hamiltonian matrices for any given angular momentum J sub-block.

NBE2MX : Maximum number of non-zero matrix elements for Q operator between any two angular momentum states.

PARAMETER(NMATRX=999, NBE2MX=110000)

COMMON/ENGR/EIGVAL(20), EIGVEC(NMATRX, 20) ! Eigensolutions

PSMGR : percentage measure of basis state in eigenstate

NZERO : basis state number of above percentage value

DIMENSION PSMGR(100), NZERO(NMATRX), LABEL(3, LABDIM)

DATA EGMIN/0.10/

IF(IPRNT.EQ.1) THEN ! print details

WRITE(6,2) J2, NDIM

2 FORMAT('0 The number of 2J =', 13, 3X, 'states is', 16)

IF(NFRNT .EQ. 0) WRITE(6,4)

4 FORMAT('0 State', 8X, 'Eigenvalue'

END IF

Run through eigenvalues

DO 50, N=1, NEVAL

IF(J2.EQ.3 .AND. N.EQ.1) EGMIN=EIGVAL(1)

EIGVAL(N)=EIGVAL(N)-EGMIN
IF(IPRNT.EQ.1) THEN ! End of fitting, print results.
IF(N.EQ.1 .AND. J2.EQ.JMIN) THEN
  WRITE(6,10) EDMIN
  FORMAT('0',11X,'... Eigenvalue of the ground state:',
        1X,1PD13.4,/,END IF
IF(NPRNT.EQ.1 .AND. N.LE.NVECT) THEN
  WRITE(6,12) N,EIGVAL(N),(JJ,EIGVEC(JJ,N),JJ=1,NDIM)
  FORMAT('0 State',I3,3X,'with eigenvalue',1PD13.4,3X,
        'has eigenvector:'/(7(15,1PD13.4))
ELSE
  WRITE(6,14) N,EIGVAL(N)
  FORMAT(4X,I3,6X,1PD13.4)
END IF

C C
C Set up logical array for print control of selected eigenstates
IF(NCOMP .GE. 1) THEN
  C
  C Generate basis state labels.
  IF(N.EQ.1) CALL PACKSU3B(J2,IFILEIRR,NETAP,NDXM,LABDIM,LABEL,*60)
  C
  C Find eigenstates for which detailed output desired.
  CALL TESTCOND(J2,N,NTMX,NTESTDXM,TEST)
  C
  C Output eigenvectors with components > 0.1% amplitude
  C
  C Check if current eigenstate is one of those listed above.
  DO 40,NTRN=1,NTMX
    IF(TEST(NTRN)) THEN
      IR=0
      JR=0
      C Run through components
      DO 20,JX=1,NDIM
        PCH=SNGL(100.D0*EIGVEC(JX,N)**2)
        IF(PCH.LE.0.1D0) THEN ! 0.1%
          JR=JR+1
        ELSE
          IR=IR+1
          NZERO(IR)=JX
          PSMGR(IR)=PCH
        END IF
      20 CONTINUE
      JRMAX=JR
      IRMAX=IR
      WRITE(6,22) J2,N
      FORMAT('0 Analysis of the eigenstate: 2J =',I3,3X,
            'N =',I3)
      WRITE(6,24) JRMAX
      FORMAT('0 Components with < 0.1% amplitude:',I5/
            'Remaining eigenstate analysis ...')
      WRITE(6,26) J2,N
      FORMAT('0',T5,'IBASIS',T14,'PERCENT',T23,'...',
            'T41',2S',T44,'2T',T47,'2P0',T51,'2P1',T55,'2P2')
      C      DO 30,JX=1,IRMAX
      ISTATE=NZERO(JX)
CALL UNPKSU3B (ISTATE, LABEL, NPAR, IALPHA, LM, MU, KAP, LANG, IP0, IP1, IP2, IBETA, I2S, I2T)

WRITE (6, 28) ISTATE, PSMGR(JX), IALPHA, LM, MU, KAP, LANG, IBETA, I2S, I2T, IP0, IP1, IP2


CONTINUE

Output wavefunctions for input into other programs.

