A RIGOROUS TREATMENT OF NUCLEAR ROTATION

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ABSTRACT

A fundamental formulation of nuclear rotation is developed using a separation of variables method. When applied to the Hamiltonian of the system, this procedure gives a clear separation into collective and non-collective or intrinsic parts. By using conservation of angular momentum the collective portions of the energy eigenfunctions can be determined exactly. Then, approximate solutions of the intrinsic problem are obtained by using a variational principle in the redundant space of all the particle coordinates. This procedure is carried out by treating the coupling between the rotational and intrinsic motions perturbatively using a basis of deformed Hartree-Fock states. The resulting moment of inertia of the ground state band in lowest order is just the Thouless-Valatin result, currently accepted as the best estimate. Corrections to this answer are shown to be small in general, though anomalies in particular cases are quite likely.

Besides giving rise to a moment of inertia formula, this method provides a theoretical justification for much of the content of the Bohr-Mottelson model. In particular, it is shown that their model Hamiltonian follows naturally from the separation method and, more important, a precise definition of the somewhat nebulous intrinsic angular momentum is obtained. Also, concepts such as symmetries of the wavefunctions, expressions for multipole moments, and values of transition amplitudes are studied from this fundamental formulation. In most cases, the Bohr-Mottelson results appear in lowest order. Correction terms and discussions in disparities are presented where applicable.

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BIOGRAPHICAL NOTE

The author was born in Rockford, Illinois, on November 25, 1942. He lived there until 1960 when he went to the University of Illinois. After receiving a B.S. there in Physics in 1964, he came to M.I.T. as a graduate student. During his first three years, he was supported by the Atomic Energy Commission under a nuclear science fellowship. His final semester was on a research assistantship.

In August of 1963 the author married the former Carolyn Weith. A daughter, Lisa, was born in May of 1965.
I. INTRODUCTION

A. Historical Background

The problem of nuclear rotation was initiated around 1950\(^{(1)}\) by the discovery that certain energy level bands exhibited a sequence very similar to that for a rigid rotor. These bands occurred in clusters throughout the periodic table in regions where the nuclei were known to deviate significantly from spherical symmetry as characterized by large quadrupole moments. Quite naturally, this led to the interpretation that the rotational levels arose from the collective rotation of the nucleus as a whole without a change of shape. The idea of characterizing nuclear motion in this manner was reminiscent of the liquid drop model developed by Bohr and Kalckar in 1937. Expanding the concepts of this model, A. Bohr\(^{(2)}\) and later A. Bohr and B. Mottelson\(^{(3)}\) presented the unified model which contained as one of its features a description of nuclear rotation.

In essence, the unified model pictured the nucleus as a quantized hydrodynamical system capable of performing
surface vibrations and rotations. To account for observed single particle characteristics in non-even-even nuclei, valence nucleons were appended to this hydrodynamical core and particle-core interactions were introduced. The Hamiltonian used for this model had the form

$$H = H_{\text{vib}} + H_{\text{rot}} + H_{\text{part}} + H_{\text{coup}}$$  \hspace{2cm} (1.1)

and operated in a space defined by the following coordinates:

- \{x\} = set of all valence particle coordinates
- \{\theta\} = set of Euler angles defining orientation of core
- \{\beta, \gamma\} = deformation variables defining the extension of the core along the principal axes by

$$R_j = R_0(1 + \sqrt{\beta_j} \beta_j) \quad \beta_j = \beta \cos \left( \alpha - \frac{2\pi j}{3} \right) \quad j = 1, 2, 3$$  \hspace{2cm} (1.2)

and the \beta_j's are assumed much smaller than one. Of particular interest is

$$H_{\text{rot}} = \frac{1}{2} \sum_{j=1}^{3} \frac{J_j}{I_j} (J_j - I_j)^2$$  \hspace{2cm} (1.3)

where

$$\beta_j = \frac{3}{2\pi} \beta \epsilon A \kappa \sin^2 \left( \alpha - \frac{2\pi j}{3} \right) \quad \text{A= the number of nucleons with mass m in the core}$$  \hspace{2cm} (1.4)

$$J_j = \text{component of total angular momentum along the principal axis } j$$  \hspace{2cm} (1.5)
I = component of intrinsic angular momentum along
the principal axis \( j \) \hspace{1cm} (1.6)

The concept of an intrinsic angular momentum was
borrowed from molecular theory where it had a precise defi-
nition in terms of the angular momenta of the electrons and
nuclei of the atoms making up the molecule. In the nuclear
model, its definition was vague but necessary to fit the
observed results.

Applying this model in the region of well defined
rotation, one takes the deformation variables as constant,
signifying a stable nuclear surface. Specializing to even-
even nuclei with axial symmetry along the 3-axis gives

\[
H = H_{nr} + \frac{1}{2\alpha} (J^2 - I_3^2 - I_2^2) + \frac{1}{2\beta \gamma} (J_3^2 - I_3^2) - \frac{1}{J}(J_1 I_2 + J_2 I_3)
\]  \hspace{1cm} (1.7)

with

\[
\mathcal{O}_1 = \mathcal{O}_2 = \mathcal{O}_3 = \beta \gamma \frac{3}{2} A R_0^2 \hspace{0.5cm} ; \hspace{0.5cm} \mathcal{O}_3 = 0
\]  \hspace{1cm} (1.8)

and

\[
H_{int} = \text{the intrinsic energy of the axially symmetric}
\text{core}
\]

\hspace{1cm} (1.9)

Except for a special case mentioned later, one may drop the
last term of \( H \). Then the eigenvalues take on the structure
\[ \psi_{JmK} = D^{*J}_{mK}(\theta) \chi_\nu \]  

(1.10)

where \( D^{*J}_{mK}(\theta) \) are the Wigner D-functions\(^4\) and are eigenfunctions of \( J^2 \), \( J_z \) and \( J_3 \) with eigenvalues \( J(J+1) \), \( m \) and \( K \) respectively. The intrinsic wavefunctions satisfy

\[ (H_{\text{int}} + \frac{J^2}{2}) \chi_\nu = E_\nu \chi_\nu \]  

(1.11)

\[ L_3 \chi_\nu = \mathcal{N} \chi_\nu \]  

(1.12)

\[ E_\nu = E_{-\nu} \]  

(1.13)

Thus

\[ H \psi_{JmK} = (E_\nu + \frac{J(J+1) - \mathcal{N}^2}{2J_3} + \frac{K^2}{2J_3}) \psi_{JmK} \]  

(1.14)

and since \( L_3 = 0 \) one must choose \( K = \nu \).

Because of a redundancy introduced in the definition of the coordinates of this model Hamiltonian, the wave function must satisfy certain symmetry requirements. When these are applied the eigenfunctions assume the form

\[ \psi_{JmK} \propto (D^{*J}_{mK} \chi_\nu + (-1)^{J-K} D^{*J}_{m-K} \chi_{-\nu}) \]  

(1.15)

For \( K = 0 \), since in general \( \chi_{-0} = + \chi_{+0} \), this restricts the rotational spectrum to only even values of \( J \), while \( K \neq 0 \) admits all values.
One exception to the above mentioned energy spectrum results in odd-A nuclei with $k=\frac{1}{2}$. In this case, the term in the Hamiltonian which was dropped couples the $\pm K$ parts of $\psi_{Jm|kl}$ to give an added term to the energy of the form

$$E_{oc} = \frac{L}{2d} a (-i)^{s+\frac{1}{2}} (J + \frac{1}{2})$$

(1.16)

where $a$, known as the decoupling parameter, depends on the details of the intrinsic wavefunction.

When compared with the observed energy spectra, the predictions of this model met with much success, especially in describing the qualitative features. Applications of the eigenfunctions to calculation of the various moments and transition probabilities produced very reasonable results. The only place where the model really exhibited a weakness was in the prediction of the value of the moment of inertia. By using experimental values of the quadrupole moment, it was possible to obtain the parameter $\beta^2$. However, with this value of $\beta^2$, the hydrodynamical value of the moment of inertia was found to be about a factor of five too small. This indicated that the picture of the rotating nucleus as a hydrodynamical system devoid of any internal structure was too extreme.
Extending the ideas of the very successful shell model, D. R. Ingles\(^{(5)}\) added the next step in the development of nuclear rotation theory. His model, the cranking model, placed the nucleons in a non-spherical shell model potential and then imagined the axes of the potential as rotating with a small, constant velocity, \(\vec{\omega}\). The effect of the rotation was to introduce a perturbation, due to coriolis effects, of the form

\[
\nabla_{\text{pert}} = -\vec{\omega} \cdot \vec{J}
\]

Arguing classically, the moment of inertia was defined by

\[
\langle \omega | \vec{J} \cdot \vec{\omega} | \omega \rangle \equiv J | \vec{\omega} |
\]

\(\hat{\omega} = \frac{\vec{\omega}}{|\vec{\omega}|}\) and parallel to a principal axis of the well

(1.18)

where \(| \omega \rangle\) is the wave function obtained using first order perturbation theory. The resulting moment of inertia was found to be

\[
J = \sum_n' \sum_m \frac{|\langle \omega | \vec{J} \cdot \vec{\omega} | n \rangle|^2}{E_n - E_\omega}
\]

(1.19)

where the sums are over the single particle states of the deformed potential, \(\Sigma'\) means only occupied states, and the \(E\)'s are the unperturbed energies.
The treatment, though limited by being semi-classical, has the advantage of presenting the moment of inertia in a form which exhibits the role played by the individual nucleons in the formation of rotational states. It establishes a bridge between the collective aspects of nuclei and the single particle aspects as exemplified in the shell model. As far as numerical accuracy goes, this formula predicts a moment of inertia approximately equal to that found considering the nucleus as a rotating rigid body. This is about a factor of 2 too large, but as will be seen later is in error more because of the shell model approximation than the cranking approximation.

Aiding in the next step of development of the theory was the Hartree-Fock approximation. Calculations in the regions of observed deformations indicated that the self consistent Hartree-Fock single particle potentials tended to also assume a deformed nature. This gives rise to Hartree-Fock solutions which aren't eigenstates of the total angular momentum. Thus, even though one invokes an individual particle approximation seemingly incompatible with the concept of collective motion, the existence of collective behavior manifests itself in the type of potential the particles move in. Using the result of a deformed well, the theory splits off into two distinct approaches.
The first, the Peierls-Yoccoz method, is the only truly workable quantum mechanical treatment of the problem of nuclear rotation. The procedure is to project out of the determinental Hartree-Fock solution, states with good angular momentum. Assuming that the Hartree-Fock solution is a superposition of low lying states of the nucleus, the projected result should contain a significant portion of the rotational state of the lowest band. This method gives satisfactory numerical results but is not very useful in exhibiting the mechanism involved in forming rotational levels.

Looking very much like the cranking model, the second method uses a time dependent Hartree-Fock scheme to find the self consistent solution to the problem of a rotating deformed potential. By requiring a stationary solution in the rotating frame, one can reduce the problem to a time independent Hartree-Fock one with a modified Hamiltonian

\[ \hat{H} = H - \vec{\omega} \cdot \vec{J} \tag{1.20} \]

where \( \vec{\omega} \) is again the angular velocity and is assumed small. The resulting Hartree-Fock problem is solved by perturbation theory and the moment of inertia is defined as in the cranking model. It can be stated succinctly, in a
form known as the Thouless-Valatin equations, as follows:
Let \( |0\rangle \) be the Hartree-Fock state for \( H \), and \( G \) be a
one particle-hole operator defined by
\[
\langle n | i \hat{J} \omega | 0 \rangle = \langle n | \hat{J} \hat{\omega} | 0 \rangle \quad (\hat{\omega} \text{ parallel to a principal
axis of the H.F. well}) \tag{1.21}
\]
for all one particle-hole states \( | n \rangle \); then the moment
of inertia is given by
\[
\mathcal{I} = \langle 0 | i [\hat{J} \hat{\omega}, G] | 0 \rangle \tag{1.22}
\]
The first equation represents a complicated set of coupled
equations for the matrix elements of the operator \( G \). If
one ignores the off diagonal terms of \( H \) in the Hartree-
Fock representation, the matrix elements of \( G \) can be
determined as follows:
\[
i \langle n | [H, G] | 0 \rangle = i \langle n | [H_{\text{HF}}, G] | 0 \rangle \tag{1.23}
= i (E_n - E_0) \langle n | G | 0 \rangle = \langle n | \hat{J} \hat{\omega} | 0 \rangle
\]
where \( H_{\text{HF}} \) is the diagonal part of \( H \) and satisfies
\[
|H_{\text{HF}}|_0 \rangle = E_0 |0\rangle, \quad E_0 = \text{ground state energy} \tag{1.24}
\]
\[
H_{\text{HF}} |n\rangle = E_n |n\rangle, \quad E_n = \text{energy of the one particle hole state} \tag{1.25}
\]
Thus
\[ \langle n | G | 0 \rangle = \frac{i \langle n | J \cdot \hat{\omega} | 0 \rangle}{E_n - E_0} \]  \hspace{1cm} (1.26)

and hence
\[ \mathcal{Q} = 2 \sum_n \frac{1}{E_n - E_0} |\langle n | J \cdot \hat{\omega} | 0 \rangle|^2 \]  \hspace{1cm} (1.27)

In most cases the potential possesses axial symmetry and so \( \hat{\omega} \) is perpendicular to the axis of symmetry.

This result is identical to that of the cranking model except for two differences. First, the energies and states refer to those in the Hartree-Fock well and not a simple shell model potential. This is a crucial distinction since recent calculations\(^{(7)}\) have shown that in deformed nuclei an energy gap between the ground state and first particle hole state exists which isn't present in a simple shell model solution. Numerically, this lowers the moment of inertia from the rigid body value to a value in good agreement with experimental values, i.e. \( E_n - E_0 \) increases. The second difference in this approach results if one does not ignore the off diagonal elements of \( H \) since then \( \mathcal{Q} \) is not given by a cranking model type formula. Inclusion of the off diagonal elements essentially takes into account the change to the Hartree-Fock well due to Coriolis corrections, but this is only a small effect.
The above brief resume of the development of a theoretical understanding of nuclear rotation was presented to put the problem in perspective and to indicate what features should result from a more rigorous treatment. From the Bohr-Mottelson model one learns mostly how to make systematic classifications of energy levels. In particular, the symmetry properties of the wave functions indicate when levels will be missing or won't fit the proper sequence because of decoupling effects. Since the model works so well it will be interesting to see what assumptions were implicitly made and why they hold. Finally, the Bohr-Mottelson model contains a few hazy concepts such as an intrinsic angular momentum which must be clarified.

Information gained from the cranking model and later the time dependent Hartree-Fock theory consists mainly of the fact that it is possible, maybe even mandatory, to base the theory on an independent particle picture. The shape and extent of the deformed Hartree-Fock potential are clearly collective concepts so that even though the nucleons move independently, they move in a collectively parameterized environment.
B. **Philosophical Background**

The aim of this thesis is to develop a consistent quantum mechanical theory of nuclear rotation starting from the Hamiltonian describing the nucleus. Since the "true" nuclear Hamiltonian is not known, the theory must be constructed on very general arguments without reference to specific properties of the internucleon potential. This is not an entirely hopeless task since it appears that much of the problem is founded upon kinematical properties of the nuclear many body system. Augmenting the kinematics, certain generally believed symmetry and conservation laws are available which reduce the problem to a more tractable level. The most important of these is of course conservation of angular momentum.

It is necessary still to know something more about the nuclear potential than its symmetries in order to make certain specific statements in the development of the theory. For a minimal set of properties the following are assumed:

a) $V$, the potential, is only 2-body

b) $V$ is a function of the nucleon positions, spin, and isospin but not velocities

c) $V$ is local
In order to render the problem more transparent, it will be advantageous to work in a framework where the collective and intrinsic degrees of freedom are clearly separated. The obvious step is to transform from the original coordinates and momenta describing the nuclear system to a new set consisting of collective and intrinsic variables. This is doomed to failure, though, since specification of the intrinsic variables is a far too complicated procedure. Fortunately, there exists a procedure due to Tomonaga\(^8\) whereby it is possible to decompose the operators of the theory into collective and intrinsic parts without actually specifying the intrinsic coordinates. The essence of the method is to develop the operators in a power series in the collective variables with the coefficients in the expansion being intrinsic operators. In principle, these coefficients could be expressed in terms of the intrinsic variable, but in reality they are actually expressed in terms of the original variables of the nuclear system.

The technique of explicitly displaying collective variables while using all of the variables of the problem in non collective operators is not new to many body physics. It was used extensively by Bohm and Pines\(^9\) in their
treatment of the electron gas. In their work, they also introduced the concept of using redundant variables and subsidiary conditions to solve problems stated in this manner. This technique will be useful also in treating the nuclear rotation problem where the subsidiary conditions will appear as certain delta function constraints in overlap integrals and matrix elements.

Once the Hamiltonian has been decomposed using Tomonaga's method, various methods of solution are open. One could, of course, state how to solve the problem exactly, in principle. The main task, though, is to develop an approximation scheme whereby one may arrive at a practical solution to the eigenvalue problem. At this point the independent particle approximation can be introduced. It will be found that by using the Hartree-Fock states of the Hamiltonian as a basis for expressing intrinsic functions, one can arrive at the Thouless-Valatin equations for the moment of inertia. That this result occurs serves as an indication that solving the nuclear rotation problem using redundant variables is a meaningful procedure.

By rewriting the decomposed Hamiltonian, it will be found that one may generate, in a rigorous manner, the
model Hamiltonian assumed by Bohr and Mottelson. Of special interest, it is possible to make a precise definition of the intrinsic angular momentum which, though satisfying the commutation relations of angular momentum, are purely intrinsic operators. The application of this form of the Hamiltonian to axially symmetric nuclei exhibits two important features present in the Bohr-Mottelson model. First, in the absence of coupling between the rotational and intrinsic degrees of freedom, the component of the intrinsic angular momentum along the symmetry axis is conserved though the total intrinsic angular momentum is not necessarily constant. Second, the zero order moment of inertia about the symmetry axis is very small but not exactly zero as in the model. This latter effect indicates that it is necessary to use intrinsic basis functions which are eigenstates of the conserved component of the intrinsic angular momentum in order to eliminate the $\frac{1}{2\theta_{sym}}$ times $(J_3-J_{sym}^{intrinsic})^2$ from the energy of the low lying rotational bands. It will be seen that this basis can be constructed from the deformed Hartree-Fock states by use of a suitable projection operator. Using this basis and treating the rotation-intrinsic coupling by perturbation theory one again finds the Thouless-Valatin equations, a
result available also from the Bohr-Mottelson model if the definition of the intrinsic angular momentum would have been known.

All of the approximate diagonalizations will be carried out using trial functions which are lacking certain required symmetries. This is done to make the methods of solution more transparent. Later on the symmetries are investigated and it will be found that their inclusion, though complicating the algebra somewhat, lead to only minor rectification.

In deriving the symmetries, exact statements can be made only about the collective parts of the wavefunctions since symmetry properties of the intrinsic parts required a detailed knowledge of the intrinsic coordinates. To extract the intrinsic symmetries, it is necessary to assume that the symmetries of the deformed Hartree-Fock solutions represent them to a sufficient degree of approximation. Classification of states by approximate symmetries is of course not a new concept, but is used in most branches of physics to some extent.

Once the properly symmetrized approximate solutions are generated, other quantities of interest such as moments and transition probabilities can readily be found.
As with the Hamiltonian, these operators can be decomposed into collective and intrinsic parts and the contribution from each part to the final result will be immediately available. Since the wavefunctions include corrections due to the rotation-intrinsic coupling, improvements over the results from the Bohr-Mottelson model are obtained. These corrections should prove to be significant since, as is known from shell model calculations including configuration mixing, small corrections to the energy eigenfunctions can lead to large effects on the above mentioned quantities.
II. SEPARATION METHOD

A. Basic Principle

In order to explicitly exhibit the collective variables in an operator while leaving the intrinsic parts in a convenient form, the following technique due to Tomonaga (8) is used. This consists of expanding the operator, say \( F(\hat{p}_1 \ldots \hat{p}_A; \hat{\tau}_1 \ldots \hat{\tau}_A) \), in a Taylor series in the collective variables and then expressing the coefficients of this expansion in a form which does not depend explicitly on the remaining non-collective variables. Proceeding, call the conjugate collective coordinate and momentum \( q \) and \( \Pi \) respectively. For all of the following purposes, it will be sufficient to specialize to the problem to the case where \( F \) is independent of \( q \) or equivalently \([F,\Pi] = 0\). Then, if \( F \) were a numerical function, one would write

\[
\begin{align*}
F(\hat{p}_1 \ldots \hat{p}_A; \hat{\tau}_1 \ldots \hat{\tau}_A) &= F|_{\Pi=0} + \Pi \frac{\partial F}{\partial \Pi}|_{\Pi=0} + \frac{1}{2} \Pi^2 \left( \frac{\partial^2 F}{\partial \Pi^2} \right)|_{\Pi=0} + \cdots \\
&= \sum_{\Pi=0}^\infty \frac{1}{n!} \Pi^n \left( \frac{\partial^n F}{\partial \Pi^n} \right)|_{\Pi=0} + \cdots
\end{align*}
\]  

(2.1)

assuming \( \Pi = 0 \) is the proper expansion point. It should be noted at this point that \( F|_{\Pi=0}, \frac{\partial F}{\partial \Pi}|_{\Pi=0} \), etc. are all intrinsic in the sense that they are in principle expressible in terms of the variables which, in addition to \( q \)
and $\Pi$, are required to complete the canonical transformation from the $r$'s and $p$'s. A disadvantage here is that in general one doesn't know $F$ as a function of $\Pi$ so that these intrinsic operators are seemingly incalculable. Moreover, in order to find the required partial derivatives, one must hold the intrinsic, and completely unknown, variables constant.