FILE=FILESTART + J2 ! File for output wavefns

IF (NCOMP .EQ. 1) THEN
WRITE (JFILE, *) J2, N, IRMAX
DO JX=1, IRMAX
   ISTATE=ZERO(JX)
   WRITE (JFILE, *) (LABEL(I,ISTATE),1-1,3), EIGVEC(ISTATE,N)
END DO
ELSE
WRITE (JFILE, *) J2, N, NDIM
DO ISTATE=1, NDIM
   WRITE (JFILE, *) (LABEL(I,ISTATE),1-1,3), EIGVEC(ISTATE,N)
END DO
END IF
WRITE (6, 32) FORMAT ('0 End of analysis for this eigenstate',/)
ENDIF ! TEST construct

CONTINUE

ENDIF ! NCOMP construct

END IF

CONTINUE
RETURN

CALL TKO( ' OUTEIG: No basis states for given J2.0')
END

SUBROUTINE TESTCOND (J2, NJSTATE, NLIST, NTESDIM, TEST)

-----------------------------------------------

Program Description:
Routine to check if current eigenstate is amongst list of ones for which a detailed basis state decomposition is desired. The list of state is contained in the file attached to unit number JFILE.

-----------------------------------------------

Parameters:

J2 : twice total angular momentum of current eigenstate
NJSTATE : number of eigenstate
NLIST : number of states in list
NTESDIM: dimension of test array in calling routine
TEST : logical array for test comparison

-----------------------------------------------

CHARACTER RECORD*80
LOGICAL TEST(NTESDIM)
IFILE : unit number for file containing list of states
PARAMETER (IFILE=8)

READ (IFILE,*) NLIST ! Number of conditions
IF (NLIST .GT. NTESTDIM)
& CALL TKO ('TESTCOND: Too many conditions for array.')
READ (IFILE, '(A)') RECORD ! Skip line.
DO N=1,NLIST
READ (IFILE,*) JVAL, NSTATE
TEST (N)=J2.EQ.JVAL .AND. NJSTATE.EQ.NSTATE
END DO
REWIND (IFILE)
RETURN
END

SUBROUTINE DSHENG (VALPAR, J2, LM, MU, NCASE, LSLLOPER, RATIOLLLS,
& KJOPER, NEVAL, NVECT, NPARM, NDIM)

Program Description:
Program to calculate eigenvalues and eigenvectors.

Input variables:
VALPAR : Array of variable parameters from least squares fit.
J2 : Twice angular momentum value for which matrix to be
constructed.
CASE : Which hamiltonian type to construct.
NEVAL : Number of eigenvalues desired.
NVECT : Number of eigenvectors desired.
NPARM : Number of interactions in hamiltonian for given case.
NDIM : Returns dimension of matrix constructed on output.

CPUTIME: routine to determine current cputime
LANEUVV : Lanczos routine for diagonalizing large symmetric
matrices

Note: Input matrices must have indices packed in IMSL form.
INDEX (I,J,MATDIM)=J + I*(I-1)/2 ! J .LE. I

IMPLICIT REAL*8 (E, F, H, R, W, X)
LOGICAL LSLLOPER, KJOPER

NZMAX : Maximum number of non-zero matrix elements for
any J sub-block of hamiltonian matrix.
NMATRIX : Maximum dimension of hamiltonian matrices for given
angular momentum J sub-block.
PARAMETER (NZMAX=499500, NMATRIX=999)

B : hamiltonian matrix
COMMON/HAMM/H(NZ1MAX)

IDIMIM : dimension for array IM
IDIMFM : dimension for array FM
PARAMETER(IDIMIM=100000, IDIMFM=100000)

IM : array for packed matrix indices
FM : array for non-zero values of matrix
COMMON/MEDATA/ FM(IDIMFM), IM(IDIMIM)

EIGVAL : array for eigenvalues
EIGVEC : array for eigenvectors
COMMON/ENG/EIGVAL(20), EIGVEC(NMATRX, 20)

DIMENSION VALPAR(*)
DATA NOTX/O/!, XPI/3.1415926535897932D0/

Statement to pack matrix indices in ESSL format. INDEX(I,J,MATDIM)=I + ((2*MATDIM-J)*(J-1))/2 ! J .LE. I

Hamiltonian parameters

XHM=DBLE(VALPAR(1))
XQQ=DBLE(VALPAR(2))
XMAJORANA=DBLE(VALPAR(3))
XSPINO=DBLE(VALPAR(4))
IF(.NOT. LSLOPER) THEN
XORBORB=DBLE(VALPAR(5))
ELSE
XORBORB=DBLE(RATIOLLLS*VALPAR(4))
END IF
IF(KJOPER) THEN
XLM1=DFLOAT(-LM+MU)/3.0
XLM2=DFLOAT(-LM-2*LM+MU-3)/3.0
XLM3=DFLOAT(2*LM+MU+3)/3.0
XDENOM=2.0*XLM3**2 + XLM1*XLM2
XUCl=DBLE(VALPAR(6)) + DBLE(VALPAR(7))*XLM1*XLM2/XDENOM
XX3A=DBLE(VALPAR(7))*XLM3/XDENOM
XX4A=DBLE(VALPAR(8))/XDENOM
ELSE
XJJ=DBLE(VALPAR(6))
XX3A=DBLE(VALPAR(7))
XX4A=DBLE(VALPAR(8))
END IF