Fortunately, both of these objections can quite easily be remedied. The latter is rectified by using the result from the canonical formulation of classical mechanics that

$$\frac{\partial}{\partial \Pi} = -\{, q\} \quad (2.2)$$

where $\{, \}$ is the Poisson bracket. Now since one knows $q$ as a function of the $r$'s and $p$'s, one can readily calculate this bracket using the fact that it is representation independent. In other words, one may use the $(r,p)$ variables instead of the set $(q, \Pi + \text{intrinsic})$ to find $\{, q\}$.

As for finding the intrinsic coefficients in the above power series, one merely expands them in a power series about $\Pi$. That is
\[ F \bigg|_{\pi^2 = 0} = F - \pi \frac{2F}{\pi^2} + \frac{1}{2} \pi^2 \frac{2F}{\pi^2} + \ldots \quad (2.3) \]

\[ = F + \pi \{ F, g \} + \frac{1}{2} \pi^2 \{ \{ F, g \}, g \} + \ldots \]

\[ \frac{2F}{\pi^2} \bigg|_{\pi^2 = 0} = -\{ F, g \} - \pi \{ \{ F, g \}, g \} + \ldots \quad (2.4) \]

\[ \frac{2F}{\pi^2} = \{ \{ F, g \}, g \} + \ldots \quad (2.5) \]

And since \( F, q \) and \( \pi \) are all known functions of the \( \hat{r} \)'s and \( \hat{p} \)'s, everything here can be calculated as desired. Furthermore, everything may be expressed entirely in terms of the \( \hat{r} \)'s and \( \hat{p} \)'s, a result needed for the redundant variables treatment.

To make the above results correct for quantum mechanical operators one need only make the usual replacement (\( \hbar \equiv 1 \))

\[ \{ , g \} \rightarrow -i \{ , g \} \quad (2.7) \]

Then one has the second order result

\[ F(\hat{r}_1, \ldots, \hat{r}_n, \hat{p}_1, \ldots, \hat{p}_n) = (F - i \pi \{ F, g \} - \frac{1}{2} \pi^2 \{ \{ F, g \}, g \}) + \quad (2.8) \]

\[ i [F, g] + \pi [\{ F, g \}, g] \pi - \frac{1}{2} [\{ F, g \}, g] \pi^2 \]
Even though this is actually the identity $F = F$, it is still a second order result because the coefficients are only intrinsic to second order. For example, consider the first one which if intrinsic should commute with $g$ and $\pi$, the general criterion for intrinsic operators.

\[
\begin{align*}
[\left(F - i \pi \left[ F, g \right] - \frac{1}{2} \pi^2 \left[ \left[ F, g \right], g \right] \right), \pi] &= \left[ F, \pi \right] - i \pi \left[ \left[ F, g \right], \pi \right] - \\
&\frac{1}{2} \pi^2 \left[ \left[ \left[ F, g \right], g \right], \pi \right]
\end{align*}
\] (2.9)

The first term is zero since $F$ is independent of $g$ by definition. To calculate the second term use the Jacobi identity

\[
\left[ \left[ A, B \right], C \right] + \left[ \left[ C, A \right], B \right] + \left[ \left[ B, C \right], A \right] = 0
\] (2.10)

plus the fact $[g, \pi] = i$ to get

\[
\left[ \left[ F, g \right], \pi \right] = \left[ \left[ \pi, g \right], F \right] + \left[ \left[ F, \pi \right], g \right] = 0
\] (2.11)

In exactly the same manner one shows the third term is zero. Thus, this coefficient does commute with $\pi$. The trouble arises in the commutator with $g$. 

\[
\begin{align*}
\left[ \left( F - i \pi \left[ F, g \right] - \frac{1}{2} \pi^2 \left[ \left[ F, g \right], g \right] \right), g \right] &= \left[ F, g \right] - i \pi \left[ \left[ F, g \right], g \right] + \frac{1}{2} \pi^2 \left[ \left[ \left[ F, g \right], g \right], g \right] - \\
&\frac{1}{2} \pi^2 \left[ \left[ \left[ F, g \right], g \right], g \right] \left[ \left[ F, g \right], g \right]
\end{align*}
\] (2.12)

\[
= -\frac{1}{2} \pi \left[ \left[ \left[ F, g \right], g \right], g \right]
\]
This is zero only to second order in the commutators. Fortunately in the nuclear rotation case, it can be arranged that all commutators higher than second order vanish so that an expansion of the type of equation (8) is rigorously valid.

For the sake of completeness and to aid in later cases where it will be necessary to abandon the luxury of the previous condition, the above procedure will be extended to complete accuracy. Instead of equation (8), one now has the expansion

\[ F = \sum_{n=0}^{\infty} \frac{1}{n!} F^n \]  

where

\[ F^n = \sum_{n=0}^{\infty} \frac{1}{n!} (-i)^n \left[ \frac{\ldots}{n} F, \ldots \right] \]  

That this is the proper expansion is evident by considering the arguments leading to (11) and (12). An explicit verification will be given for the case of two dimensional rotation a bit later.

Before doing nuclear rotation, consider as an illustration the application of this procedure to the center-of-mass motion. Here one has

\[ H = \sum_{j=1}^{A} \frac{\bf p_j^2}{2m} + \frac{1}{2} \sum_{i,j} V_{ij} \]  

(2.15)
Define

$$\vec{P} = \sum_{j=1}^{A} \vec{p}_j = \text{center of mass momentum} \quad (2.16)$$

For an isolated system \([H, \vec{P}] = 0\). Thus \(H\) is a function only of the \(\vec{P}\) and the remaining 6A-6 coordinates and momenta required to describe the system. Denote these remaining variables by \(\eta\).

The variable conjugate to \(\vec{P}\) is of course the center of mass position \(\vec{x} = \frac{1}{A} \sum_{j=1}^{A} \vec{r}_j\), and for the Hamiltonian (15), one finds

$$i[H, \vec{x}] = \dot{\vec{x}} = \frac{\vec{p}}{M} \quad \text{and} \quad [H, x_i] = \frac{\partial H}{\partial p_i} = -\frac{i}{\hbar} \delta_{i,j} \quad (2.17)$$

where \(M = \sum_{j=1}^{A} m_j = Am\). Since all higher commutators vanish one has

$$H = (H - \frac{\vec{p}^2}{2M}) + \frac{\vec{p}^2}{2M} \quad (2.18)$$

which is the well known, trivial result. The first term is the "intrinsic energy" and is independent of both \(\vec{P}\) and \(\vec{x}\), and the second is the collective energy. In this case there exists no coupling between the intrinsic and collective motions as evidenced by the absence of a term linear in \(\vec{P}\). Because of no coupling, the eigenfunctions of \(H\) are of the form

23
\[ \psi_{n\kappa}(r_1, \ldots, r_n) = f_n(q) e^{i\mathbf{k} \cdot \mathbf{r}} \]  \hspace{1cm} (2.19)

where

\[ H_0(q)f_n = \left( H - \frac{\mathbf{p}^2}{2M} \right) f_n = \epsilon_n f_n \]  \hspace{1cm} (2.20)

and

\[ H \psi_{n\kappa} = \left( \epsilon_n + \frac{k^2}{2M} \right) \psi_{n\kappa} \]  \hspace{1cm} (2.21)

B. Decomposition of Two-Dimensional Hamiltonian

Denoting the coordinate axes by \( x \) and \( y \) and ignoring spin which will be included only in three dimensions, one has as the collective variable

\[ J \equiv \sum_{i=1}^{A} (\dot{x}_i \rho_{y_i} - \dot{y}_i \rho_{x_i}) \]  \hspace{1cm} (2.22)

Since the Hamiltonian commutes with \( J \), it is only a function of \( J \) and the appropriate remaining intrinsic coordinate. Thus, the coefficients in the expansion of the Hamiltonian in powers of \( J \) will be intrinsic. In order to perform this expansion it is necessary to find the angle \( \varphi \) conjugate to \( J \) i.e. satisfying

\[ [J, e^{i\varphi}] = e^{i\varphi} \]  \hspace{1cm} (2.23)
This relation is insufficient to determine \( \varphi \) uniquely, a fact which is to be exploited later to cause the expansion of the Hamiltonian to terminate after three terms. At this time only the existence of \( \varphi \) is assumed.

To affect the decomposition of \( H \), still defined by equation (15), introduce the following definitions:

\[
H^{(0)} = H; \quad H^{(i)} = [H, \varphi]; \quad H^{(n+)} = [H^{(n)}, \varphi]
\]  

(2.24)

Then in analogy to equations (13) and (14)

\[
H^{(n)}(\vec{r}_1 \ldots \vec{r}_N; \vec{p}_1 \ldots \vec{p}_N) = \sum_{n=0}^{\infty} \frac{J^n}{n!} \lambda^n H_n
\]  

(2.25)

with

\[
H_n = \sum_{k=0}^{\infty} \frac{(-J)^k}{k!} \lambda^{kn} H^{(k+n)} = \text{intrinsic operator.} \tag{2.26}
\]

To demonstrate that the \( H_n \) are intrinsic it is necessary to verify that they commute with both \( J \) and \( \varphi \). From the fact that \([H, J] = 0\), one can immediately show that \([H^{(n)}, J] = 0\) by induction as follows: assume \([H^{(n-1)}, J] = 0\), then

\[
[H^{(n)} J] = [[H^{(n-1)}, \varphi], J] = [[H^{(n-1)} J], \varphi] + [[J, \varphi], H^{(n-1)} \varphi] \tag{2.27}
\]

\[
= [0, \varphi] + [-\lambda \varphi, H^{(n-1)} \varphi] = 0
\]
Here use was made again of the Jacobi identity.

Now since \( J \) commutes with itself, it follows trivially from the definition of \( H_n \) that \( J \) commutes with \( H_n \). That \( \varphi \) commutes with \( H_n \) follows from the facts

\[
[J^k, \varphi] = -i K J^{k-1}
\]  
(2.28)

\[
[H^{(n)}, \varphi] = H^{(n+1)}
\]  
(2.29)

Then

\[
[H_n, \varphi] = \sum_{k=0}^{\infty} \frac{1}{k!} (-i)^k (J^k \varphi) H^{(k+n)} + J^k [H^{(k+n)}, \varphi]
\]  
(2.30)

\[
= \sum_{k=0}^{\infty} \frac{1}{k!} (-i)^k (J^k H^{(n+1)}) + J^k H^{(k+n)}
\]

\[
= \sum_{k=0}^{\infty} \frac{1}{(k+n)!} (-i)^k J^{k+n} H^{(k+n)} + \frac{1}{k!} (-i)^k J^k H^{(k+n+1)}
\]

Changing the summation index on the first term via \( K \rightarrow K+1 \) gives

\[
[H_n, \varphi] = \sum_{k=0}^{\infty} \left( \frac{i^{k+n}}{k!} J^{k+n} H^{(k+n)} + \frac{i^{k+n}}{k!} J^k H^{(k+n+1)} \right) \rightarrow 0
\]  
(2.31)

Thus the \( H_n \) are indeed intrinsic operators and are in principle expressible in terms of a suitable set of intrinsic variables.
Now that the decomposition has been made, the next question is whether it has any meaning in the sense that the infinite sums above converge when applied to states of physical interest. This is, of course, a difficult problem in analysis as long as $\varphi$ is defined only by equation (23). Fortunately, due to the ambiguity in $\varphi$, the problem can be circumvented by ascribing certain subsidiary conditions along with equation (23). In particular, if one requires $\varphi$ to be a function of the particle coordinates only, the $H^{(n)}$ vanish for $n \geq 3$ and hence all series terminate. To show this, remember that the potential was assumed local and independent of momentum and hence commutes with $\varphi (\vec{r}_1, \ldots, \vec{r}_A)$. Thus one has

$$H^{(n)} = \left[ \sum_{\vec{r}_i} \frac{\vec{p}_i^2}{2m_i}, \varphi \right] = \frac{i}{\hbar} \sum_{\vec{r}_i} \sum_{\vec{r}_j} \left( \vec{p}_i \cdot \nabla_i \varphi + (\nabla_i \varphi) \cdot \vec{p}_i \right)$$

(2.32)

$$H^{(w)} = \left[ H^{(w)}, \varphi \right] = \frac{-i}{\hbar} \sum_{\vec{r}_i} \left\{ \left( \frac{\partial \varphi}{\partial \vec{r}_i} \right)^2 + \left( \frac{\partial \varphi}{\partial \nabla_i} \right)^2 \right\}$$

(2.33)

and since $H^{(2)}$ is independent of momentum, all higher $H^{(n)}$ vanish.

The question still remains if it is possible to choose $\varphi$ as a function of the coordinates only. This can be
affirmed by explicitly demonstrating the existence of one such angle as follows: consider the mass quadrupole eigenvalue problem

$$\sum_{j=1}^{A} (\hat{r}_j \cdot \hat{e}_c) \hat{r}_j = Q_c \hat{e}_c$$

where the $\hat{e}_c$'s are the eigenvectors and the $Q_c$'s the eigenvalues (quadrupole moments). Now defining $\varphi$ by $\hat{e}_1 \cdot \mathbf{x} = \cos \varphi$, it will be shown to be conjugate to $J$ and independent of momenta as desired. Equations (2.34) now become for $c=1$,

$$\begin{align*}
\sum_j x_j (x_j \cos \varphi + y_j \sin \varphi) &= Q_1 \cos \varphi \\
\sum_j y_j (x_j \cos \varphi + y_j \sin \varphi) &= Q_1 \sin \varphi
\end{align*}$$

(2.35)

These are consistent only if

$$\det \begin{vmatrix} \sum x_j^2 - Q_1 & \sum x_j y_j \\ \sum x_j y_j & \sum y_j^2 - Q_1 \end{vmatrix} = (\sum x_j^2 - Q_1)(\sum y_j^2 - Q_1) - (\sum x_j y_j)^2 = 0$$

(2.36)

or

$$Q_1 = \frac{\sum (x_j^2 + y_j^2) \pm \sqrt{(\sum (x_j^2 - y_j^2))^2 + 4(\sum x_j y_j)^2}}{2}$$

(2.37)

Then taking + sign (and dropping $j$-subscripts)

$$\tan \varphi = \frac{\sum x y}{Q_1 - 2y^2} = \frac{2\sum x y}{\sum (x^2 - y^2) + [\sum (x^2 + y^2)]^2 + 4(\sum x y)^2}$$

(2.38)
Using the relation \( \tan \varphi = \frac{\tan 2\varphi}{1 + \tan^2 2\varphi} \) one sees that

\[
\tan^2 \varphi = \frac{2 \Sigma \times \varphi}{\Sigma (x^2 - y^2)} \quad \text{or} \quad (2.39)
\]

\[
\varphi = \frac{1}{2} \tan^{-1} \left( \frac{2 \Sigma \times \varphi}{\Sigma (x^2 - y^2)} \right) + \text{specification of branches} \quad (2.40)
\]

Note that this \( \varphi \) is a function of positions only. Thus, if it is conjugate to \( J \) the existence condition is proved.

To show this one merely calculates the commutator of \( \varphi \) and \( \tan 2\varphi \) which should give \(-2i(1 + \tan^2 2\varphi)\) if \( \varphi \) is conjugate.

\[
[J, \tan \varphi] = -2i \left[ \Sigma (x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}), \frac{\Sigma \times \varphi}{\Sigma (x^2 - y^2)} \right] \quad (2.41)
\]

\[
= -2i \left( \frac{\Sigma \times \varphi}{\Sigma (x^2 - y^2)} - \frac{\Sigma \times \varphi}{(\Sigma \times \varphi)^2} (-2 \Sigma \times \varphi - 2 \Sigma \times \varphi) \right)
\]

\[
= -2i \left( 1 + \frac{4(\Sigma \times \varphi)^2}{\Sigma (x^2 - y^2)} \right) = -2i (1 + \tan^2 2\varphi)
\]

which is the desired result. One may wonder why the commutator \([J, \varphi]\) was not calculated. The answer is purely a technical one; namely, until the branches in equation (40) are completely specified \( \varphi \) is not really defined and so its commutator should not be calculated.

However, in this particular case, since the proper branch
definition requires just adding multiple of $\mathbf{\nabla}$ to the principal value of the arc-tangent, commutators of the incomplete operator are the same as those for the true operator. With this in mind, then, all latter developments will be done using $\mathbf{\Psi}$ which is easier to work with.

This particular choice of $\mathbf{\Psi}$ will be used later in order to establish certain approximations. For reference purposes, $H^{(1)}$ and $H^{(2)}$ as calculated from (30) and (31) are given here. Since they can be found by trivial algebraic manipulations, the results will just be stated.

$$H^{(1)} = -i \mathbf{\dot{\Psi}} = -i \left( \frac{\Sigma (x^2 + y^2) - \Sigma (x^2 - y^2) \tan^2 \mathbf{\Psi}}{m \Sigma (x^2 - y^2) (1 + \tan^2 \mathbf{\Psi})} \right)$$  \hspace{0.5cm} (2.42)

$$H^{(2)} = -Q = - \left( \frac{\Sigma (x^2 + y^2)}{m (x^2 - y^2) (1 + \tan^2 \mathbf{\Psi})} \right)$$  \hspace{0.5cm} (2.43)

Returning to the separated Hamiltonian for a general $\mathbf{\Psi} (\mathbf{\vec{r}}_1, ..., \mathbf{\vec{r}}_A)$ and using the notation introduced in equations (42) and (43), one finds the form

$$\mathbf{\mathcal{H}} = (\mathbf{H} - \mathbf{\dot{\Psi}} J + \frac{1}{2} Q J^2) + (\mathbf{\dot{\Psi}} - Q J) J + \frac{1}{2} Q J^2$$  \hspace{0.5cm} (2.44)

Note that the three terms above give $\mathbf{\mathcal{H}}$ the structure of intrinsic plus coupling plus rotation respectively.

However, since all nuclei do not possess rotational spectra,
this form does not establish the existence of nuclear rotation. That can only be established by a more detailed study of the intrinsic structure as exemplified by the intrinsic energy spectrum and strength of intrinsic-rotation coupling.

Two other points should be mentioned. First, the choice of subsidiary condition on $\mathcal{J}$ is in accord with the basic philosophy of this thesis since now the decomposition of $H$ is essentially a kinematical effect. It depends in no way upon the potential. Second, the final results should, and will, be independent of any specific properties of $\mathcal{J}$ beyond this subsidiary condition. This is because the introduction of $\mathcal{J}$ is actually only an intermediate step needed to render the problem transparent.

C. **Decomposition of Three-Dimensional Hamiltonian**

Extending the above procedure to the case of three dimensions requires the introduction of a body fixed coordinate system in order to exhibit the intrinsic dynamics in a clear fashion. This is analogous to using the body fixed principal axes in the classical rotation of a rigid body. The usual procedure is to introduce the Euler angles to specify the orientation of the body fixed system.

However, this expresses the variables in a very complicated
and unsymmetric manner. To accomplish a symmetric specification of the body fixed axis introduce three unit vectors to specify the directions of the axes. These vectors, \( \vec{e}_i \), must satisfy

\[
\vec{e}_i \cdot \vec{e}_j = \delta_{ij} \quad ; \quad \vec{e}_i \times \vec{e}_j = \vec{e}_k \quad (i,j,k \ cycl.)
\]

(2.45)

Also, in order that they specify a body fixed system, one imposes the requirement that if body fixed angular momenta components are defined by

\[
\mathbf{J}_A = \vec{e}_A \cdot \vec{J} = \vec{J} \cdot \vec{e}_A
\]

(2.46)

then

\[
[\mathbf{J}_A, \mathbf{J}_K] = 0 \quad \forall A,K
\]

(2.47)

where \( \mathbf{J}_K \) are space fixed angular momentum components defined by

\[
\mathbf{J}_k = \hat{k} \cdot \vec{J}
\]

(2.48)

with \( \hat{k} \) being the set of unit vectors along the non-rotating laboratory axes.

For a notation use \( A, B, C, \ldots \) body fixed, \( k, \ell, m, \ldots \) space and the convention that if three alphabetically sequent indices appear, they represent all cyclic permutations of the alphabetical ordering.
It is assumed all of the $\vec{e}'s$ and their components commute, in which case equations (46) and (47) give

\[ [J_k, e_{pA}] = i \epsilon_{mA} \]  \hspace{1cm} (2.49)

\[ [J_A, e_{kB}] = -i \epsilon_{kC} \] \hspace{1cm} (2.50)

\[ [J_A, J_B] = -i J_0 \] \hspace{1cm} (2.51)

where

\[ \epsilon_{kA} = \hat{k} \cdot \vec{e}_A \] \hspace{1cm} (2.52)

With this apparatus the decomposition of $H$ can now be made. The aim is to express $H$ in the form

\[ H = \sum_{n=0}^{N} \sum_{i_A, \ldots, A_n} H_{i_A, \ldots, A_n} J_{i_A} \cdots J_{A_n} \] \hspace{1cm} (2.53)

where the $H_{i_A, \ldots, A_n}$ must be intrinsic to satisfy

\[ [H, \vec{J}] = 0 \] \hspace{1cm} (2.54)

In order to find these operators, it is necessary to find a way to take "derivatives" with respect to the $J_A$'s. Unfortunately, the body fixed angular momenta do not possess conjugate angles so that differentiation can not be expressed in terms of simple commutation. However, from equation (48) one knows
\[
[J_A, \hat{e}_\theta] = -i \hat{e}_c
\]  \hfill (2.55)

and since the \( \hat{e} \)'s are unit vectors

\[
[J_A, \hat{e}_\theta] \cdot \hat{e}_c = -i
\]  \hfill (2.56)

Thus, if \( f(J_A) = \sum a_n J_A^n \), then

\[
[f(J_A), \hat{e}_\theta] \cdot \hat{e}_c = \sum a_n \left( J_A^n \hat{e}_\theta \right) \cdot \hat{e}_c
\]  \hfill (2.57)

\[
= \sum a_n \left\{ -i J_A^{n-1} + [J_A^{n-1}, \hat{e}_\theta] \cdot J_A \hat{e}_c \right\}
\]

But

\[
[J_A^{n-1}, \hat{e}_\theta] = -i J_A^{n-2} \hat{e}_c + J_A \left[ J_A^{n-2}, \hat{e}_\theta \right] \]  \hfill (2.58)

Thus

\[
[f(J_A), \hat{e}_\theta] \cdot \hat{e}_c = \sum a_n \left\{ -i J_A^{n-1} + J_A \left[ J_A^{n-2}, \hat{e}_\theta \right] \cdot J_A \hat{e}_c \right\}
\]  \hfill (2.59)

where

\[
\hat{e}_c \cdot J_A \hat{e}_c = J_A + i \hat{e}_\theta \cdot \hat{e}_c = J_A
\]  \hfill (2.60)

was used. This can be continued until finally one gets

\[
[f(J_A), \hat{e}_\theta] \cdot \hat{e}_c = -i \sum n a_n J_A^{n-1} = -i \frac{\partial f}{\partial J_A}
\]  \hfill (2.61)

Also note that a similar argument gives

\[
[f(J_A), \hat{e}_c] \cdot \hat{e}_\theta = i \frac{\partial f}{\partial J_A}
\]  \hfill (2.62)
so that one has the hermitian, formal statement

\[
\frac{\partial}{\partial \mathcal{A}} \leftrightarrow \frac{i}{\hbar} \left\{ \left[ \hat{\mathcal{E}}_\theta, \hat{\mathcal{E}}_\phi \right], \hat{\mathcal{E}}_\theta - \left[ \hat{\mathcal{E}}_\phi, \hat{\mathcal{E}}_\theta \right], \hat{\mathcal{E}}_\phi \right\} \quad (2.63)
\]

Now that differentiation has been defined it is possible to generalize the two dimensional results. From the outset, it will be assumed that the \( \hat{\mathcal{E}} \)'s are functions of position only and later on a specific calculation for the axes defined by the quadrupole eigenvalue problem will be made. As generalizations of \( \mathcal{V} \) and \( Q \) define

\[
\eta_A = -\frac{i}{\hbar} \left\{ [H_j, \hat{\mathcal{E}}_\theta], \hat{\mathcal{E}}_\theta - [H_j, \hat{\mathcal{E}}_\phi], \hat{\mathcal{E}}_\phi \right\} \equiv \frac{\partial \mathcal{H}}{\partial \mathcal{A}} \quad (2.64)
\]

\[
Q_{\mathcal{E}A} = -\frac{i}{\hbar} \left\{ [\mathcal{E}_\theta, \hat{\mathcal{E}}_\theta] \cdot \hat{\mathcal{E}}_\theta - [\mathcal{E}_\phi, \hat{\mathcal{E}}_\phi] \cdot \hat{\mathcal{E}}_\phi \right\} \equiv \frac{\partial \mathcal{E}H}{\partial \mathcal{A}, \mathcal{E}} \quad (2.65)
\]

Note that because of the orthogonality of the \( \hat{\mathcal{E}} \)'s

\[
Q_{\mathcal{E}F} = -\frac{i}{\hbar} \left\{ [\mathcal{E}_\theta, \hat{\mathcal{E}}_\theta] \cdot \hat{\mathcal{E}}_\theta - [\mathcal{E}_\phi, \hat{\mathcal{E}}_\phi] \cdot \hat{\mathcal{E}}_\phi \right\} \quad (2.66)
\]

\[
= -\frac{i}{\hbar} \left\{ \mathcal{E}_\theta \cdot (\mathcal{E}_\phi \cdot H \mathcal{E}_\theta - \mathcal{E}_\theta \cdot H \mathcal{E}_\phi) \mathcal{E}_F - G \leftrightarrow F \right\}
\]

\[
= -\frac{i}{\hbar} \left\{ \mathcal{E}_\phi \cdot (\mathcal{E}_\theta \cdot H \mathcal{E}_\phi - \mathcal{E}_\phi \cdot H \mathcal{E}_\theta) \mathcal{E}_F - G \leftrightarrow F \right\}
\]

\[
= -\frac{i}{\hbar} \left\{ \mathcal{E}_\theta \cdot (\mathcal{E}_\phi \cdot H \mathcal{E}_F - \mathcal{E}_F \cdot H \mathcal{E}_\phi) \mathcal{E}_\theta - B \leftrightarrow C \right\}
\]

\[
= Q_{\mathcal{E}A}
\]

confirming the usual commutability of the order of differentiation. Also, as with \( Q \), the \( Q_{\mathcal{E}A} \)'s are independent
of momentum so that all higher derivatives of $H$ vanish as desired.

The stage is now set for the decomposition of $H$ by using the obvious generalization of the previous case and defining

$$H_0 = H - \sum A \eta_A J_A + \frac{1}{2} \sum_{A\delta} Q_{A\delta} J_A J_\delta$$

(2.67)

$$H_A = \eta_A - \sum \delta Q_{A\delta} J_\delta$$

(2.68)

$$H_{AB} = Q_{AB}$$

(2.69)

Proving that these operators are intrinsic requires showing that they commute with both $J$ and the $\xi$'s. To do this, one needs the following commutators.

$$[Q_{A\delta}, \xi_\epsilon] = 0$$

A, B and E

(2.70)

since the $Q$'s and $\xi$'s are both momentum independent. Next

$$\lambda (Q_{AE} \xi_F - Q_{AF} \xi_E) = \frac{1}{2} \left\{ ([\eta_A, \xi_\delta] \cdot \xi_F - [\eta_A, \xi_\delta] \cdot \xi_E) \xi_F + ([\eta_A, \xi_E] \cdot \xi_F - [\eta_A, \xi_E] \cdot \xi_\delta) \xi_\delta \right\}$$

$$= [\eta_A, \xi_\delta]$$

(2.71)

where the following facts were used

(a) the $\xi$'s form a complete Euclidean vector set
(b) \[ \{ \hat{e}_A, \hat{e}_B \} = \{ \hat{e}_A, \hat{e}_A \hat{e}_B \} - \hat{e}_A \cdot \hat{e}_A = -\hat{e}_A \cdot \hat{e}_B \]

(c) \[ [\eta_A, \hat{e}_C] \]

is momentum independent and thus commutes with the \( \hat{e} \)'s.

Continuing in the list of required results,

\[
[\eta_A, J_n] = \frac{i}{2} \sum \{ (\epsilon_{ec} H \epsilon_{fo} - \epsilon_{eo} H \epsilon_{fc}) J_n \}
\]

\[
= \frac{i}{2} \sum \{ (\vec{\lambda} \vec{n}) \cdot \vec{e}_c H \vec{\lambda} \vec{e}_o + \vec{\lambda} \cdot \vec{e}_c H (\vec{\lambda} \times \vec{n}) \cdot \vec{e}_o - (c \leftrightarrow e) \}
\]

\[= 0 \]

since terms containing the antisymmetric dyadic \( \frac{i}{2} (\vec{\lambda} \times \vec{n}) \cdot \vec{e}_c \) cancel in pairs and \([H, J_n] = 0\). Finally, by exactly the same reason except with \([\eta_A, J_n] = 0\)

\[
[Q_{O_A}, J_n] = 0 \quad (2.73)
\]

Now to show that (65)-(67) are intrinsic, note that they all commute with the \( J_n \) since all of their constituents do. Next the \( Q_{AB} \) are definitely intrinsic by virtue of (70) and (73). To establish this property for the \( H_A \) notice that (50) and (71) give

\[
[\hat{H}_A, \hat{e}_C] = [\eta_A, \hat{e}_C] + \frac{2}{\alpha} [\eta_A, \hat{e}_C] = [\eta_A, \hat{e}_C] + \frac{2}{\alpha} Q_{AB} (\hat{e}_A \times \hat{e}_C)
\]

\[
= \hat{\lambda} (Q_{AF} \hat{e}_F - Q_{AE} \hat{e}_E) - \hat{\lambda} (Q_{AF} \hat{e}_F - Q_{AE} \hat{e}_E) = 0
\]

Showing that \( H_0 \) is intrinsic reduces to calculating

37
\[
\begin{align*}
[H_0, \vec{E}_G] & = [H - \frac{1}{2} \sum_a H_A J_A - \frac{1}{2} \sum_a \eta_A J_A, \vec{E}_G] \\
& = [H, \vec{E}_G] + \frac{i}{2} \sum_a \left\{ (\eta_a - \sum_a \alpha_{AE} J_B)(\vec{E}_A \times \vec{E}_G) + \eta_a (\vec{E}_A \times \vec{E}_G) - (\alpha_{AE} \vec{E}_A - \alpha_{AE} \vec{E}_G) J_a \right\} \\
& = [H, \vec{E}_G] + \sum_a \eta_a (\vec{E}_A \times \vec{E}_G) - \frac{1}{2} \sum_a (\alpha_{AE} (\vec{E}_A \times \vec{E}_G) - \alpha_{AE} (\vec{E}_A \times \vec{E}_A))
\end{align*}
\]

which is zero because
\[
\sum_a \eta_a (\vec{E}_A \times \vec{E}_G) = \eta_E \vec{E}_E - \eta_F \vec{E}_F
\]
\[
= \frac{i}{2} \left\{ ([H, \vec{E}_E] \cdot \vec{E}_G - [H, \vec{E}_G] \cdot \vec{E}_E) \vec{E}_E - ([H, \vec{E}_E] \cdot \vec{E}_E - [H, \vec{E}_F] \cdot \vec{E}_G) \vec{E}_F \right\} \\
= i [H, \vec{E}_E] + \frac{i}{2} \left\{ [\vec{E}_E, [H, \vec{E}_E]] \vec{E}_E + [\vec{E}_E, [H, \vec{E}_F]] \vec{E}_F \right\}
\]

and hence
\[
\begin{align*}
[H_0, \vec{E}_E] & = -\frac{1}{2} \left\{ [\vec{E}_E, [H, \vec{E}_E]] \vec{E}_E + [\vec{E}_E, [H, \vec{E}_F]] \vec{E}_F + \sum_a (\alpha_{AE} (\vec{E}_E \times \vec{E}_G) - \alpha_{AE} (\vec{E}_E \times \vec{E}_A)) \right\} \\
& = 0
\end{align*}
\]
since the left side is antihermitian while the right side is hermitian.

This completes the proof that $H_0$, $H_A$ and $Q_{AB}$ are indeed intrinsic operators. Now all that remains is to write $H$ down.

\[
H = H_0 + \sum_a H_A J_A + \frac{1}{2} \sum_a Q_{AB} J_A J_B
\]
Inserting definitions (65)-(67) reduces (76) to the identity $H=H$, thus confirming that this is the correct result.

In order to simplify the diagonalization of $H$, it will be convenient to use a specific choice of body fixed axes defined by diagonalizing the quadrupole tensor as was done for two dimensions. This set of axes will render $Q_{AB}$ diagonal and thus eliminate the need of handling the messy cross terms introduced by off diagonal elements. Another advantage of using these axes is that they cast the operators of the theory in a form which can be directly related to physically observed phenomena such as axial symmetry of the nucleus.

Proceeding in the construction of this set of axes, introduce the quadrupole tensor

$$T_{K\ell} = \sum_{\bar{\sigma}_A} \sum_{\bar{\sigma}_B} (\hat{r}_A \cdot \hat{k})(\hat{r}_B \cdot \hat{k})$$

(2.79)

then the desired eigenvalue problem is

$$\sum_{\ell} T_{K\ell} \epsilon_{\ell A} = Q_A \epsilon_{KA}$$

(2.80)

where the $Q_A$ are the principal quadrupole moments and are purely intrinsic and the $\epsilon_{KA}$ are defined in equation (50).
To show that the eigenvectors above specify a body fixed system, it is necessary to verify that equation (49) holds, which for reference is

\[ [\mathcal{J}_k, \varepsilon_{\mathbf{k}A}] = i \varepsilon_{mA} \quad (2.49) \]

From its definition, \( T_{KL} \) satisfies

\[ [T_{KL}, \mathcal{J}_n] = i \sum_i \left\{ (\mathbf{r}_i \cdot (\varepsilon_{\mathbf{k}A})(\mathbf{r}_i \times \dot{\mathbf{r}}) + (\mathbf{r}_i \cdot \dot{\mathbf{r}})(\mathbf{r}_i \cdot (\varepsilon_{\mathbf{k}A})) \right\} \quad (2.81) \]

\[ = i (T_{KmK} + T_{KkKn}) \]

with the obvious notation for the indices. Thus

\[ \sum_{L} [T_{KL}, \mathcal{J}_n] \varepsilon_{L\mathbf{A}} \overset{?}{=} \sum_{K} \left( [T_{KL} \varepsilon_{\mathbf{k}A}, \mathcal{J}_n] - T_{KL} [\varepsilon_{\mathbf{k}A}, \mathcal{J}_n] \right) \quad (2.82) \]

\[ = Q_{A}[\varepsilon_{\mathbf{k}A}, \mathcal{J}_n] - \sum_{K} T_{KL} [\varepsilon_{\mathbf{k}A}, \mathcal{J}_n] = i \sum_{K}(T_{KmK} + T_{KkKn}) \varepsilon_{L\mathbf{A}} \]

\[ = i Q_{A} \varepsilon_{mK} \mathbf{A} + i \sum_{K} T_{KkKn} \varepsilon_{L\mathbf{A}} \]

Changing the summation index on the last term to \( \mathcal{J} \times n \) and using the identity \( \mathbf{r} = \mathbf{r} \times (\mathbf{r} \times \dot{\mathbf{r}}) \), (82) reduces to

\[ Q_{A}[\varepsilon_{\mathbf{k}A}, \mathcal{J}_n] - i \varepsilon_{mK} \mathbf{A} = \sum_{K} T_{KL} (\varepsilon_{\mathbf{k}A}, \mathcal{J}_n) - i \varepsilon_{mK} \mathbf{A} \quad (2.83) \]

In general the eigenvalues are non-degenerate so that one has at most

\[ [\varepsilon_{\mathbf{k}A}, \mathcal{J}_n] - i \varepsilon_{mK} \mathbf{A} = C_{A} \varepsilon_{\mathbf{k}A} \quad (2.84) \]
with $C_A$ some intrinsic operator or a constant. Multiplying by $\epsilon_{LA}$ and summing over $l$ one finds
\[ -i \sum_l \epsilon_{LA} \epsilon_{Lkn,A} = C_A \] (2.85)

But $\sum_l \epsilon_{LA} \epsilon_{Lkn,A} = \hbar \cdot (\hat{e}_A \times \hat{e}_A) = 0$ and thus the $C_A$ are zero showing that
\[ [J_n, \epsilon_{LA}] = i \epsilon_{nkn,A} \] (2.86)
as desired, establishing that the $\hat{e}$'s do specify a body fixed system.

Now consider the equivalent form of the eigenvalue problem
\[ \sum_{k \theta} \epsilon_{kA} T_{k\theta} \epsilon_{L\theta} = Q_A \delta_{AB} \] (2.87)
which upon taking the commutator with $H$ for $A \neq B$ leads to
\[ \sum_{k \theta} \left( [H, \epsilon_{kA}] T_{k\theta} \epsilon_{L\theta} + \epsilon_{kA} T_{k\theta} [H, \epsilon_{L\theta}] + \epsilon_{kA} [H, T_{k\theta}] \epsilon_{L\theta} \right) \] (2.88)
\[ = \sum_{k \theta} \left( [H, \epsilon_{kA}] Q_{\theta} \epsilon_{L\theta} + Q_{\theta} \epsilon_{kA} [H, \epsilon_{kA}] \right) + \sum_{k \theta} \epsilon_{kA} [H, T_{k\theta}] \epsilon_{L\theta} \]
\[ = 0 \]
or using the completeness of the $\hat{k}$'s
\[ -\left( [H, \hat{e}_A] \cdot \hat{e}_A Q_\theta + Q_\theta \hat{e}_A \cdot [H, \hat{e}_A] \right) = \sum_{k \theta} \epsilon_{kA} [H, T_{k\theta}] \epsilon_{L\theta} \] (2.89)
But since \( A \neq B \)

\[
Q_A \vec e_A \cdot [H, \vec e_B] = [H, Q_A \vec e_A \cdot e_B] - [H, Q_A \vec e_A] \cdot e_B
\]

\[
= - [H, \vec e_A] \cdot Q_A \vec e_B
\]

thus

\[
[H, \vec e_A] \cdot e_B = \sum_{k_A} \epsilon_{kA} [H, T_{kA}] e_{kA} \epsilon_{kA} (Q_A - Q_B)^{-1}
\]

(2.91)

and one sees from the definition of \( \eta_A \) in equation (64) that

\[
\eta_A = \pm \sum_{k_A} \epsilon_{kA} [H, T_{kA}] e_{kA} + \epsilon_{kA} [H, T_{kA}] e_{kA} \epsilon_{kA} (Q_A - Q_B)^{-1}
\]

(2.92)

Note that \( \eta_A , (Q_B - Q_C)^{-1} \) and \( \frac{1}{2} \{ \cdots \} \) are all hermitian and hence commute among themselves.