Construct hamiltonian matrix

JFILE=10+J2

Run through the interactions.
IF(NCASE .LE. 3) THEN
NUMINT=NPARM
ELSE
NUMINT=NPARM-1
END IF
DO 30, INT= 1 , NUMINT
READ(JFILE) J2FILE, INTRACT, NDIM
IF(J2FILE .NE. J2)
6 CALL TKO(' DSHENG: J value of file does not match J2.0')
IF(INTRACT .NE. INT)
6 CALL TKO(' DSHENG: Interaction numbers do not match.8')
CALL IODATA(1,0,JFILE,NOTZ,NOTZ) ! read in matrix elements
IF(NOTZ .GT. NIMAX)
6 CALL TKO(' DSHENG: Too many nonzero matrix elements.8')
NEVAL=MINO(NEVAL,NDIM)
NVECT=MINO(NVECT,NDIM)

C Array initializations
C IF(INT .EQ. 1) THEN
  KMAX=NDIM*(NDIM+1)/2
  IF(KMAX .GT. NIMAX) CALL
6 TKO(' DSHENG: Overflow in the H matrix8')
DO 10,K=1,KMAX
  H(K)=0.D0
10 END IF
C IF(NOTZ .NE. 0) THEN
C Start matrix construction.
C DO 20,JK = 1 , NOTZ
  INDX=IM(JK) ! IMSL packing order.
  IROW=INT(SQR(2.0*INDX))
  JCOL=INDX - IROW*(IROW-1)/2
  JSS=INDX(IROW,JCOL,NDIM) ! ESSL packing order.
C Construct Hamiltonian matrix according to case.
C NCASE= 1: H.O.
C 2: H.O. + Q.Q (algb)
C 3: H.O. + Q.Q (algb) + M + l(i).s(i) + l(i).l(i)
C 4: H.O. + Q.Q (algb) + M + l(i).s(i) + l(i).l(i)
C + J.J + Y3A + Y4A
C 5: H.O. + Q.Q (algb) + M + l(i).s(i) + l(i).l(i)
C + J.J + Y3A + Y4A + L.L
C IF(NCASE .EQ. 1) THEN
C H.O. hamiltonian only.
C IF(INT .EQ. 1) H(JSS)=H(JSS) + XHN*FM(JK)
ELSE IF(NCASE .EQ. 2) THEN
C H.O. + Q.Q (algb) hamiltonian
C IF(INT.EQ.1) THEN
  Add H0 term.
  H(JSS)=H(JSS) + XHN*FM(JK)
ELSEIF(INT.EQ.2) THEN
  Add Q.Q (algb) contribution.
  H(JSS)=H(JSS) - 0.5D0*XQQ*FM(JK)
ENDIF
ELSE IF(NCASE .EQ. 3) THEN
C H.O. + Q.Q (algb) + M + l(i).s(i) + l(i).l(i)
C IF(INT.EQ.1) THEN
  Add H0 and centroid terms for Q.Q (coll).
  H(JSS)=H(JSS) + XHN*FM(JK)
ELSEIF(INT.EQ.2) THEN
  Add Q.Q (algb) contribution.
$H(JSS) = H(JSS) - 0.5D0 \times QQ \times FM(JK)$

ELSEIF (INT. EQ. 3) THEN
  Add Majorana contribution.
  $H(JSS) = H(JSS) + XMAJORANA \times FM(JK)$

ELSEIF (INT. EQ. 4) THEN
  Add spin-orbit contribution.
  $H(JSS) = H(JSS) + XSPINO \times FM(JK)$

ELSEIF (INT. EQ. 5) THEN
  Add orbit-orbit contribution.
  $H(JSS) = H(JSS) + XORBORB \times FM(JK)$

ENDIF

ELSE IF (NCASE .EQ. 4) THEN
  $H.O. + Q.Q (algb) + M + 1(i).s(1) + 1(1).l(1) + J^2 + Y3A + Y4A$

  IF (INT. EQ. 1) THEN
    Add HO $\times J^2$ contribution.
    $H(JSS) = H(JSS) + XHW \times FM(JK) + XJJ \times DELOAT(J2*(J2+2)) \times 0.25D0$

  ELSEIF (INT. EQ. 2) THEN
    Add Q.Q (algb) contribution.
    $H(JSS) = H(JSS) - 0.5D0 \times QQ \times FM(JK)$

  ELSEIF (INT. EQ. 3) THEN
    Add Majorana contribution.
    $H(JSS) = H(JSS) + XMAJORANA \times FM(JK)$

  ELSEIF (INT. EQ. 4) THEN
    Add spin-orbit contribution.
    $H(JSS) = H(JSS) + XSPINO \times FM(JK)$

  ELSEIF (INT. EQ. 5) THEN
    Add orbit-orbit contribution.
    $H(JSS) = H(JSS) + XORBORB \times FM(JK)$

  ELSEIF (INT. EQ. 6) THEN
    Add Y3A contribution.
    $H(JSS) = H(JSS) + XY3A \times FM(JK)$

  ELSEIF (INT. EQ. 7) THEN
    Add Y4A contribution.
    $H(JSS) = H(JSS) + XY4A \times FM(JK)$

ENDIF

ELSE IF (NCASE .EQ. 5) THEN
  $H.O. + Q.Q (algb) + M + 1(i).s(1) + 1(1).l(1) + J^2 + J^2 + Y3A + Y4A$

  IF (INT. EQ. 1) THEN
    Add HO $\times J^2$ contribution.
    $H(JSS) = H(JSS) + XHW \times FM(JK) + XJJ \times DELOAT(J2*(J2+2)) \times 0.25D0$

  ELSEIF (INT. EQ. 2) THEN
    Add Q.Q (algb) contribution.
    $H(JSS) = H(JSS) - 0.5D0 \times QQ \times FM(JK)$

  ELSEIF (INT. EQ. 3) THEN
    Add Majorana contribution.
    $H(JSS) = H(JSS) + XMAJORANA \times FM(JK)$

  ELSEIF (INT. EQ. 4) THEN
    Add spin-orbit contribution.
    $H(JSS) = H(JSS) + XSPINO \times FM(JK)$

  ELSEIF (INT. EQ. 5) THEN
    Add orbit-orbit contribution.
    $H(JSS) = H(JSS) + XORBORB \times FM(JK)$

  ELSEIF (INT. EQ. 6) THEN
    Add Y3A contribution.

ENDIF
H(JSS) = H(JSS) + XY3A*FM(JK)
ELSEIF (INT.EQ.7) THEN
  C  Add Y4A contribution.
  H(JSS) = H(JSS) + XY4A*FM(JK)
ELSEIF (INT.EQ.8) THEN
  C  Add L**2 contribution.
  H(JSS) = H(JSS) + XLSQ*FM(JK)
ENDIF
ELSE
  CALL TKO(' DSHENG: Invalid NCASE value.')
END IF NCASE construct.
20 CONTINUE
END IF
30 CONTINUE
C ---------------------------------------------------------------
C Diagonalize hamiltonian matrix
C ---------------------------------------------------------------
REWIND JTILE ! Rewind data file for next set of parameters.
WRITE(6,40) NDIM
40 FORMAT('0 Entering the eigenvalue routine ... dimension =',I6)
   CALL CPUTIME(XBEG,I)
   IF (I.NE.0) THEN
     CALL OUT('0***** Error encountered in determining cputime@')
   ENDIF
   CALL LANEXV(0,-NEVAL,NDIM,H)
   CALL CPUTIME(XEND,I)
   IF (I.NE.0) THEN
     CALL OUT('0***** Error encountered in determining cputime@')
   ELSE
     XDIF = (XEND-XBEG)*1.E-06
     WRITE(6,50) XDIF
   ENDIF
50 FORMAT('0 CPU time for diagonalization =',E12.5)
ENDIF
RETURN
END
SUBROUTINE NQANTA(QTOT,NTOT,NPI,NNU,NSP,NSN,NVP,NVN)
C --------------------------------------------------------------
C Program Description:
C --------------------------------------------------------------
C EVALUATE NUMBER OF PARTICLES IN THE REAL OR NORMAL SPACE (NTOT)
C AND EIGENVALUE OF THE HARMONIC OSCILLATOR HAMILTONIAN (QTOT)
C
C Parameters:
C QTOT = RETURNED VALUE FOR EIGENVALUE OF THE H.O. HAMILTONIAN
C NTOT = RETURNED VALUE FOR THE TOTAL NUMBER OF NUCLEONS
C NPI = RETURNED VALUE FOR THE TOTAL NUMBER OF PROTONS
C NNU = RETURNED VALUE FOR THE TOTAL NUMBER OF NEUTRONS
C
C ... CLEARLY NTOT = NPI + NNU
C NSP = PROTON SHELL NUMBER
C NSN = NEUTRON SHELL NUMBER
C NVP = NUMBER OF VALENCE PROTONS
C
NVN = NUMBER OF VALENCE NEUTRONS