To find the \( \frac{1}{2} \{ \eta, \eta, \eta \} \cdot e_B \) must be calculated which according to (90) reduce to finding

\[
[\sum_{kA} [H, T_{kA}] e_{kA} \cdot e_B = - [T_{kA}, [H, e_{kA}] \cdot e_B]
\]

(2.93)

\[
= - \sum_{kA} \epsilon_{kA} [T_{kA}, [T_{kA}, H]] e_{kA} (Q_A - Q_B)^{-1}
\]

Since the \( T \)'s commute with the potential, one has

\[
[T_{kA}, [T_{kA}, H]] = - \frac{1}{m} \sum_{j \neq kA} \frac{2T_{kA} \cdot 2T_{kA}}{s_{X_j} s_{X_j}} = - \frac{1}{m} \{ T_{kA} x_{kA} + T_{kA} x_{kA} + T_{kA} x_{kA} + T_{kA} x_{kA} \}
\]

(2.94)
and so

\[
\left[ \mathbf{\eta}_e, \mathbf{\hat{c}}_c \right] \cdot \mathbf{\hat{c}}_\theta = \frac{i}{2m} \sum_{\mathbf{\hat{c}}_c} \left\{ \epsilon_{ek} \epsilon_{ek} \left( Tr d_{ek} + Tr _{k_{c_{ek}}} + Tr _{k_{ec_{ek}}} + Tr _{k_{c_{ec_{ek}}}} + Tr _{k_{c_{ec_{ek}}}} \right) \right\} \epsilon_{ek} \epsilon_{ek} \\
+ \left( \frac{F \leftrightarrow \gamma}{} \right) \right\} \left( \mathbf{Q}_c - \mathbf{Q}_c \right)^{\dagger} \left( \mathbf{Q}_c - \mathbf{Q}_c \right)^{\prime} \tag{2.95}
\]

\[
= \frac{i}{2m} \left\{ \left( \mathbf{Q}_c - \mathbf{Q}_c \right) \left( \mathbf{F} \leftrightarrow \gamma \right) \right\} \left( \mathbf{Q}_c - \mathbf{Q}_c \right)^{\dagger} \left( \mathbf{Q}_c - \mathbf{Q}_c \right)^{\prime} \\
= \frac{i}{m} \frac{\left( \mathbf{Q}_c + \mathbf{Q}_c \right)}{\left( \mathbf{Q}_c - \mathbf{Q}_c \right)} \delta_{AE}
\]

Finally, since \( \left[ \mathbf{\eta}_e, \mathbf{\hat{c}}_c \right] \cdot \mathbf{\hat{c}}_c = - \left[ \mathbf{\eta}_e, \mathbf{\hat{c}}_c \right] \cdot \mathbf{\hat{c}}_c \), one sees from equation (65)

\[
\mathbf{Q}_{AE} = \frac{\left( \mathbf{Q}_c + \mathbf{Q}_c \right)}{\left( \mathbf{Q}_c - \mathbf{Q}_c \right)} \delta_{AE} \equiv \frac{1}{\delta_{AE}} \delta_{AE} \tag{2.96}
\]

This completes the construction of the explicit forms of the operators. It should be noted that if the quadrupole eigenvalues in equation (96) are replaced by their average values for a nuclear system, \( \mathbf{\ell}_A \) reduces to the Bohr-Mottelson hydrodynamical moment of inertia. Thus, this particular choice of axes gives as a zero order moment of inertia the one derived from the unified model. In the next section this fact is used to arrive at a precise definition of the intrinsic angular momentum.
D. Derivation of the Bohr-Mottelson Hamiltonian

As mentioned in the Introduction, since the Bohr-Mottelson unified model has successfully accounted for most of the observed properties of rotational nuclei, any more fundamental treatment of the problem should provide insight into why this is true. The present formulation of the problem does this by putting the separated Hamiltonian in a manifestly Bohr-Mottelson form. Then during the course of diagonalizing this Hamiltonian, some of the implicit assumptions of the model will become apparent. Also some of the empirical information contained in the model can be used as an aid in the solution of the problem in the present case by indicating what properties of the nuclear system should be studied or assumed.

Considering first a two dimensional system, the aim is to put the separated Hamiltonian given by equation (44) in the Bohr-Mottelson form

\[ H = H_{\text{int}} + \frac{1}{2\alpha} (J - \mathbf{I})^2 \]  \hspace{1cm} (2.97)

where \( H_{\text{int}} \) is some intrinsic operator, \( \mathbf{I} \) is the so-called intrinsic angular momentum, and \( \alpha \) is the hydrodynamical moment of inertia. Using the particular angle specified by equation (39), this latter quantity is just \( \frac{1}{Q} \) defined
in equation (43). Then with the definitions, motivated by completing the square in equation (44),

\[ H_{\text{int}} \equiv H - \frac{i}{\hbar} \langle \dot{\varphi} \rangle \]

(2.98)

\[ I \equiv J - \frac{1}{\hbar} \dot{\varphi} \]

(2.99)

one finds

\[ H_{\text{int}} + \frac{\alpha}{2} (J-I)^2 = \frac{1}{\alpha} (\dot{\varphi})^2 + 2 \sum \left( J \cdot \dot{J} + (\dot{\varphi})^2 \right) \]

(2.100)

\[ = H \]

indicating that this is a meaningful decomposition. To show that \( H_{\text{int}} \) and \( I \) are intrinsic note first that they both commute with \( J \) since \( H, \dot{\varphi} \) and \( Q \) do. Thus only commutation with \( \varphi \) need be shown. First of all

\[ [H_{\text{int}}, \varphi] = [H, \varphi] - \frac{1}{\alpha} \left[ \dot{\varphi}, \varphi \right] = -i \dot{\varphi} - \frac{1}{\alpha} \left( \dot{\varphi} \right)^2 \]

(2.101)

Now \( [\dot{\varphi}, \varphi] = -i Q \) and

\[ [\dot{\varphi}, Q] = i [\dot{\varphi}, [\varphi, Q]] = i [\varphi, [\dot{\varphi}, Q]] = i [\varphi, [Q, \dot{\varphi}]] \]

(2.102)

\[ = i [\varphi, [Q, \dot{\varphi}]] = i [\varphi, [Q, \dot{\varphi}]] J = 0 \]

where the facts \( J \) commutes with \( Q \) and \( \dot{\varphi} \) as well as the fact \( [Q, \dot{\varphi}] \) contains no derivatives and thus commutes with \( \varphi \) were used. This result immediately establishes that \( [H_{\text{int}}, \varphi] = 0 \) and so \( H_{\text{int}} \) is
intrinsic. That \( \mathcal{I} \) is intrinsic follows from

\[
[I, \mathcal{I}] = [J, \mathcal{I}] - \frac{\lambda}{\sigma} [\dot{\mathcal{I}}, \mathcal{I}] = -\mathcal{I} - \frac{\lambda}{\sigma} \eta = 0
\]  \hspace{1cm} (2.103)

Thus \( \mathcal{H} \) can indeed be decomposed in a manner described by the unified model. Again note that this form does not imply rotational spectra since it applies for all nuclear systems.

The three dimensional analogue can be made by paralleling the above arguments. Using the particular set of body fixed axes discussed in the previous section, the separated Hamiltonian becomes

\[
\mathcal{H} = (H - \sum \left( \eta_a - \frac{\partial}{\partial \eta_a} \right) J_a) + \sum (\eta_a - \frac{\partial}{\partial \eta_a}) J_a + \frac{1}{2} \sum \frac{1}{A} \dot{J}_a^2 \]  \hspace{1cm} (2.104)

Then with

\[
\mathcal{H}_{\text{int}} = \mathcal{H} - \frac{1}{2} \sum \frac{1}{A} J_a \left( \eta_a \right)^2
\]  \hspace{1cm} (2.105)

\[
I_A \equiv J_A - J_a \eta_a
\]  \hspace{1cm} (2.106)

it is again possible to complete the square in the angular momentum terms and get

\[
\mathcal{H} = \mathcal{H}_{\text{int}} + \frac{1}{2} \sum \frac{1}{A} J_a (J_a - I_A)^2
\]  \hspace{1cm} (2.107)

Now, since \( \oint \) commutes with the \( J_a \)'s, \( \eta_a \)'s, \( \chi_a \)'s and \( \mathcal{H} \),
it commutes with $H_{\text{int}}$ and the $I_A$'s and so only commutation with the $\hat{e}$'s is required to prove them intrinsic.

Starting with $H_{\text{int}}$ note that since $H_0 = H - \sum_A (\eta_A - J_A) J_A$ commutes with the $\hat{e}$'s, one has

$$\left[ H, \hat{e}_G \right] = \sum_A \left[ (\eta_A J_A - \frac{J_A}{2 J_A}), \hat{e}_G \right] = \sum_A \left[ H_A J_A + \frac{J_A}{2 J_A}, \hat{e}_G \right]$$

$$= \left( J_A \hat{e}_F - H_A \hat{e}_G \right) + \frac{J_A}{2 J_A} \hat{e}_F + \hat{e}_F \frac{J_A}{2 J_A} \hat{e}_e - \hat{e}_e \frac{J_A}{2 J_A} \hat{e}_F$$

$$= \frac{J_A}{2} (\eta_A \hat{e}_F + \hat{e}_F \eta_A - J_A \hat{e}_e - \hat{e}_e J_A)$$

Using equation (71) one also has

$$\sum_A \left[ J_A (\eta_A), \hat{e}_G \right] = \left( J_A \hat{e}_F + \hat{e}_F J_A - \hat{e}_e J_A - \hat{e}_e J_A \right)$$

and so by looking at equation (105), $H_{\text{int}}$ obviously commutes with $\hat{e}_G$ and is hence intrinsic. Finally, the $I_A$ are intrinsic because

$$I_A = J_A - \Delta_A \eta_A = J_A H_A$$

and both $J_A$ and $H_A$ are intrinsic.

Now that a Bohr-Mottelson type of Hamiltonian has been derived, there still exists one crucial question and that is how to interpret the $I_A$. In particular do they satisfy the proper space fixed angular momentum commutation rules.
\[ [I_A, I_B] = i I_C \]  

(2.111)

as ascribed to them in the unified model.

The answer to this question is that these rules hold approximately. To demonstrate this, first consider

\[ [I_A, Q_G] = [-J_A \eta_A + J_A \sum_{x_k} \epsilon_{x_k}, T_{x_k} \epsilon_{x_G}] \]  

(2.112)

\[ = -J_A \sum_{x_k} \epsilon_{x_G} [\eta_A, T_{x_k}] \epsilon_{x_G} \]

\[ = \frac{1}{2} J_A \sum_{r_k \neq s_k} (\epsilon_{x_G} \epsilon_{x_B} [T_{x_k}, \delta_{s_k}] T_{s_k} \delta_{r_k} + T_{s_k}, \delta_{r_k} + T_{r_k}, \delta_{s_k}) \epsilon_{x_G} \epsilon_{x_B} \]  

(1 \leftrightarrow C)

\[ = 0 \]

where some of the steps above depend on the facts \([J_A', Q_G] = 0\) since \(Q_G\) is intrinsic, and \(\sum_{x_k} \epsilon_{x_k} T_{x_k} \epsilon_{x_B} = 0\) for \(A \neq B\). With this commutation property, one has

\[ [I_A, I_B] = [J_A - J_A \eta_A, J_B - J_B \eta_B] = -J_A [\eta_A, J_B - J_B \eta_B] \]  

(2.113)

since \(J_A\) depends only on the \(Q_G\) 's. To reduce things further, note that equation (112) also shows that \([\eta_A', Q_G] = 0\) so that

\[ [I_A, I_B] = -J_A [\eta_A, J_B] + J_A J_B [\eta_A, \eta_B] \]  

(2.114)

Using the fact that \(H_A = \eta_A - J_A J_A \) is intrinsic, one finds
\[
[\eta_A, J_B] = \frac{1}{J_A} [J_A, J_B] = \frac{i}{J_A} J_C
\]  \hspace{1cm} (2.115)

Calculating the other commutator is a tedious task relegated to Appendix A with the result

\[
\eta_A \eta_B [\eta_A, \eta_B] = -i \left[ \frac{(q_A - q_B)(q_A - q_C)}{(q_A + q_B)(q_A + q_C)} L_C + \frac{2(q_A + q_B)q_C}{(q_A + q_B)(q_A + q_C)} \eta_C \right]
\]  \hspace{1cm} (2.116)

where \( L_C \) is the component of the total orbital angular momentum along \( \hat{e}_C \). It should be noted that this is the only place where the spin of the particles explicitly need be mentioned. In this context one has \( J_C = L_C + S_C \) and thus

\[
[\eta_A, \eta_B] = i J_C - i \left[ \frac{(q_A - q_B)(q_A - q_C)}{(q_A + q_B)(q_A + q_C)} (J_C - S_C) - i \frac{2(q_A + q_B)q_C}{(q_A + q_B)(q_A + q_C)} \eta_C \right]
\]  \hspace{1cm} (2.117)

\[
= i \frac{2(q_A + q_B)q_C}{(q_A + q_B)(q_A + q_C)} L_C + i \frac{(q_A - q_B)(q_A - q_C)}{(q_A + q_B)(q_A + q_C)} S_C
\]

Obviously the \( S_C \) are intrinsic, a result stemming from the fact that the \( \hat{e}'s \) here are independent of spin.

Now that the commutators of the intrinsic angular momenta have been found, it is possible to make some statements about the domain of applicability of the Bohr-Mottelson model. In order to bring (117) in accord with (111), two conditions seem necessary. First, the nuclear system must have a stable shape so that the \( Q_A \)'s may be replaced by their average values. Second, the deformation
of the nucleus should be small compared to the average radius. Then, writing

\[ Q_c = \langle Q_c \rangle \] (2.118)

\[ Q_A = \langle Q_A \rangle \equiv \langle Q_c \rangle + \Delta_{AC} \]

\[ Q_B = \langle Q_B \rangle \equiv \langle Q_c \rangle + \Delta_{BC} \]

one find that (116) gives

\[ [I_A, I_B] = i \frac{2\langle Q_c \rangle (2\langle Q_c \rangle + \Delta_{AC} + \Delta_{BC})}{(2\langle Q_c \rangle + \Delta_{AC})(2\langle Q_c \rangle + \Delta_{BC})} I_c + i \frac{\Delta_{AC} \Delta_{BC}}{2\langle Q_c \rangle + \Delta_{AC} + \Delta_{BC}} S_c \] (2.119)

\[ = i I_c + O(\Delta_{AC}; \Delta_{BC}) I_c + \ldots \]

which is the desired result. Note that the two conditions required to get (119) are indeed those assumed in the unified model.
III. EVALUATION OF MATRIX ELEMENTS AND INTRODUCTION OF REDUNDANT VARIABLES

A. Two-Dimension

Now that the Hamiltonian has been written in a form which explicitly exhibits the collective variables, there still exists the problem of finding the eigenvalues. In the two chapters following this one, various approximate diagonalization techniques will be introduced. However, before these can be carried out, one must find a way to evaluate matrix elements in a manner which does not destroy the benefits gained by performing the separation of variables. This means that the original integrations over all of the particle coordinates must be replaced by integrations over the collective and intrinsic sets. Since the intrinsic coordinates are not specified, it is obvious that some scheme be introduced to perform the intrinsic integrations which represents the intrinsic coordinates only implicitly. This can be accomplished by noting that the intrinsic degrees of freedom are equivalent to the degrees of freedom of all of the particles restricted to a surface of constant collective coordinate. Operationally, the identity

$$\int d\vec{r}_1 \cdots d\vec{r}_n \equiv \int d\vec{r}_1 \cdots d\vec{r}_n \int d\vec{\varphi} \int (\vec{\varphi} - \Psi(\vec{r}_1 \cdots \vec{r}_n))$$

(3.1)
can be used to exhibit this fact as will now be shown. To simplify the writing abbreviate the set \( \{ \vec{r}_1, \ldots, \vec{r}_A \} \) by \( r \) and the set of intrinsic coordinates by \( \eta \). Then consider functions of the form \( g_k(\varphi(r)) f_\eta(\eta(r)) \) and operators of the form \( A(\eta, \partial / \partial \eta, \ldots) B(\varphi, J) \), these being the types encountered in the present theory. Matrix elements can then be written

\[
\int dr \, g_k^*(\varphi(r)) f_\eta^*(\eta(r)) A B \, g_k(\varphi(r)) f_\eta(\eta(r)) =
\]

\[
\int d\varphi \, \int d\eta \, \delta(\varphi - \phi_k) g_k^*(\phi) f_\eta^*(\eta) A B \, g_k(\phi) f_\eta(\eta) =
\]

\[
\int d\varphi \, g_k^*(\phi) \bar{B} g_k(\phi) \int dr \, \delta(\varphi - \phi) f_\eta^*(\eta) A \, f_\eta(\eta)
\]

where \( \bar{B} \) is defined by

\[
B(\varphi, J) g_k(\phi) \Rightarrow \bar{B} g_k(\phi) = C(\phi) \tag{3.3}
\]

and the fact that the collective and intrinsic coordinates define independent spaces was used to perform the commutations necessary to put (2) in its final form.

The next step in putting the integrations in matrix elements in a convenient form comes from noting that \( A \) and the \( f \)'s are independent of the orientation of the coordinate system. In particular, if one considers the rotation
\[ r' = R_r r \]  

such that

\[ \Psi(r') = -\bar{\Psi} + \Psi(r) \]  

then

\[ A(\eta(r), \ldots) = A(\eta(r'), \ldots) \]  

and

\[ f(\eta(r)) = f(\eta(r')) \quad \text{for } n \text{ and } n'. \]  

Thus one has

\[ \int dr \, S(\bar{\Psi} - \Psi) f_n^*(\eta(r)) A(\eta(r), \ldots) f_{n'}(\eta(r)) = \]  

\[ \int dr' \, S(\bar{\Psi}(r')) f_n^*(\eta(r')) A(\eta(r'), \ldots) f_{n'}(\eta(r')) \]  

This gives the final form for matrix elements, dropping primes on the dummy integration variable \( r' \),

\[ \int dr \, g_k^* (\Psi) f_n^*(\eta) A B g_{k'} (\Psi) f_{n'} (\eta) = \]  

\[ \int d\bar{\Psi} \, g_k^*(\bar{\Psi}) B g_{k'} (\bar{\Psi}) \int dr \, S(\Psi) f_n^*(\eta) A f_{n'}(\eta) \]  

At this point, it should be noted that this is the first place where \( \Psi(r) \) appears explicitly. To be entirely correct, one must really face the problem mentioned in
Chapter II of defining \( \varphi \) properly, i.e. all of its branches. Obviously, this is a very difficult proposition if the number of particles of the system is larger than two. Fortunately, there is again a way to circumvent this problem. This comes from noting that the intrinsic integrations give the same answer regardless of the value of \( \tilde{\varphi} \). Thus, if one defines \( \varphi \) using a principal value, the results will be the same except for a normalization factor. This factor arises because the principal value is zero at points where \( \varphi \) is not so there is an over counting. However, since all of the matrix elements in the present treatment are to be divided by a normalization integral with the same over counting, it is clear that no mistake is made in using \( \varphi \) defined in this manner.

As a particular application of this technique consider matrix elements of the Hamiltonian from Chapter II,

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 J + \frac{1}{2} Q J^2
\]  

(3.10)

Since \([\mathcal{H}, J] = 0\), the eigenstates of \( \mathcal{H} \) can be taken in the form

\[
\psi_{n\kappa}(r) = \frac{1}{\sqrt{\mathcal{N}}} e^{i\kappa r} \phi_{n\kappa}(\eta)
\]  

(3.11)
and so equation (9) gives after simple algebra

$$\langle \psi_{n',k'} | H | \psi_{n,k} \rangle = \delta_{n,n'} \int d\eta \phi_{n,k}^\dagger (\eta) \phi_{n',k'} (\eta)$$

(3.12)

The problem of finding eigenstates of $H$ now reduces to diagonalizing the reduced matrix

$$\hat{H}_{n',n}^K = \int d\eta \phi_{n,k}^\dagger (\eta) \phi_{n',k} (H_0 + H \frac{1}{2} Q \kappa^2)$$

(3.13)

which means using some complete intrinsic set, $\{ \chi_n (\eta) \}$$$, and writing

$$\phi_{n,k} (\eta) = \sum m a_{n,m} \chi_m (\eta)$$

(3.14)

Then, the condition that $\hat{H}_{n',n}^K$ be diagonal is equivalent to finding the $a$'s such that

$$\sum_m a_{n,m}^* \int d\eta \chi_m^\dagger (\eta) (H_0 + H \frac{1}{2} Q \kappa^2) \chi_m \sum_m a_{n,m} = \delta_{n,n'}$$

(3.15)

This is, of course, how to solve the problem in principle; the real task is finding meaningful approximate diagonalizations.