... APPLIES TO BOTH REAL AND PSEUDO SHELL CASES ...
EXAMPLES: 24Mg --> NSP=2, NSN=2, NVN=4, NVP=4 (REAL)
238U --> NSP=4, NSN=5, NVP=6, NVN=12 (PSEUDO)

---

NSPF=NSP-1
NSNF=NSN-1
NSUM1=0
NSUM2=0

IF(NSP.EQ.NSN) THEN
  DO 100 K=0,NSPF
    NSUM1=NSUM1+(K+1)*(K+2)
  100    NSUM2=NSUM2+K*(K+1)*(K+2)
    NFI=NSUM1+NVP
    NN=NSUM1+NVN
    NTO=NFI+NN
    QT=FLOAT(NSUM2+NSU22+NSP*(NVN+NVP))+FLOAT(3*(NTO-1))/2.E0
  ELSE
    DO 200 K=0,NSPF
      NSUM1=NSUM1+(K+1)*(K+2)
    200     NSUM2=NSUM2+K*(K+1)*(K+2)
      NFI=NSUM1+NVP
      NQP=NSUM2+NSP*NVP
      NSUM3=0
      NSUM4=0
      DO 300 K=0,NSNF
        NSUM3=NSUM3+(K+1)*(K+2)
      300     NSUM4=NSUM4+K*(K+1)*(K+2)
        N=NSUM3+NVN
        NQ=NSUM4+NSP*NVN
        NTO=NFI+NN
        QT=FLOAT(NQP+NQ)+FLOAT(3*(NTO-1))/2.E0
  ENDIF
RETURN
END

SUBROUTINE NQFIND(NP,NN,QS)
C
--------------
C Program Description:
C EVALUATE THE EIGENVALUE OF THE OSCILLATOR HAMILTONIAN (QS)
C
--------------

C Parameters:
NP = NUMBER OF PROTONS (input)
NN = NUMBER OF NEUTRONS (input)
QS = TOTAL QUANTA (output)

C

DIMENSION NPAR(2)
NPAR=0
NPAR(1)=NP
NPAR(2)=NN
DO 200 J=1,2
NSUM=0
DO 100 K=0,25
\[ \text{NAD1} = (K+1) \times (K+2) \]
\[ \text{NAD2} = K \times \text{NAD1} \]
\[ \text{NSUM} = \text{NSUM} + \text{NAD1} \]
\[ \text{IF} (\text{NSUM} \leq \text{NPAR}(J)) \text{ THEN} \]
\[ \quad \text{NQAN} = \text{NQAN} + \text{NAD2} \]
\[ \text{ELSE} \]
\[ \quad \text{NQAN} = \text{NQAN} + K \times (\text{NPAR}(J) - \text{NSUM} + \text{NAD1}) \]
\[ \quad \text{GOTO 200} \]
\[ \text{ENDIF} \]

100 CONTINUE
200 CONTINUE
\[ \text{QS} = \text{FLOAT(NQAN)} + (1.5E0) \times \text{FLOAT(NP+NN-1)} \]
RETURN
END
Husney Ahmed Naqvi was born on February 12, 1951 in Khairpur, Pakistan. He graduated from Naz High School in Khairpur. He joined University of Karachi in Karachi, Pakistan, where he graduated in 1980 with a Bachelor of Science degree securing first class first position for which he was awarded Gold Medal by the President of Pakistan. He received an academic scholarship to continue graduate studies at University of Karachi, where he received his Master of Science degree in Physics in 1982 securing first class first position and was awarded a Gold medal by Philips Electrical Company of Pakistan. In 1984 he accepted a graduate teaching assistantship in the Department of Physics and Astronomy at Louisiana State University in Baton Rouge, Louisiana. In 1985 he received his Master of Science degree in Physics from Louisiana State University. He is currently a candidate for the degree of Doctor of Philosophy in the department of Physics and Astronomy at Louisiana State University.
DOCTORAL EXAMINATION AND DISSERTATION REPORT

Candidate: Husney A. Naqvi

Major Field: Physics

Title of Dissertation: Shell-Model Description of Rotational Motion in Odd-Mass Nuclei.

Approved:

[Signature]

Major Professor and Chairman

[Signature]

Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination:

April 14, 1992