To illustrate the above procedure for calculating matrix elements, consider the simple case of the rotation of two particles about their center of mass. In this case
there are just two degrees of freedom which can be taken as the \( x \) and \( y \) components of the vector giving the separation of the two particles. Then using the definition of \( \Psi \) which specifies the orientation of the principal quadrupole axes, one has

\[
\Psi = \frac{1}{2} \tan^{-1} \left( \frac{2xy}{x^2 - y^2} \right) = \tan^{-1} \left( \frac{y}{x} \right)
\]

(3.16)

Also, in this simple case, one can write down an intrinsic coordinate which is conventionally taken as

\[
\gamma = \sqrt{x^2 + y^2}
\]

(3.17)

Now consider for example matrix elements of the potential, \( V(r) \), with functions of the type given in (11).

\[
\frac{i}{2\pi} \int dxdy e^{-ik\Psi} \Phi_{n\kappa}^{(r)} \cdot V(r) e^{iK\Psi} \Phi_{n\kappa'}^{(r)} =
\]

(3.18)

\[
\frac{i}{2\pi} \int dxdy d\tilde{\Psi} \delta(\tilde{\Psi} - \Psi) e^{i(K-k)\Psi} \Phi_{n\kappa}^{(r)} \cdot V(r) \Phi_{n\kappa'}^{(r)} =
\]

\[
\frac{i}{2\pi} \int d\tilde{\Psi} e^{i(K-k)\tilde{\Psi}} \int dxdy d\tilde{\Psi} \delta(\tilde{\Psi} - \Psi) \Phi_{n\kappa}^{(r)} \cdot V(r) \Phi_{n\kappa'}^{(r)} =
\]

\[
\delta_{\kappa\kappa'} \int dxdy \delta(\tilde{\Psi} - \Psi) \Phi_{n\kappa}^{(r)} \cdot V(r) \Phi_{n\kappa'}^{(r)}
\]

Next define

\[
x' = x \cos \tilde{\Psi} + y \sin \tilde{\Psi}
\]

(3.19)

\[
y' = -x \sin \tilde{\Psi} + y \cos \tilde{\Psi}
\]

(3.20)
Then, of course

\[ r' = \sqrt{x'^2 + y'^2} = \sqrt{x^2 + y^2} = r \]  \hspace{1cm} (3.21)

while

\[ \Psi(x', y') = \tan^{-1}\left( \frac{y \cos \varphi - x \sin \varphi}{x \cos \varphi + y \sin \varphi} \right) \]

\[ = \tan^{-1}\left( \frac{x}{1 + \frac{y}{r} \tan \varphi} \right) = \Psi(x, y) - \varphi \]  \hspace{1cm} (3.22)

So, since the Jacobian of the above transformation is 1, one finds

\[ \frac{1}{2\pi} \int dx' dy' e^{-i k' \Psi} \phi_{nk}(r') V(r') e^{i k \Psi} \phi_{nk}(r) = \]  \hspace{1cm} (3.23)

\[ \delta_{kk'} \int dx' dy' S(\Psi(x', y')) \tilde{\phi}_{nk}(r') \phi_{nk}(r) \]

Finally, using the identity (in this case \( \Psi = 0 \) is easy to find)

\[ S(\Psi(x, y)) = \Theta(x) S(tan^{-1}(\frac{y}{x})) = \frac{\Theta(x) S(y)}{\left| \frac{\partial}{\partial y} tan^{-1}(\frac{y}{x}) \right|_{y=0}} = \Theta(x) S(y) \]  \hspace{1cm} (3.24)

where \( \Theta(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases} \), one has

\[ \int dx' dy' S(\Psi(x', y')) \tilde{\phi}_{nk}(r') \phi_{nk}(r) = \]  \hspace{1cm} (3.25)

\[ \int_0^\infty dx' \tilde{\phi}_{nk}(x') \phi_{nk}(x') \]

which is the trivial result gotten by just performing the transformation from \( x, y \) to \( r, \varphi \). In this case the
equivalence of

\[ \int d\xi d\eta d^2 \delta(\eta, \xi) \quad \text{and} \quad \int \phi(\eta, \xi) \delta'(\eta, \xi) \]

was explicitly shown but, of course, for the many body case where the intrinsic coordinates are not known this must remain an implicit relation.

B. **Three-Dimensions**

Extending this procedure to three dimensions is a straightforward task. Instead of using the \( \hat{z}'s \) of Chapter II, it will be convenient here to employ the Euler angles describing the orientation of the system and then put the results in a manifestly symmetric form as a final step. Again adopting the abbreviations \( \{x_1, \ldots, x_N\} \to r \) and \( \{\text{intrinsic coordinates}\} \to \eta \) as well as using \( \varpi \) for the Euler angles, one relies on the identity

\[
\int dr = \int dr \int d\varphi \int d\varpi \delta(r - \eta(n))
\]

\[
= \int dr \int d\omega d\varphi \int d\varpi \delta(\varpi - \omega) \delta(\varphi - r) \delta(\cos(\varphi - r) - 1)
\]

For the present purposes, an explicit form for the set \( \eta(n) \) is not required.

Matrix elements of operators of the form \( A(\eta, \eta^2, \ldots) \cdot B(\varpi, J) \) with functions \( \phi(n) D_k(\eta) \) now become in analogy with equation (2)
\[ \int dr' D^*(r') \overline{B} D_k(r') \int dr' \delta(\eta(r')) \phi^*_n(\eta) A \phi_n(\eta) \]  \quad (3.27)

Next, if one performs the transformation from \( r \) to \( r' \) defined by

\[
\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} (\cos \beta \cos \gamma - \sin \beta \sin \gamma \cos \phi) & (-\sin \beta \cos \gamma - \cos \beta \sin \gamma \cos \phi) & (\sin \gamma \sin \phi) \\ (\sin \beta \cos \gamma + \cos \beta \sin \gamma \cos \phi) & (-\cos \beta \cos \gamma + \sin \beta \sin \gamma \cos \phi) & (-\sin \gamma \sin \phi) \\ (-\cos \beta \sin \phi) & (\sin \beta \sin \phi) & (\cos \beta) \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad (3.28)
\]

which is just a rotation through the set of Euler angles, \( \gamma, \beta, \phi \), then

\[ \{ \mathbf{r}(r') \} = \{ \mathbf{r}(r) - \mathbf{r} \} \]

Thus, equation (27) becomes

\[ \int dr' D^*(r') \overline{B} D_k(r') \int dr' \delta(\eta(r')) \phi^*_n(\eta(r')) A \phi_n(\eta(r')) \]  \quad (3.29)

where the scalar properties of the \( \phi \)'s and \( A \) were used as before.

To achieve a more symmetrical form, note that equation (28) with \( \mathbf{r} \) replaced by \( \mathbf{r}(r) \) defines a transformation between the lab system, \( r \), and the body fixed system, \( r' \). If one now uses the specific choice of angle introduced in Chapter II, the one defining the principal quadrupole...
axes, then the following relation holds
\[
\mathcal{S}(\eta(n)) = \left| \frac{\partial(\Sigma x, \Sigma y, \Sigma z)}{\partial (\eta)} \right|_{n=0} \delta(\Sigma x) \delta(\Sigma y) \delta(\Sigma z) \tag{3.30}
\]
i.e. \(\eta = 0\) means that the principal axes coincide with
the lab axes. The calculation of the Jacobian involves
only tedious algebra which will be bypassed as it contains
no important results. Upon setting \(\eta = 0\) in all non-
singular terms and terms not cancelling singularities one
finds
\[
\left| \frac{\partial(\Sigma x, \Sigma y, \Sigma z)}{\partial (\eta)} \right|_{n=0} = \left| \begin{array}{ccc}
(q_1-a_1) & 0 & (a_1-a_2)(a_2-a_3) \\
0 & (a_1-a_3) & (a_3-a_2)(a_2-a_3) \\
(a_1-a_2) & (a_2-a_3) & 0
\end{array} \right| \left. \right|_{\eta \to 0} \tag{3.31}
\]
\[
= |(a_1-a_2)(a_1-a_3)(a_2-a_3)-(a_1-a_3)(a_1-a_2)(a_2-a_3)|
\]
\[
= |(a_1-a_2)(a_1-a_3)(a_2-a_3)|
\]
where the \(Q\)'s are the principal quadrupole moments as
defined in Chapter II by
\[
Q_k = \sum_{j=1}^{A} \nu_j^k \tag{3.32}
\]
Thus one has
\[
\mathcal{S}(\eta(n)) = |(a_1-a_2)(a_1-a_3)(a_2-a_3)| \delta(\Sigma x) \delta(\Sigma y) \delta(\Sigma z) \tag{3.33}
\]
\[
= |(\Sigma x^4, \Sigma y^4, \Sigma z^4)(\Sigma y^4, \Sigma z^4)| \delta(\Sigma x) \delta(\Sigma y) \delta(\Sigma z)
\]
\[
= \delta(\frac{\Sigma x}{y^2}) \delta(\frac{\Sigma x}{y^2}) \delta(\frac{\Sigma y}{z^2}) \tag{3.33}
\]
where the last step follows from the fact that the $\mathcal{S}$-functions allow the replacement of $r'_k$ by $r_k$ and the identity $\mathcal{S}(a\chi) = \frac{1}{|a|} \mathcal{S}(\chi)$ was used. With this result and dropping primes and tildas one has the final symmetric form for matrix elements of

$$\int d\eta \mathcal{D}^*_{n}(\eta) \mathcal{B}_c(\eta) \int dr \mathcal{S}(\frac{r+x}{|x|}) \cdots \mathcal{D}^*_{n}(\eta) A \mathcal{\phi}^*_n(\eta)$$

(3.34)

For the sake of simplicity, the less symmetric $\mathcal{S}(\eta)$ will be used in all subsequent developments, but equation (33) should be kept in mind when an actual calculation is to be made.

Now one can calculate matrix elements of the Hamiltonian decomposed via Tomonaga's method. Since $[H, J] = 0$, the eigenfunctions of $H$ take on the general form

$$\Psi_n(r) = \sum_{j=1}^{J} \mathcal{D}^*_m(r) \phi^*_n(\eta)$$

(3.35)

where the $\mathcal{D}^*_m(r)$ are the usual Wigner D-functions as used in the Introduction in describing the Bohr-Mottelson model. Employing the notation

$$[J_K | J_A | J' K'] = \int d\eta \mathcal{D}^*_m J_A \mathcal{D}^*_m'$$

(3.36)

and

$$\langle J_n k | A | J'_n k' \rangle = \int dr \mathcal{S}(\eta) \phi^*_n A \phi^*_{n'}$$

(3.37)
and using the decomposed form of the Hamiltonian of equation (2.78)

$$H = H_0 + \sum_A H_A J_A + \frac{1}{2} \sum_A \frac{J_A^2}{J_A}$$  

(3.38)

one sees that the eigenvalue problem

$$H \psi_{nJm} = E_{nJ} \psi_{nJm}$$  

(3.39)

is equivalent to the matrix statement

$$H_{nn'}^{T} = \sum_{kk'} \langle n k | H_0 | k n' \rangle + \sum_A \langle h_A [J_{kk'} J_{kk'}] + \frac{J_{kk'}}{2 J_A} [J_{kk'} J_{kk'}^T + J_{kk'}^T J_{kk'}] | n k' \rangle \delta_{kk'}$$  

(3.40)

$$\equiv \sum_{kk'} \langle n k | H_{kk'}^T | n k' \rangle \delta_{kk'} = E_{nJ} \delta_{nn'}$$

where the obvious abbreviation has been made. In this case one must determine the coefficients of the expansion in a complete set, \( \chi_m(\eta) \)

$$\phi_{nK}^T(\eta) = \sum_m a_{nk,m} \chi_m(\eta)$$  

(3.41)

such that

$$\sum_{kk'} \sum_{mm'} a_{nk,m}^* \langle n k | s(\eta) \chi_m^* H_{kk'}^T \chi_{m'} | m' \rangle a_{nk',m} = E_{nJ} \delta_{nn'}.$$  

(3.42)

Finding approximate solutions to this still exact problem will be the main concern of much of the remainder of this thesis.

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C. **Introduction of Redundant Variables**

Since it is nearly impossible to find intrinsic variables for the general nuclear rotation problem, it is obvious that finding a complete set of intrinsic functions, \( \{ \phi(\eta) \} \), is also an impractical feat. Thus the necessity of producing an alternative formulation of the energy eigenvalue problem in a way which sidesteps the explicit use of such a set of functions is clear. This can be accomplished by the introduction of redundant variables, the 6A coordinates and momenta of the nucleons, instead of the 6A-6 intrinsic variables (for two dimensions it is a replacement of 4A-2 variables by 4A).

As usual, the two-dimensional case will be treated first to indicate simply the logic involved. Considering equation (15), note that instead of using the basis \( \chi_n(\eta) \) to diagonalize the reduced Hamiltonian one could just as well have used the set \( \{ \tilde{\chi}_n(\eta) = \chi_n(\eta) + f_n(\eta, \varphi) \} \) where the \( f \)'s are arbitrary nice functions satisfying \( f(\eta,0)=0 \). The \( \mathcal{S}(\varphi) \) insures that one gets the same results. Conversely, can use any set of functions, \( \{ \tilde{\Phi}_m(\eta) \} \), as long as they reduce to a complete set of intrinsic functions when \( \varphi = 0 \). One way to achieve this is to let \( \{ \tilde{\Phi}_m(\eta) \} \) be a complete set in \( \eta \) space. Then, as will be shown
below, \( \{ \hat{\phi}_m(r) |_{\eta=0} \} \) can be used to expand any intrinsic function. However, this set suffers from the defects of being overly complete and non-orthogonal in \( \eta \) space, both of which are only technical problems. The proof of completeness is as follows: rewrite \( \hat{\phi}_m(r) \) as

\[
\hat{\phi}_m(r) = \psi_m(\eta) + g_m(\varphi, \eta) 
\]

(3.43)

where

\[
\psi_m(\eta) = \frac{\hat{\phi}_m}{|_{\eta=0}}
\]

(3.44)

and

\[
g_m(\varphi, \eta) = \phi_m(r) - \psi_m(\eta)
\]

(3.45)

Obviously \( g_m(0, \eta) = 0 \) as desired. Now since \( \{ \hat{\phi}_m(r) \} \) is complete in \( r \) space, any function of the intrinsic coordinates, say \( t(\eta(r)) \), can be expanded in terms of it. Thus

\[
t(\eta(r)) = \sum_m a_m \hat{\phi}_m(r) = \sum_m a_m \psi_m(\eta) + \sum_m a_m g_m(\varphi, \eta)
\]

(3.46)

But since \( t(\eta) \) is independent of \( \varphi \), one must have the last term equal to zero and so

\[
t(\eta) = \sum_m a_m \psi_m(\eta)
\]

(3.47)
Hence, any intrinsic function may be expanded in terms of 
\[ \{ \psi_m(\eta) \} \]. Unfortunately, this is an over complete set 
in the sense that there is more than one set of expansion 
coefficients for the same \( t(\eta) \). To see this note that 
for any \( P(\varphi) \) one may write

\[ P(\varphi) t(\eta) = \sum_m b_m \phi_m(\varphi) = \sum_m b_m \psi_m(\eta) + \sum_m b_m q_m(\varphi, \eta) \quad (3.48) \]

where in general \( \{ a_m \} \neq \{ b_m \} \). Considering those 
functions, \( P \), such that \( P(0)=1 \), one sees that 

\[ t(\eta) = \sum_m b_m \psi_m(\eta) \quad (3.49) \]

so that \( \{ b_m \} \) also gives \( t(\eta) \).

A simple example will prove useful at this point.

Consider the redundant Fourier expansion on the interval 
\((0, 2\pi)\) of functions of the form \( f(x-y), \{ x, y \} \) being 
a redundant set here. Then

\[ f(x-y) = \sum_{k\in \mathbb{Z}} a_{k \xi} e^{i(kx+y)} = \sum_{k \in \mathbb{Z}} a_{k \xi} e^{i(kx+y)} e^{i(kx+y)\frac{\xi}{2}} \quad (3.50) \]

\[ = \sum_{k \in \mathbb{Z}} a_{k \xi} e^{i(kx+y)\frac{\xi}{2}} + \sum_{k \in \mathbb{Z}} a_{k \xi} (e^{i(kx+y)} - e^{i(kx+y)\frac{\xi}{2}}) \]

where \( R = \frac{x+y}{2} \) and \( r = x-y \). Now since \( \partial f / \partial R = 0 \) for 
all \( x, y \) one sees that
\[ \sum_{k \neq k_L} (k + q) a_k e^{i(k + q) R} e^{i(k - q)/2} = 0 \] (3.51)

or as is well known

\[ a_{k_L} = \alpha_{k_L} \delta_{k+L} \] (3.52)

This shows that

\[ \sum_{k \neq k_L} (e^{i(dx+L)} - e^{i(k - q)/2}) = 0 \] (3.53)

as desired, and thus that \( \{ e^{i(kx + Ly)} \}_{R=0} \) can be used to expand any function of \( x-y \). To show over completeness, note that for example for any integer \( N \),

\[ e^{iN}\nu(x,y) = \sum_{k \neq k_L} a_{k-n} e^{i(k - q)/2} + \sum_{k \neq k_L} a_{k+n} (e^{i(dx+Ly)} - e^{i(k - q)/2}) \] (3.54)

so that setting \( R=0 \) one sees that \( \{ b_k \} = \{ a_{k-n}, a_{k+n} \} \) also gives \( f(x-y) \).

In review, then, to make the problem of diagonalizing the reduced Hamiltonian tractable, one introduces a complete set of functions defined in terms of redundant variables. The \( \delta(\psi) \) in the integration assures one that this redundancy will be removed. Only one problem remains, the fact one must use an over complete set, but this is the price one must pay.
As a final step in putting the redundant variable technique in a workable form, note that \((H_0+H_1K^2+\frac{1}{2}QK^2, \varphi) = 0\). Thus, after the basis \(\hat{\Phi}_m(r)\) has been introduced, one need only simultaneously diagonalize the matrices

\[
\hat{H}^K_{nn'} = \int dr \; \hat{\varphi}^*_n(r)(H_0+H_1K^2+\frac{1}{2}QK^2)\hat{\varphi}_{n'}(r)
\]

and

\[
\hat{N}_{nn'} = \int dr \; \hat{\varphi}^*_n(r) \delta(\varphi_n(r)) \hat{\varphi}_{n'}(r)
\]

(3.55)

In principle, diagonalizing the \(N\) matrix acts as a subsidiary condition designed to correct for using redundant variables. However, since \(H_0+H_1K^2+\frac{1}{2}QK^2\) is invariant under transformations generated by \(\varphi\) and \(J\), it is clear that the effect of redundancy is to merely make the eigenvalues of \(\hat{H}^K_{nn'}\) highly degenerate. That is, for any eigenfunction of \(H_0+H_1K^2+\frac{1}{2}QK^2\), one may generate another with the same eigenvalue by just rotating by an arbitrary angle. Simultaneously diagonalizing \(N\) and keeping only functions with a particular eigenvalue eliminates this degeneracy. Clearly, one may ignore this process if only energy eigenvalues are desired and an exact diagonalization could be achieved. If one only does an approximate calculation, then of course the eigenvalues of \(\hat{H}^K_{nn'}\) will in general become non-degenerate and the
N matrix should be used to eliminate spurious energy levels. Unfortunately, the eigenvalues of N are only 0 and $\infty$ and thus any approximate diagonalization of it would have no meaning. This is because an approximate treatment of N would usually give finite eigenvalues and thus require an infinite number of off diagonal elements to raise its value to infinity. Consequently, it will be assumed in this thesis that the diagonalization of $H^K_{nn'}$ is sufficiently accurate that spurious levels are not a serious problem. Also, as will be argued in the next chapter, the property of low lying deformed H-F states used in the approximate diagonalization to be localized near $\varphi \approx 0$ will actually enforce, to a certain extent, the condition specified by diagonalizing N.

To complete the introduction of redundant variables, one still must consider the three-dimensional case which is just a trivial extension of the previous development. Again, because of the $\delta$-function constraint in the matrix elements in equation (42), one may extend the basis functions, $\chi_m(\eta)$, to the 3A dimensional redundant space and then as above use a complete set $\hat{\phi}_m(r)$ instead. No new complications have been added by going to three dimensions. By virtue of the fact that $[H^J_{KK'}, \delta(\eta')] = 0$, 

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one may also put this problem in the form of a simultaneous diagonalization on the following matrices

\[ H_{kk',nn'}^{J} \equiv \int dr \, \hat{\phi}_{n}^{*}(r) \, H_{kk'}^{J} \, \hat{\phi}_{n}(r) \]  \hspace{1cm} (3.57)

and

\[ N_{nn'} \equiv \int dr \, \hat{\phi}_{n}^{*}(r) \, \mathcal{S}(\mathcal{N}(r)) \, \hat{\phi}_{n}(r) \]  \hspace{1cm} (3.58)

As before, the \( N \) matrix acts as a projection operator and is still a singular matrix.

In closing this section, it should be mentioned that all of the developments in it are actually too formal to be of any real interest in a practical solution of the nuclear rotation problem. However, with suitable approximations introduced along the line, one can develop a meaningful program of solution which hopefully will give sufficiently accurate results. At some points what might seem as unsuitable approximations will also be made with the only justification that they allow one to proceed.
A. **Introduction**

As a prelude to using a redundant basis of Hartree-Fock (H.F.) states, one may attempt to solve the problem of the non-rotational motion with a suitable set of intrinsic functions. This method has the advantage that intrinsic part of the eigenfunctions resulting from approximate diagonalization of the Hamiltonian resemble more closely the "true" intrinsic states. A particular circumstance where this property is desirable will be found in a later chapter where the symmetries of the wavefunctions are investigated. It is clear that to do this efficiently requires maximum knowledge of at least the approximate properties of the intrinsic functions. Another place where this type of state becomes useful is for axially symmetric nuclei. As will be seen in the next chapter, in order to solve the rotational problem for this case, one must use basis functions which are eigenstates of the component of the intrinsic angular momentum along the symmetry axis.

To find a set of intrinsic functions, one merely need look back to Chapter III where the redundant basis functions were first introduced. There it was shown that starting with a complete set of functions in \( r \) space, \( \{ \overline{\Phi}_n(r) \} \),
one may construct an overcomplete set in the intrinsic space via the prescription

$$\Psi_n(\eta) \equiv \hat{\Phi}_n(r) \bigg|_{\alpha, \epsilon = 0} \quad (4.1)$$

The overcompleteness of the $\psi$'s is only a slight disadvantage, one would like just a complete set. This is overshadowed by the relative ease by which the intrinsic states are constructed.

In this chapter, these functions will be formed from the H.F. states used in the redundant variables treatment of the problem. For deformed nuclei, the H.F. states depended strongly on the angles and were not eigenstates of the total angular momentum. After performing the above construction, which is actually a projection of $r$ space onto $\eta$ space, the $\psi$'s of course no longer are angle dependent. Also, they become eigenstates of all components of angular momentum with eigenvalue zero, or more commonly, the $\psi$'s represent a set of scalar functions.

As illustrations, the construction will be applied to the two-dimensional and three-dimensional axially symmetric cases. Also, for completeness a brief discussion of the use of these functions directly in the energy eigenvalue problem is given. Because of the extra work required to
perform the scalar projection, this does not represent a very practical method of solution. However, in the next chapters, it will be seen that using scalar functions as an intermediate step to allow definitions of eigenstates for certain intrinsic operators is extremely convenient. In fact, it is for this reason that scalar functions are even considered.

B. **Two Dimensions**

For the two-dimensional example, use the angle specifying the orientation of the quadrupole principal axes as usual. With this choice, the explicit form of the decomposed Hamiltonian as derived in Chapter II can be used. In particular, and this is important for some of the proofs, the intrinsic angular momentum is expressible in terms of known quantities.

To begin with, suppose that $\phi_0(r)$ is the Hartree-Fock (H.F.) ground state for H, some Hamiltonian, i.e.

$$\hat{\mathbf{S}} \langle \phi_0 | H | \phi_0 \rangle = 0$$  \hspace{1cm} (4.2)

for all one particle variations (see beginning of next chapter for more details), and let $\phi_n >_0 (r)$ be the remaining elements of the complete H.F. basis, i.e. one particle, two particle, ... excitations of $\phi_0$. Then, one may
construct the scalar functions, $\psi_n(\eta)$, by evaluating the $\phi$'s at $\varphi(r)=0$. This is done, of course, by replacing each $r_j$ by its "rotated" value.

$$\begin{bmatrix} \bar{X}_j \\ \bar{Y}_j \end{bmatrix} = \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix} \begin{bmatrix} X_j \\ Y_j \end{bmatrix}$$

(4.3)

for all A j's. It should be noted that this is not a unitary transformation since $\varphi$ is not an external angle but is instead determined by all of the r's. In fact, it is this property which gives the projection onto $\eta$ space. The $\bar{Y}$ coordinates thus may be expressed entirely in terms of the $\eta$'s or equivalently represent a set of intrinsic operators. To see this note that they commute with $\varphi$ since they depend only on $\varphi$ and the r's. If they also commute with J, then, their intrinsic nature will be established. So looking at

$$\begin{bmatrix} \bar{X}_j \\ \bar{Y}_j \end{bmatrix} J = \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix} \begin{bmatrix} X_j \\ Y_j \end{bmatrix} + \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix} \begin{bmatrix} X_j \\ Y_j \end{bmatrix}$$

(4.4)

$$= i \begin{bmatrix} -\sin \varphi & \cos \varphi \\ -\cos \varphi & -\sin \varphi \end{bmatrix} \begin{bmatrix} X_j \\ Y_j \end{bmatrix} + i \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix} \begin{bmatrix} X_j \\ Y_j \end{bmatrix}$$

$$= i \left\{ \begin{bmatrix} -X_j \sin \varphi + Y_j \cos \varphi \\ -X_j \cos \varphi - Y_j \sin \varphi \end{bmatrix} + \begin{bmatrix} -Y_j \cos \varphi + X_j \sin \varphi \\ Y_j \sin \varphi + X_j \cos \varphi \end{bmatrix} \right\}$$

$$= 0$$
one sees that the $\Phi$ are intrinsic. A particular consequence of this property is the fact that $\phi_n(\hat{r})$ is manifestly a scalar.

Before discussing the application of these functions to diagonalization of $H$, consider the case where the H.F. states are eigenstates of $J_z$, i.e.

$$J \phi_n(r) = K_n \phi_n(r)$$  \hspace{1cm} (4.5)

This situation, of course, precludes the existence of rotational states since there is no deformation. It is presented here in relation to the axially symmetric three dimensional system where such a state appears. The pertinent question to be answered is what the intrinsic angular momentum gives when applied to $\phi_n(\hat{r})$. Since these are scalars one has

$$I \phi_n(\hat{r}) = (J - \frac{\dot{\phi}}{\phi}) \phi_n(\hat{r}) = -\frac{1}{\phi} \frac{\dot{\phi}}{\phi} \phi_n(\hat{r})$$  \hspace{1cm} (4.6)

Now associated with no deformation is the fact that $\frac{1}{Q} \to 0$ upon neglect of fluctuations of the quadrupole moments about their average values. This would indicate that equation (6) gives zero except for the fact that $\dot{\phi}$ operating on the scalar function gives a singularity of order $Q$. To exhibit this, remember that the H.F. states are antisymmetrized products of the form $\prod_{\alpha=1}^{A} f_{\alpha}(\hat{r})$ and when
J is conserved, the $f$'s take on the structure (ignoring spin and iso-spin)

$$f_\alpha(\vec{r}_\alpha) = g_\alpha(|\vec{r}_\alpha|)(x_\alpha + i\gamma_\alpha)^{\alpha}(x_\alpha - i\gamma_\alpha)^{\alpha}$$

(4.7)

This latter fact comes from the property that conservation of $J = \sum_\alpha \vec{j}_\alpha$ in the H.F. picture means that the single particle potential is radially symmetric and thus that the single particle levels are eigenstates of $\vec{j}_\alpha$. In the present case, one has

$$\vec{f}_\alpha^*(\vec{r}_\alpha) = (m_\alpha - n_\alpha) f_\alpha(\vec{r}_\alpha)$$

(4.8)

and clearly

$$\sum_{\alpha} (m_\alpha - n_\alpha) = K_n$$

(4.9)

Then since, $(\vec{x}_\alpha \pm i\vec{y}_\alpha)^m = e^{i(m \cdot \vec{y}_\alpha)}(x_\alpha \pm i\gamma_\alpha)$ and $|\vec{r}_\alpha| = |\vec{r}_\alpha|$

one sees that

$$f_\alpha(\vec{r}_\alpha) = e^{i(m_\alpha - n_\alpha) \vec{y}_\alpha} (x_\alpha + i\gamma_\alpha)^{\alpha}(x_\alpha - i\gamma_\alpha)^{\alpha}$$

(4.10)

so that

$$\hat{\phi}_n(\vec{r}) = e^{-izK_n \vec{y}_\alpha} \phi_n(r)$$

(4.11)

Now, first of all note that since $i[\hat{\phi}, \gamma] = 0$ one has

$$-\frac{\partial}{\partial r} \phi_n(\vec{r}) = -[\frac{\partial}{\partial r}, e^{-izK_n \vec{y}_\alpha}] \phi_n(r) - e^{-izK_n \vec{y}_\alpha} (\frac{\partial}{\partial r} \phi_n(r))$$

(4.12)

$$= k_n \phi_n(\vec{r}) - e^{-izK_n \vec{y}_\alpha} (\frac{\partial}{\partial r} \phi_n(r))$$

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If \( \hat{\psi} \phi_n(r) \) does not give any singularity of order \( Q \), then
\[
\frac{1}{Q} \to 0
\]
will give the result
\[
\int \phi_n(\vec{r}) = K_n \phi_n(\vec{r})
\] (4.13)

To show that this is true, look at
\[
\hat{\psi} \phi_n(\vec{r}) = \frac{1}{m(\Sigma x^2 - y^4)(1 + \tan^2 \psi)} \left\{ \Sigma (x \rho_y + y \rho_x) - \tan \gamma \rho \right\} f_\alpha(\vec{r})
\] (4.14)

Since
\[
\frac{1}{Q} = \frac{m(\Sigma x^2 - y^4)(1 + \tan^2 \psi)}{\Sigma x^2 + y^4}
\]

it is clear that the bracket factor in equation (14) must not give a \frac{1}{(\Sigma x^2 - y^4)}
type contribution if the desired result is to prevail. An exception to this is the \( \tan 2\psi \) factor because not only is \( (\Sigma x^2 - y^4) \) zero on the average but also \( \Sigma xy \). Thus
\[
\tan 2\psi = \frac{\Sigma xy}{\Sigma x^2 - y^4}
\]
is given on the average by the ratio of the fluctuations of these two quantities and so is roughly one since
\[
\langle (\Sigma xy)^2 \rangle = \langle e^{\Sigma J} (\Sigma xy)^2 e^{-\Sigma J} \rangle = \frac{1}{\frac{1}{2}} \langle (\Sigma x^2 - y^4)^2 \rangle
\] (4.15)

using the fact that the states are eigenfunctions of \( J \).

With these conditions in mind, consider the bracket contribution in more detail. When acting on the \( q_\alpha(\vec{F}_\alpha) \)
part of \( f_\alpha \), one gets

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\[ q_\alpha (r_\alpha) = \frac{1}{r_\alpha^2 \sin^2 \theta} \left[ \cdots \right] \]

\[ = -i \frac{2}{r_\alpha^2} \frac{d}{dr_\alpha} \left[ 2x_\alpha y_\alpha = (x^2 - y^2) \tan 2\varphi \right] \]

The g's do not vary wildly in general so that this term will give no trouble. This is even enhanced when summed over \( \alpha \) as is done when one considers the products of \( f \)'s appearing in \( \phi \). The reason is, of course, because apart from the leading factors, the bracket in equation (16) sums to zero.

To complete the present analysis, consider the bracket of equation (14) acting on the factors of the form \((x_\alpha + iy_\alpha)^n\) in \( f_\alpha \).

\[ \left[ \cdots \right] (x_\alpha \pm iy_\alpha)^n = -i n \left[ (x_\alpha + iy_\alpha)^{-1} \right] \left( x_\alpha \pm iy_\alpha \right)^{n-1} \]

\[ = n \left( x_\alpha \pm iy_\alpha \right)^{n-1} \left( x_\alpha \pm iy_\alpha \right) \]

Thus, when acting on one of the products making up \( \phi \), the above bracket gives

\[ \left[ \cdots \right] \int_{x_\alpha} f_\alpha (r_\alpha) = \sum_{\beta=1}^A \left\{ (m_\beta \left[ x_\alpha^2 + \frac{y_\alpha^2}{x_\alpha} \right]) (x_\alpha \pm iy_\alpha) \right\} \]

\[ + (n_\beta \left[ x_\alpha \pm iy_\alpha \right]) (x_\alpha \pm iy_\alpha - 1) \]
Clearly, except for some freakish pathology, there is no way for the above terms to correlate to give a \( \frac{1}{(\Sigma x^2 - y^2)} \) factor.

Collecting all of the above results, one finds that

\[
\frac{i}{\hbar} \phi_n(r) \sim (\Sigma x^2 - y^2) \left[ \right] \phi_n(r) \tag{4.19}
\]

where the bracket factor contains no divergent terms. Thus, applying the approximation of replacing the quadrupole moments by their expectation values, which means setting \( \Sigma x^2 = \Sigma y^2 \), one finds that the second term in equation (12) vanishes. This result verifies the statement that the intrinsic angular momentum on the scalar functions has the same eigenvalue as the regular angular momentum on the original H.F. functions.

When one uses the scalar functions only for symmetries and to get eigenstates of the intrinsic angular momentum, the above fact may be used to define a convenient operating procedure. This consists of using the scalar functions for the desired purposes and then extending them to the redundant space by using the \( \delta \)-function. In practice, this is the only place where the use of scalar functions represents a definite advantage because as will be seen below, direct use of them for diagonalization is an impractical situation. However, for the present procedure, they are
used merely as a formal intermediate step to derive a prescription whereby the action of intrinsic angular momenta on scalars can be associated with the action of the real angular momenta on redundant H.F. functions. Then when the $\mathcal{J}$-function is used to allow expansion to redundant variables, the intrinsic angular momentum operator is replaced by the corresponding real angular momentum operator. This procedure will be used extensively in the next chapters.

Apart from using scalar functions for the previously-mentioned purposes, there is also open the possibility of using them in the diagonalization program. This gives rise to certain technical problems associated with the fact that even though $\phi_n(\vec{r})$ is a determinant, it is not a true H.F. state. The reason is, of course, since the $\vec{r}$ are not all independent, one does not have a determinant of independent particle states. As a consequence of this, Thouless theorem is inapplicable and the usual methods of the last chapter do not work. To rectify the situation two alternatives are open. First of all, one may keep the $\mathcal{J}$-function in the integrations in which case the matrix elements for the redundant and scalar functions are identical, i.e.
\[ \int dr \delta(r) \phi_n^*(r) H^K \phi_n(r) = \int dr \delta(\vec{r}) \phi_n^*(\vec{r}) H^K \phi_n(\vec{r}) \] (4.20)

It is clear that since the matrix elements are the same, approximate diagonalizations will yield identical results and thus nothing is gained doing things this way.

The alternate procedure is to drop the \( \delta \)-function. When scalar functions are used, this results in nothing more than a normalization change since \( H^K \) is intrinsic and thus integrating overall variables or just the intrinsic ones differs by only a factor of 2\( \pi \). At this point, the equality of matrix elements of equation (20) is lost. Consequently, even though \( \phi_0(r) \) is a H.F. state of \( H \), which means \( H \) does not connect it with any one particle states, the scalar function, \( \phi_0(\vec{r}) \), no longer has this property. Thus, one must start fresh by taking trial functions of the form

\[ \psi_{\text{trial}}(\vec{r}) = \phi_0(\vec{r}) + \sum_n C_n \phi_n(\vec{r}) \] (4.21)

with the \( n \)‘s some set of one particle states, and determine the \( C_n \)‘s variationally. Except for the extra computation required to make the transformation \( r \rightarrow \vec{r} \), this is a feasible procedure. However, it is doubtful whether any inaccuracy will result to justify the additional work. It is up to a more detailed numerical analysis, though, to determine if this conjecture is true.
C. Three Dimensions

Extension of the present technique of constructing scalar functions to three dimensions adds nothing but algebraic complications. The existence of these functions, though, is essential for axial symmetry so that it will be worthwhile to consider their construction in some detail. Assuming one has the H.F. ground state for the Hamiltonian, \( H \), say \( \phi_{0K}(r) \), and that this state is an eigenfunction of \( J \) with eigenvalue \( K \), the construction prescription requires the replacement

\[
\vec{p}_A^{(j)} = \sum_B R_{AB}^{(a)} \vec{r}_B^{(j)}
\]

(4.22)

where \( R_{AB} \) is the rotation matrix of Chapter III. It will be shown that the intrinsic angular momenta, \( \vec{I}_A \), operating on \( \phi_{0K}(\vec{r}) \) are approximately isomorphic to \( J_x, J_y, J_z \) operating on \( \phi_{0K}(r) \), a very desirable property.

Since the Euler angle specification is inconvenient, it will be more efficient to use the equivalent transformation

\[
\vec{r}_A^{(j)} = \vec{e}_A \cdot \vec{r}^{(j)} = \sum_k \epsilon_{kA} V_k^{(j)}
\]

(4.23)

The \( \epsilon_{kA} \) are actually the same as the \( R_{AB} \) and have well defined commutation relations with the \( J \)'s. In particular,
one has from Chapter II

\[
\left[ J_j, \varepsilon_{kA} \right] = i \epsilon_{jA} \tag{4.24}
\]

which leads immediately to

\[
\left[ J_i, \hat{r}_A \right] = \sum_n \left[ J_i, \varepsilon_{nA} r_n \right] \tag{4.25}
\]

\[
= \sum_n (i \varepsilon_{nA} r_{i+n} + i \varepsilon_{i+nA} r_n) = 0
\]

To get the final step, change the summation index in the second term to \( \hat{n}' = \hat{i} \times \hat{n} \) and use the identity \( \hat{n} = -\hat{i} \times (\hat{i} \times \hat{n}) \). Thus, the \( \Psi_A \) are indeed intrinsic and so \( \Phi_{0K}(\vec{r}) \) is a true scalar i.e. \( \tilde{J} \Phi_{0K}(\vec{r}) = 0 \).

Now, to demonstrate that \( I_3 \) on the scalar function gives \( K \), note that the single particle states of \( \phi_{0K}(r) \) assume the form

\[
f_n(\vec{r}) = \sum_{\bar{J}} C_{\bar{J}} \varphi_{Jn}(\vec{r}) \tag{4.26}
\]

For the scalar function, remember that the spherical harmonics transform under rotations according to

\[
\varphi_{Jn}(\vec{r}) = \sum_m \mathcal{O}_{mn}^{\bar{J}}(\eta(r)) \varphi_{Jm}(\vec{r}) \tag{4.27}
\]

so that

\[
f_n(\vec{r}) = \sum_{\bar{J}} C_{\bar{J}} \mathcal{O}_{mn}^{\bar{J}}(\vec{r}) \varphi_{Jm}(\vec{r}) \tag{4.28}
\]
These functions, of course, go into the determinant
making \( \phi_{0K}(\vec{r}) \) so that as before one considers products
of the form \( \prod_{\alpha=1}^{A} f_{n_{\alpha}}(\vec{r}_{\alpha}) \), where \( \sum_{\alpha=1}^{A} n_{\alpha} = K \). Thus, 
onumber
one must consider this structure when analyzing

\[
I_3 \phi_{0K}(\vec{r}) = -I_3 \eta_3 \phi_{0K}(\vec{r})
\]  

(4.29)

As with two dimensions, one must address the problem of
determining what portion of \( \eta_3 \phi_{0K}(\vec{r}) \) diverges like \( \frac{1}{\sqrt{3}} \) as \( \sqrt{3} \to 0 \).

First of all consider the \( \mathcal{D} \)-function part of \( f_n \)
coming from the rotation of the spherical harmonics. Since

\[
I_3 \mathcal{O}_{m_k}^{\tau}(n) = -\left( I_3 \mathcal{O}_{m_k}^{\tau}\right)^* \]

\[
= -\left( I_3 \mathcal{O}_{m_k}^{\tau}\right)^* = -K \mathcal{O}_{m_k}^{\tau}(n)
\]

(4.30)

and since \( I_3 \) is intrinsic, one finds

\[
\eta_3 \mathcal{O}_{m_k}^{\tau}(n) = \frac{1}{I_3} (I_3 - I_3) \mathcal{O}_{m_k}^{\tau}
\]

\[
= -\frac{1}{I_3} K \mathcal{O}_{m_k}^{\tau}
\]

(4.31)

Thus, one gets a contribution from the \( \mathcal{D} \)-functions in
the product of \( f_n \)'s equal to \( \sum_{\alpha=1}^{A} n_{\alpha} = K \) as expected, so 
that

\[
I_3 \phi_{0K}(\vec{r}) = K \phi_{0K}(\vec{r}) - \sqrt{3} \eta_3 \phi_{0K}(\vec{r})
\]

\[\text{\text{I}_{\text{non-D-function}}^*}\]

(4.32)
The second term must be investigated for \( \frac{1}{\bar{d}_3} \) type terms. However, as this is quite a lengthy process, reference will be made to the analogous result for two dimensions to see that, in general, there is no way to produce the correlation necessary to produce a \( \frac{1}{\bar{d}_3} \) singularity. Nothing in principle is changed in a three-dimensional system. As a matter of fact, since the \( z \) and \( 3 \) axes are almost parallel on the average, the results are almost identical. Thus, one has the final form

\[
I_3 \phi_{0k}(\vec{r}) = k \phi_{0k}(\vec{r})
\]

and, of course, similar results for excited states, \( \phi_{nK'} \).

The operation of \( I_1 \) and \( I_2 \) on the scalar states will in general differ from \( J_x \) and \( J_y \) on the original H.F. states. To see this, note that for these directions the moment of inertia do not go to zero. Thus one gets contributions from both the \( D \)-functions and non-\( D \)-function parts of the \( f_n \)'s. However, for typical nuclear systems, one may still argue that the latter give only a small effect, though not as small as in the \( I_3 \) case by any means. The reason for this is that the non-\( D \)-function contributions are about a factor of \( |\beta| \varepsilon |\bar{q} - q| \bar{q}^* + \bar{q}^* | \bar{q} \bar{q}^* |^{1/2} / - .3 \) smaller. This can be seen by looking at

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\[ \mathcal{J} n_i = \left( \frac{Q_k - Q_3}{Q_n + Q_3} \right) \left( \sum_{k} \varepsilon_{2k} \tilde{T}_{k3} \varepsilon_{3k} + z \leftrightarrow \bar{z} \right) \quad (4.34) \]

Now,

\[ \mathcal{J} n_1 \mathcal{O}^{\ast}_{m,n}(r) = J_1 \mathcal{O}^{\ast}_{m,n}(r) = J \mathcal{O}^{\ast}_{m,n}(r) \quad (4.35) \]

so that on the \( O \)-function part of \( f_n \), this operator gives a contribution characterized by a strength \( J \). When operating on the other parts of \( f_n, \mathcal{J} n_i \), acts like \( \beta \) times some differential operator, i.e. the second factor in equation (34). Since this operator has a structure similar to the \( J \)'s (see eq. (14)), it will give a contribution of the order \( J \) and thus \( \mathcal{J} n_i \), will give at term \( \sim \beta J \ll J \). What has happened, in words, is that uncorrelated single particle states in the H.F. function have no chance to produce the coherent effect existing in \( \mathcal{O}(r) \). Consequently, to lowest order in \( \beta, I_1 \) and \( I_2 \) do act like \( J_x \) and \( J_y \) when applied to scalar functions made from H.F. states.

More important than the above result, is how the scalar states transform under the \( I \)'s. Because of the exact commutation relations for axially symmetric systems to be derived in the next chapter,

\[ [I_1, I_3] = -i I_2 \quad ; \quad [I_2, I_3] = i I_1 \quad (4.36) \]
one easily finds, for example,

\[ e^{-i\vec{I}_3 \cdot \vec{I}_1} e^{i\vec{I}_3 \cdot \vec{I}_2} = \vec{I}_1 \cos \alpha + \vec{I}_2 \sin \alpha \]  

(4.37)

However, since

\[ [\vec{I}_1, \vec{I}_2] = i \frac{2 (\vec{a}_1 + \vec{a}_2) \vec{a}_3}{(\vec{a}_1 + \vec{a}_2) \cdot (\vec{a}_1 + \vec{a}_2)} \vec{I}_3 = i (1-\rho^2) \vec{I}_3 \]  

(4.38)

(ignoring spin contributions), one finds

\[ e^{-i\vec{I}_3 \cdot \vec{I}_1} e^{i\vec{I}_3 \cdot \vec{I}_2} = \vec{I}_3 \cos [\alpha (1-\rho^2)] - \vec{I}_2 \sin [\alpha (1-\rho^2)] \]  

(4.39)

and similarly for transformations generated by \( \vec{I}_2 \).

Since \( \beta^2 < 1 \), though, one may clearly ignore the slight correction in equation (38) in which case the \( I_A \)'s are seen to have the same rotational properties as the \( J_K \)'s. This means, in particular, that one may define \( \phi_{o-k}(\vec{r}) \) by

\[ \phi_{o-k}(\vec{r}) \equiv e^{i\pi I_1} \phi_{o-k}(\vec{r}) + O(\rho^2) \]  

(4.40)

since clearly \( I_3 \phi_{o-k}(\vec{r}) = -K \phi_{o-k}(\vec{r}) \) and one knows that

\[ \phi_{o-k}(\vec{r}) = e^{i\pi J_y} \phi_{o-k}(\vec{r}) \] .

The significance of this result will become apparent in the next chapter. Right now it just serves as an example of the utility of the scalar functions in discussions where the intrinsic angular momentum is a meaningful concept.
As far as using the scalar functions in the solution of the energy eigenvalue problem, the remarks in the two-dimensional example apply here also. The only added point is that, though a scalar basis of this sort is not computationally practical, there is a conceptual advantage of introducing them as an intermediate step, i.e. the $\lambda_A$'s are put on an easily interpretable level.
V. REDUNDANT HARTREE-FOCK

A. Statement of Method

The results of the previous three chapters will now be applied to the solution of the nuclear rotation problem. As mentioned before, the techniques developed so far are too formal to allow any practical solution for the cases of present interest. However, the formulation is such that meaningful results can be obtained for deformed nuclei in the event that one performs approximate solutions. In particular, using the crudest approximations one sees excitations corresponding to rigid body type rotation and with a moment of inertia in good agreement with that found experimentally. There will, of course, be many types of excitations missed by approximating these equations, but it is not the aim to completely solve the nuclear many body problem.

For this thesis, the main approximation will be to perform diagonalizations in a truncated basis of Hartree-Fock states e.g. the ground state and a certain number of one particle-one hole excitations. To render things complete, a brief exposition of the parts of H-F theory which are relevant here will be given. This will be done
with the aid of Thouless theorem \(^{(11)}\) which states that if 
\( |a\rangle \) is any Slater determinant (or second quantized 
analogue) and \( |b\rangle \) is any other such determinant not 
orthogonal to \( |a\rangle \), then \( |a\rangle \) and \( |b\rangle \) are related 
by

\[
|b\rangle = c e^{i f} |a\rangle
\]

(5.1)

where \( f \) is a one particle-one hole operator, i.e., an 
operator connecting only states differing by one particle-
hole state, and \( c \) is a normalization constant. If

\( a \) and \( b \) are normalized the same, one may choose

\( c = 1 \) and \( f = i s \) where \( s \) is Hermitian.

Now, the H-F approximation is a variational principle 
based on using a single determinant as a trial function. 
Stated more precisely, if \( |0\rangle \) is the H-F ground state 
then

\[
\mathcal{S} <0| H |0> = 0
\]

(5.2)

for any first order variation of \( |0\rangle \). The easiest 
way to perform the variation is through Thouless theorem 
in which case equation (2) becomes for a varied determinant

\( |\varepsilon\rangle = e^{i \varepsilon s} |0\rangle \) as \( \varepsilon \rightarrow 0 \),

\[
0 = <\varepsilon | H | \varepsilon > - <0 | H | 0>
\]

(5.3)

\[
= <0 | H + i \varepsilon [H,S] |0> - <0 | H | 0> = i \varepsilon <0 | [H,S] | 0>
\]
Since $\epsilon$ and $s$ are arbitrary except for the conditions stipulated for $s$ by the theorem, one has

\[ \langle 0 | [H, S] | 0 \rangle = 0 \]  \hspace{1cm} (5.4)

for all Hermitian one particle operators, $s$. This is known as the Brillouin theorem and from it follows the H-F equations in their usual form. Since these are not needed here they will be omitted.

Another use of Thouless theorem is performing first order perturbation calculations with the H-F ground state as the unperturbed wavefunction. In this case one assumes the Hamiltonian has the form $\tilde{H} = H + \lambda V$ and that

\[ \delta \langle 0 | H | 0 \rangle = 0 \]  \hspace{1cm} (5.5)

Then, considering $|f\rangle = e^{i\lambda \hat{f}} |0\rangle$, one defines the perturbation problem by requiring

\[ \langle f | \tilde{H} | f \rangle = \langle 0 | e^{-i\lambda \hat{f}} \tilde{H} e^{i\lambda \hat{f}} | 0 \rangle \]

\[ \equiv \langle 0 | \tilde{H} | 0 \rangle \]

be a minimum to first order in $\lambda$. From the last form, one sees that this is equivalent to the statement the $|0\rangle$ also be the H-F ground state for $\tilde{H}(f)$. Thus using equation
(4) one sees that \( f \) is determined from the condition

\[
\langle 0 | \hat{H}(f) | s \rangle | 0 \rangle = 0
\]  

(5.7)

for all one particle operators, \( s \). Since \( s \) is arbitrary, this is equivalent to requiring

\[
\langle 0 | \hat{H}(f) | ph \rangle = 0
\]  

(5.8)

for all one particle-one hole states, \( | ph \rangle \). To first order in \( \lambda \), remembering that \( | 0 \rangle \) is the H-F for \( H \) so that \( \langle 0 | H | ph \rangle = 0 \) , one finds

\[
\langle 0 | \hat{H}(f) | ph \rangle = \langle 0 | H + \lambda (i[H,f'] + V) + o(\lambda^2) | ph \rangle
\]  

(5.9)

\[
= \lambda \langle 0 | i[H,f'] + V | ph \rangle = 0
\]

This is a system of linear equations for \( f \), which when solved gives the corrected energy of

\[
\langle f | \hat{H} | f \rangle = \langle 0 | H | 0 \rangle + \lambda \langle 0 | V | 0 \rangle + \frac{\lambda^2}{2} \langle 0 | i[H,f'] | 0 \rangle
\]  

(5.10)

With these results it is now possible to outline the methods of solution to be used in this section. All of these are based on treating the intrinsic-rotation interaction term of the Hamiltonian, the one linear in angular momentum, by the above H-F perturbation program. The problem will be formulated in the redundant space of the
coordinates of the nucleons (2A for two dimensions). Thus, one must also consider the associated subsidiary conditions be they including the $\mathcal{S}$-functions in all matrix elements or simultaneously diagonalizing the H and N matrices. These extra complications, though, will only be treated in places where they are absolutely required. This is because, as mentioned in a previous chapter, the N matrix plays only a minor role in the energy eigenvalue problem. And since the problem is going to be solved in only a small region of the redundant space, the fact that this space is too big is not likely to cause any trouble except in rare instances where many of the functions differ only by the value of the collective coordinate. Using just low lying one particle excitations, as is done in practical calculations, insures that this possibility is practically non-existent. The reason for this is that states differing only in the collective coordinate, the orientation of the nucleus, differ by many particle-hole excitations.

The first way the problem is solved is by approximately diagonalizing the Hamiltonian matrix formed by not including the $\mathcal{S}$-function in the matrix elements. In principle one should also then diagonalize the associated N matrix but this will not be done in light of the arguments of
Chapter III where it was shown that the simultaneous diagonalization is not crucial in determining the energy eigenvalues. With this treatment of the problem, the primary aim is to establish the fact that a meaningful solution for the ground state rotational band is possible. To this end, it will be shown that it is possible to derive the Thouless-Valatin equations for the moment of inertia mentioned in the introduction.

Once it has been established that one does not get nonsense, the next step is to try to find better solutions to the problem. For this aspect of the treatment there will be a competition between getting better answers and keeping the computation at a reasonable level. Since there are no numerical calculations in this thesis, it may seem odd to be concerned over computational ease. However, one of the main purposes here is to develop the problem in such a manner that the results can be worked into a useful numerical procedure. Because of this, most of the answers will appear in an incomplete form in the sense that definite results readily checked against experimental data won't arise.
B. Two Dimensions

As usual, the problem will first be considered in two dimensions for simplicity. Here, the crudest approximation of dropping the $\mathcal{F}$-function and the $N$ matrix will be employed. In this case one has a perturbation separation of the form $H^k = h_k + V_k$ where

$$h_k = H_0 + \frac{1}{2} Q K^2$$  \hspace{1cm} (5.11)

$$V_k = H_1 K$$  \hspace{1cm} (5.12)

The quantities $H_0$, $H_1$ and $Q$ are those defined in Chapter II and $K$ is an eigenvalue of $J$.

To simplify matters, make the approximation of replacing $Q$ by its expectation value in the $H$-$F$ ground state of $H_0$. This can be corrected for by considering also the off diagonal elements as a perturbation. However, these elements physically represent fluctuations of the nuclear shape about its equilibrium position and for deformed nuclei can be shown to have a negligible effect on the rotational spectrum. In other words, one neglects the rotation-vibration coupling effects. Since no ambiguity exists, the symbol $Q$ will also be used for the expectation value.
Now to continue let \( |0\rangle \) be the H–F ground state for \( H_0 \), that is

\[
\delta \langle 0 | H_0 | 0 \rangle = 0 \tag{5.13}
\]

Obviously, then, since \( Q \) and \( K \) are just numbers, this is also the H–F ground state for the unperturbed Hamiltonian, \( h_k \). With this fact it is possible to use the perturbation formulas developed above. In this case the first order determinant is

\[
|f\rangle = e^{ikf} |0\rangle \tag{5.14}
\]

where \( f \) is determined from equation (9) which here gives

\[
\langle 0 | [H_0, f] - iH_1 | 0 \rangle = 0 \tag{5.15}
\]

One then finds that the energy is

\[
E_k \simeq \langle 0 | h_k | 0 \rangle + K \langle 0 | H_1 | 0 \rangle + \frac{i}{2} \langle 0 | [H_0, f] | 0 \rangle K^2 \tag{5.16}
\]

For even nuclei, \( |0\rangle \) is time reversal invariant and since \( H_1 \) is odd under this operation the term linear in \( K \) vanishes. Thus one finds

\[
E_k \simeq \langle 0 | H_0 | 0 \rangle + \frac{i}{2} K^2 \langle 0 | [H_0, f] + Q | 0 \rangle \tag{5.17}
\]
This immediately allows an identification of the moment of inertia, $\Theta$, as

$$\frac{1}{\Theta} = \langle 0 | \hat{J}_f [H_1, \hat{f}] | 0 \rangle + Q$$

(5.18)

showing the first order renormalization effect caused by the interaction $H_1$. Had there been no coupling between the intrinsic and rotational motions, the moment of inertia would merely have been $\frac{1}{\Theta} = \frac{-1}{\langle 0 | [H, \hat{f}], \hat{f} | 0 \rangle}$. 

To achieve the Thouless-Valatin equations it is necessary to introduce the following two approximations:

$$[J_f] \simeq 0$$

(5.19)

$$i [\dot{\phi}, J_f] \simeq \langle 0 | \hat{J}_f [\dot{\phi}, J_f] | 0 \rangle \equiv J$$

(5.20)

The first equation is made reasonable by noting that since $f$ results from the fact one has a perturbation, $H_1$, and since this is purely intrinsic, $f$ should essentially be intrinsic and thus commute with $J$. The fact that this is not rigorously true is because a redundant basis is being used and so for the best possible variational result, collective parts should also be allowed to occur in $f$. But, since $H_0$ and $H_1$ are intrinsic, one may perform the "gauge" transformation $f \rightarrow f + \lambda \phi$ in equations
(15) and (16) without changing the results. This means that if

\[ [\mathcal{J}, f] = \alpha + \text{(small off-diagonal terms)} \]  \hspace{1cm} (5.21)

then with \( f' = f - i\alpha \Psi \)

\[ [\mathcal{J}, f'] = \text{(small off-diagonal terms)} \]  \hspace{1cm} (5.22)

One may question the fact that \( f' \) is no longer a one body operator since \( \Psi \) is not. The reason this causes no problem is that \( f' \) is introduced after Thouless theorem, which requires a one body operator, has been used. Thus there is quite a bit of latitude for the redundancy to correct itself.

Using equations (19) and (20) one can now rewrite equation (15) as

\[ \langle 0| [H - \hat{\Psi} \mathcal{J} + \frac{i}{2} \mathcal{Q} \mathcal{J}^2, f] - i(\hat{\Psi} - \mathcal{Q} \mathcal{J})|\rho_h \rangle = \]  \hspace{1cm} (5.23)

\[ \langle 0| [H, f] + i\mathcal{Q} \mathcal{J} - i(\hat{\Psi} - \mathcal{Q} \mathcal{J})|\rho_h \rangle = \]

\[ \langle 0| [H, f + \Psi] + i(\mathcal{Q} + \Psi) \mathcal{J} |\rho_h \rangle = 0 \]

while equation (18) for the moment of inertia becomes

\[ \frac{1}{\Theta} = \Psi + \mathcal{Q} \]  \hspace{1cm} (5.24)
Now if one defines $G \equiv \frac{f+\varphi}{Q+\varphi}$, then (23) becomes

$$\langle 0| i[H,G]|ph\rangle = \langle 0| J|ph\rangle$$  \hspace{1cm} (5.25)

And, since $\varphi$ is conjugate to $J$

$$\langle 0|i[J,G]|0\rangle = \langle 0| J_i \left[ J_i f + \varphi \right] |0\rangle$$  \hspace{1cm} (5.26)

$$= \frac{1}{Q+\varphi} = \Theta$$

These last two equations have exactly the same form as the Thouless-Valatin equations. They would be such if 1) and 1) referred to H-F states of H instead of $H_0$; and 2) $G$ were a one particle operator. Neither of these are serious differences and in fact they can be compensated for to some extent. It is of no interest for the present investigation to do so.

Another form for the moment of inertia can be gotten by abandoning the approximations required to get the Thouless-Valatin equations. Instead introduce what might be called the cranking model approximation into equation (15). This consists of neglecting off diagonal elements of $H_0$ in its H-F representation. Then one gets

$$\langle 0| (\varepsilon_{\varphi} - \varepsilon_{ph}) f - i H |ph\rangle = 0$$  \hspace{1cm} (5.27)

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where $\epsilon_0 = \langle 0 | H_0 | 0 \rangle$ and $\epsilon_{ph} = \langle ph | H_o | ph \rangle$.

Consequently, one can solve directly for $f$ and find

$$\langle 0 | f | ph \rangle = \frac{i}{\epsilon_0 - \epsilon_{ph}} \langle 0 | H_i | ph \rangle$$ (5.28)

Finally, the moment of inertia formula (18) becomes

$$\frac{1}{\Theta} = \sum_{ph} \frac{|\langle 0 | H_i | ph \rangle|^2}{\epsilon_0 - \epsilon_{ph}} + Q$$ (5.29)

It is interesting to note that since $\epsilon_0 < \epsilon_{ph}$, the renormalized moment of inertia is always larger than that for the non-interacting case for the ground state rotational band. This fact will be used in a later section to define a variational program for finding $\Theta$.

There exists another path of approach to this problem which has a number of advantages over the ones just given. This consists of going back to the reduced Hamiltonian with the $s$-functions included in the matrix elements.

$$H_{nn}^k = \int dr \, \phi_n^*(r) \, S(q(n)) \left( H_0 + H_i + \frac{1}{2} Q K^2 \right) \phi_n(r)$$ (5.30)

with the $\phi_n(r)$'s still a redundant basis. Now in the expressions for $H_0$, $H_1$ and $Q$, one will in general find terms proportional to functions of $q(r)$ and in particular certain functions which are zero at $q = 0$. Since these terms will drop out in the end anyway, the procedure will
be to eliminate them at the beginning of the problem and thereby achieve a considerable simplification of the form of the operators.

To be specific, the remainder of the work will be done with the operator constructed in Chapter II, that is, the one defined by diagonalizing the quadrupole tensor. Referring back, one sees that

\[
\hat{\varphi} = \left\{ \Sigma \left( \rho_y + \gamma \rho_x \right) - \varphi \left( \rho_x - \gamma \rho_y \right) \tan^2 \varphi \right\} \sqrt{\left\{ m \varphi \left( x^2 - y^2 \right) \left( 1 + \tan^2 \varphi \right) \right\}} \\
= \left\{ \Sigma \left( \rho_y + \gamma \rho_x \right) \varphi \left( x^2 - y^2 \right) - \varphi \left( \rho_x - \gamma \rho_y \right) \varphi \left( x^2 \right) \right\} \sqrt{\left\{ m \left( \varphi \left( x^2 - y^2 \right) \right) ^2 + 4 \left( 3 \varphi ^2 \right) \right\}}
\]

and

\[
Q = \frac{\Sigma \left( x^2 + y^2 \right)}{m \left( \varphi \left( x^2 - y^2 \right) \right) ^2 + 4 \left( 3 \varphi ^2 \right)}
\]

In Q, there is no problem in setting \( \varphi = 0 \), or equivalently \( \Sigma (xy) = 0 \), since no differential operators occur to cause an ambiguity. However, one must be careful in \( \varphi \) because of the p's. Fortunately, the second form of \( \varphi \) above has the desirable property that the numerator and denominator commute as do the factors in the two products in the numerator. This is now shown.

\[
\left[ \Sigma \left( \rho_y + \gamma \rho_x \right), \Sigma \left( x^2 - y^2 \right) \right] = -2i \left( \varphi \left( xy \right) - \varphi \left( yx \right) \right) = 0
\]
\[ \left[ \Sigma (x \rho_x - y \rho_y), \Sigma x y \right] = -\lambda' \left( \Sigma x y - \Sigma y x \right) = 0 \quad (5.34) \]

Finally,

\[ \left[ \Sigma (x \rho_y + y \rho_x), \Sigma x y \right] - 2 \left[ \Sigma (x \rho_y - y \rho_x), \Sigma x y \right] \Sigma x y, \left( \Sigma x^2 - y^2 \right)^2 + 4 \left( \Sigma x y \right)^2 \right] = \quad (5.35) \]

\[ 4 \left[ \Sigma (x \rho_y + y \rho_x), \Sigma x y \right] \Sigma x^2 - y^2 \right] - 2 \left[ \Sigma (x \rho_y - y \rho_x), \Sigma x^2 - y^2 \right] \Sigma x y = \]

\[ -\lambda' 8 \Sigma (x^2 + y^2) \Sigma x y \Sigma x^2 - y^2 \right] + 4 \Sigma (x^2 + y^2) \Sigma x^2 - y^2 \right] \Sigma x y = 0 \]

This means that one may set the \( \Sigma x y \) terms = 0 in all places and not worry about the derivatives giving a non zero result. Thus, the simplified forms of the operators are

\[ \tilde{H}_o = \hat{H} - \frac{1}{2m \left( x^2 - y^2 \right)} \left( \Sigma (x \rho_y + y \rho_x) J + h.c. \right) + \frac{\Sigma (x^2 + y^2)}{2m \left( x^2 - y^2 \right)^2} J^2 \quad (5.36) \]

\[ \tilde{H}_1 = \frac{\Sigma (x \rho_y + y \rho_x)}{m \left( x^2 - y^2 \right)} - \frac{\Sigma (x^2 + y^2)}{m \left( x^2 - y^2 \right)^2} J \quad (5.37) \]

\[ \tilde{Q} = \frac{\Sigma (x^2 + y^2)}{m \left( x^2 - y^2 \right)^2} \quad (5.38) \]

It should be noted that these operators are not manifestly Hermitian since \( J \) does not commute with operators multiplying it. However, a simple calculation shows that
the commutators are all proportional to $\Sigma_{xy}$ and thus may be set equal to zero.

Before continuing, it should be pointed out that the device of setting $\psi = 0$ in the terms which vanish destroys the intrinsic nature of the operators. This is because the condition ($\psi = 0$) is not enforced in the non-vanishing terms where it is more difficult to apply. It should be clear, and can be checked, that the commutators of $\mathcal{S}(\psi)H_0$, $\mathcal{S}(\psi)H_1$ and $\mathcal{S}(\psi)Q$ with $J$ and $\psi$ will all be proportional to $\Sigma_{xy}$ and thus vanish when the $\mathcal{S}(\psi)$ condition is enforced. Thus, in matrix elements these operators do indeed remain intrinsic though not explicitly so.

The matrix to be diagonalized is now

$$H_{nn'}^k = \int dr \phi^*_n(r) \mathcal{S}(\psi(r))(\tilde{H}_0 + \tilde{H}_1 + \frac{i}{2} \tilde{Q} \tilde{K}^e) \phi_n(r)$$

and except for the $\mathcal{S}$-function is somewhat easier to calculate in a practical approximate program. To render this problem tractable for a numerical treatment, one must find a way now to eliminate the $\mathcal{S}$-function. One way is, of course, to replace it by, say, some sort of gaussian approximation. This still leads to more than two body operators, a result which is difficult to handle numerically.
An insight into what must be done can be gained by seeing what the $\mathcal{S}$-function achieves in the present case. Clearly, its main function is to keep out all components of the $\phi$'s which have $\psi \neq 0$ and thus ruin the equality of matrix elements of the tilded and untilded operators. So, if one can find a way to insure this condition, at least approximately, then the $\mathcal{S}$'s may be dropped.

As a practical approximation, remembering that variational methods are used to solve the eigenvalue problems, one chooses imposing a subsidiary condition via a Lagrange multiplier. To determine the most efficient condition, one would have to make a detailed examination of the system in question. For the present purposes, the simplest requirement, $\langle \mathcal{Z}(xy) \rangle = 0$, will be employed. This has the advantage of being the expectation value of a one particle operator. Moreover, as will be presently shown, this operator commutes with the tilded operators which means that in practice they can be simultaneously diagonalized, i.e. it is consistent to require a condition on $\mathcal{Z}(xy)$ since it is a conserved quantity.

Before continuing, it must be mentioned that the procedure of replacing the $\mathcal{S}$-function by a simple subsidiary conditions can be employed only with certain reservations. It definitely won't work in a general situation. However,
in the present case, one may make arguments based on the fact that the theory is developed in a basis of deformed H-F states. As a result of the deformation, these functions are not eigenstates of the total angular momentum but instead appear as wavepackets made up from superpositions of these eigenstates with a spread of eigenvalues. For deformed nuclear states, this spread is considerable as reflected in the fact that they give a large expectation value of $J^2$. By the uncertainty principle, this means that the spread in angle, which is given roughly by $\frac{1}{\langle J^2 \rangle}$, is small, i.e. the wavepackets are localized in angle about their mean value. Now if one chooses the axes of H-F well such that this mean is zero for the ground state, the small angular spread indicates that the $J$-function condition is automatically approximately enforced. Moreover, the low lying single particle excited states will also fulfill this condition, though not as well since there is a chance for a small shift in the mean value of the angle. Since these are the states used in the perturbation program, one sees that in a lowest approximation the $J$-functions may just be dropped, period. However, to insure that no spurious results appear, it is prudent to adopt the subsidiary condition. Clearly, this helps eliminate states whose mean angle has "slid" too far from zero.
Continuing now to prove the commutation relations for $\Sigma(xy)$ and the simplified operators, introduce the following approximations and notations

\[ m \Sigma(x^2 + y^2) \approx m \langle \Sigma(x^2 + y^2) \rangle = R \]  \hspace{1cm} (5.40)

\[ m \Sigma(x^2 - y^2) \approx m \langle \Sigma(x^2 - y^2) \rangle = \Delta \]  \hspace{1cm} (5.41)

\[ Q \approx \frac{R}{\Delta} = B \]  \hspace{1cm} (5.42)

\[ \Sigma(xp_y + yp_x) \approx M \]  \hspace{1cm} (5.43)

where the expectation values are with respect to H-F states to be defined later. The approximations are, of course, the usual ones as discussed previously. With these simplifications one finds

\[ \tilde{H}_o = H - \frac{i}{\hbar} (mJ + JM) + \frac{i}{2} B J^2 \]  \hspace{1cm} (5.44)

\[ \tilde{H}_r = \frac{M}{\Delta} - BJ \]  \hspace{1cm} (5.45)

Now note that

\[ [ J, \Sigma xy ] = -i \sum \left( x \frac{\partial \Sigma}{\partial y} - y \frac{\partial \Sigma}{\partial x} \right) \approx -i \frac{\Delta}{M} \]  \hspace{1cm} (5.46)
and that
\[
\begin{align*}
[M, \Sigma_{xy}] &= -\hbar \left( x \frac{\partial}{\partial Y} + y \frac{\partial}{\partial X} \right) \Sigma_{xy} = -\hbar \frac{R}{\tilde{m}} \\
\end{align*}
\]
(5.47)

Also, remembering that the potential is momentum independent, one has
\[
\begin{align*}
[H, \Sigma_{xy}] &= \frac{i}{\hbar} \left[ [\Sigma p^2, \Sigma_{xy}] \right] \\
&= \frac{-\hbar^2}{\tilde{m}} \left( p_x \frac{\partial}{\partial X} + p_y \frac{\partial}{\partial Y} \right) + \text{h.c.} = -\frac{M}{\tilde{m}} \\
\end{align*}
\]
(5.48)

Consequently,
\[
\begin{align*}
[H_o, \Sigma_{xy}] &= -\hbar \frac{M}{\tilde{m}} - \frac{M}{\tilde{m}} \left( \frac{-\hbar^2}{\tilde{m}} \right) - \frac{M}{\tilde{m}} \frac{-i \hbar}{\tilde{m}} J + \beta \left( \frac{-i \hbar}{\tilde{m}} \right) J \\
&= 0 \\
\end{align*}
\]
(5.49)

since
\[
\frac{R}{\tilde{A}} - B \Delta = \frac{R}{\tilde{A}} - \left( \frac{R}{\tilde{A}} \right) \Delta = 0 \\
\]
(5.50)

Next
\[
\begin{align*}
[H_1, \Sigma_{xy}] &= \frac{1}{\tilde{A}} \left( \frac{-i \hbar}{\tilde{m}} \right) - B \left( \frac{-i \hbar}{\tilde{m}} \right) = 0 \\
\end{align*}
\]
(5.51)

as above. Thus, as stated, \(\Sigma(xy)\) is a conserved quantity with respect to the tilded operators.

Proceeding now to the solution of the energy eigenvalue problem, the aim is to find the best variational determinant for
\[ \hat{H}_k(\lambda) = \hat{H}_0 + \hat{H}_1 K + \frac{1}{2} B K^2 + \lambda \Sigma(xy) \]  

(5.52)

where \( \lambda \) is determined by the subsidiary condition that the average value of \( \Sigma(xy) \) be zero. To this end the usual perturbation-variation technique will be employed based on the H-F states for \( H \). This is in contrast to the previous case where state of \( H_0 \) were used and is designed to make the problem more realizable in terms of known H-F results. Also, make the symmetry assumptions to the ground state, \( |0\rangle \), of

\[ \langle 0 | \Sigma(x,y) | 0 \rangle = \langle 0 | J | 0 \rangle = \langle 0 | M | 0 \rangle = 0 \]  

(5.53)

corresponding to an even \( A \) nucleus and with the axes of the H-F well along the principal axes of the average quadrupole tensor. Moreover, introduce the approximations

\[ \langle 0 | J^2 | \phi \rangle \approx 0 \approx \langle 0 | M J | \phi \rangle \]  

(5.54)

for all one particle states, i.e. one also has approximate H-F states for \( H_0 \).

This is done for simplicity and is crudely based on the observation that when H-F is done with \( H - \frac{1}{\mu} J^2 \) (\( \mu = \text{moment of inertia} \)) instead of \( H \) the results are not very different in terms of total energy. The last
two terms of $H_0$ are roughly $\frac{j^2}{\alpha d}$ as long as the coupling is small, i.e., if $H_1 = 0$, then $H_0 = H - \frac{j^2}{2} B j^2$. Corrections due to this approximation can be included as a perturbation, but here this won't be done.

To do the perturbation theory, the usual method based on Thouless theorem will be employed using the trial function

$$|F\rangle = e^{iF}|0\rangle$$

(5.55)

where $F$ is a one body operator. As an aid in the systematics, write it in terms of two one-body operators,

$$F = Kf + \lambda g$$

(5.56)

assuming the subsidiary condition may be treated as a perturbation. The program is then to require $\langle F | \hat{H}_k(\lambda) | F \rangle$ be a minimum to first order in $K$ and $\lambda$ independently. This can be restated as requiring the transformed "Hamiltonian",

$$\hat{\tilde{H}} = e^{-iF} \hat{H}_k(\lambda) e^{iF} = \hat{H}_k(\lambda) + i[\hat{H}_k(\lambda), F] + \ldots$$

(5.57)

to have $|0\rangle$ as a $H-F$ ground state to lowest order in $K$ and $\lambda$. To this end expand $\hat{\tilde{H}}$ to second order, anticipating a later calculation of the energy. Thus
\[ \hat{H} = \hat{H}_0 + K \{ \hat{H}_1 + i [\hat{H}_0, f] \} + \lambda \{ \Sigma_{xy} + i [\hat{H}_0, g] \} + \]

\[ K \times \{ \frac{1}{2} \hat{B} + i [\hat{H}_0, f] - \frac{1}{2} [\hat{H}_0, f] f \} + \lambda \times \{ i [\Sigma_{xy}, g] - \frac{1}{2} [\hat{H}_0, g] g \} + \]

\[ K \lambda \times \{ -\frac{1}{2} [\hat{H}_0, f], g] - \frac{1}{2} [\hat{H}_0, f], f \} + i [\hat{H}_1, f] + i [\Sigma_{xy}, f] \} + \ldots \]

Now since \( \langle 0 | \hat{H}_0 | \phi \rangle = 0 \), one sees that \( f \) and \( g \) are determined from the equations

\[ \langle 0 | i [\hat{H}_0, f] + \hat{H}_1 | \phi \rangle = 0 \] \hspace{1cm} (5.59)

and

\[ \langle 0 | i [\hat{H}_0, g] + \Sigma_{xy} | \phi \rangle = 0 \] \hspace{1cm} (5.60)

respectively.

With these equations, one may now go back and calculate the energy to second order. To do this one may use (59) and (60) to express the expectation values of double commutators of \( \hat{H}_0 \) in terms of single commutators with the perturbations. That is, for example,

\[ \langle 0 | [\hat{H}_0, f] f | 0 \rangle = i \langle 0 | [\hat{H}_1, f] | 0 \rangle \] \hspace{1cm} (5.61)

since \( f \) is a one particle operator and connects only vacuum to one particle states. Thus, with this set of
results, which won't be explicitly listed, one has

\[ \langle 0 | \hat{H} | 0 \rangle = \langle 0 | \hat{H}_0 | 0 \rangle + K^2 \left\{ \frac{i}{2} B + \frac{i}{2} \langle 0 | [\hat{J}, f] | 0 \rangle \right\} + \lambda^2 \left\{ \frac{i}{2} \langle 0 | [\Sigma xy, g] | 0 \rangle \right\} + K \lambda \left\{ \frac{i}{2} \langle 0 | [\hat{J}, g] + [\Sigma xy, f] | 0 \rangle \right\} + \cdots \]  

(5.62)

The terms linear in \( K \) and \( \lambda \) disappear as a result of the assumed symmetry conditions as well as the H-F conditions, \( \langle 0 | [\hat{J}, \alpha] | 0 \rangle = 0 \) for any one particle operator, \( \alpha \).

To get the energy, one must first determine \( \lambda \) from the subsidiary condition. This takes on the form

\[ \langle F | \Sigma xy | F \rangle = 0 \leq \langle 0 | \Sigma xy + i [\Sigma xy, F] + \cdots | 0 \rangle \]  

(5.63)

\[ = i \langle 0 | [\Sigma xy, Kf + \lambda g] | 0 \rangle \]

which gives

\[ \lambda = - \frac{\langle 0 | [\Sigma xy, f] | 0 \rangle}{\langle 0 | [\Sigma xy, g] | 0 \rangle} \]  

(5.64)

Then one gets for the energy,

\[ E = \langle F | \hat{H}_e(\lambda) - \lambda \Sigma xy | F \rangle = \langle F | \hat{H}_e(\lambda) | F \rangle \]  

(5.65)

\[ = \langle 0 | \hat{H} | 0 \rangle \]

i.e. for the particular subsidiary condition chosen, the expectation values of the Hamiltonian and Hamiltonian plus...
Lagrange condition are the same. Thus, putting $\lambda$ into (62) gives

$$E = \langle 0 | \hat{H}_0 | 0 \rangle + k^2 \left\{ \frac{1}{2} B + \frac{i}{2} \langle 0 | [\hat{H}_1, f] | 0 \rangle + \right.$$  

$$\frac{i}{2} \left( \frac{\langle 0 | [\hat{E}_Y, f] | 0 \rangle}{\langle 0 | \hat{E}_Y | 0 \rangle} \langle 0 | \hat{E}_Y | 0 \rangle - \frac{i}{2} \langle 0 | \hat{E}_Y | 0 \rangle \langle 0 | [\hat{H}_1, \hat{g}] + [\hat{E}_Y, f] | 0 \rangle \right) \}$$ 

$$= \langle 0 | \hat{H}_0 | 0 \rangle + \frac{k^2}{2} \left\{ B + i \langle 0 | [\hat{H}_1, f] | 0 \rangle - \frac{\langle 0 | [\hat{E}_Y, f] | 0 \rangle}{\langle 0 | \hat{E}_Y | 0 \rangle} \langle 0 | [\hat{H}_1, \hat{g}] | 0 \rangle \right\}$$

giving immediately the identification for the inverse moment of inertia of

$$\frac{1}{\Theta} = B + i \langle 0 | [\hat{H}_1, f - \frac{\langle 0 | [\hat{E}_Y, f] | 0 \rangle}{\langle 0 | \hat{E}_Y | 0 \rangle} \hat{g}] | 0 \rangle \} \tag{5.67}$$

As it stands, this result is not readily interpretable. To get a reasonable form, assume that the commutators of $M$ and $J$, with $g$ and $f$ may be replaced by their expectation value as was done in the previous example.

This is again a simplification assumption and may, in a particular case, require rectification. Then equation (59) assumes the form, when the explicit expression for $H_0$ and $H_1$ are used, of

$$\langle 0 | [\hat{H}_0, f] | 0 \rangle = \langle 0 | [\hat{H}_0, f] - \frac{i M}{\Theta} \hat{g} | 0 \rangle - \frac{i \langle 0 | [\hat{M}_0, f] | 0 \rangle}{\Theta} + i BJ \cos(\theta) | 0 \rangle \tag{5.68}$$

$$= \langle 0 | BJ - \frac{M}{\Theta} \hat{g} | 0 \rangle$$
Now remembering from equation (48) that $M = i [H, m \Sigma(xy)]$, one finds

$$
\langle 0 | i [H, \phi + \frac{i}{\hbar} (1 - i \langle \phi | \Sigma(xy) \phi \rangle) \Sigma(xy)] | ph \rangle = (5.69)
$$

$$
\langle 0 \left( B(1 - i \langle \phi | \Sigma(xy) | \phi \rangle) + \frac{i \langle \phi | M | \phi \rangle}{A} \right) J | ph \rangle
$$

and defining

$$
G \equiv \frac{f + \frac{i}{\hbar} (1 - i \langle \phi | \Sigma(xy) | \phi \rangle) \Sigma(xy)}{B(1 - i \langle \phi | \Sigma(xy) | \phi \rangle) + \frac{i \langle \phi | M | \phi \rangle}{A}} (5.70)
$$

gets

$$
\langle 0 | i [H, G] | ph \rangle = \langle 0 | J | ph \rangle (5.71)
$$

As this looks like one of the Thouless-Valatin equations, it is tempting to follow through and see what the second relation gives. This is

$$
\langle 0 | i [J, G] | 0 \rangle = \frac{1}{B(1 - i \langle \phi | J | \phi \rangle) + i \langle \phi | M | \phi \rangle} (5.72)
$$

using the fact from equation (46) that $\langle 0 | i [J, \Sigma(xy)] | 0 \rangle = \frac{\Delta}{\hbar}$. According to the Thouless-Valatin results, this should be the moment of inertia. However, consulting equation (67), one sees

$$
\frac{1}{\theta} = B(1 - i \langle \phi | J | \phi \rangle) + i \frac{\langle \phi | M | \phi \rangle}{\Delta} - \frac{\langle \phi | \Sigma(xy) | \phi \rangle}{\Delta} \langle 0 | i [\phi - \delta J, \phi] | 0 \rangle (5.73)
$$
when the explicit form of $H_{\perp}$ is introduced. This indicates that the subsidiary condition, which is responsible here for the last term, introduces a correction to the moment of inertia when compared with the Thouless-Valatin form. The extent of the correction will now be investigated.

Looking back at the argument upon which the substitution of a subsidiary condition for the $J$-function was based, one sees that the correction term above should be small if the preceding discussion is to have any validity. In other words, effects caused by basis states "sliding" from a zero mean value for the angle should not be large. That this is the case can be shown for highly deformed systems as will now be shown.

First of all, equations (59) and (60) give

$$\langle 0 | [\tilde{\hat{h}}, \hat{g}] | 0 \rangle = -i \langle 0 | [\tilde{\hat{A}}_0, \tilde{\hat{f}}] | 0 \rangle$$  \hspace{1cm} (5.74)

$$= -i \langle 0 | [\tilde{\hat{A}}_0, \tilde{\hat{g}}] + [\tilde{\hat{g}}, \tilde{\hat{f}}], \tilde{\hat{A}}_0 \rangle | 0 \rangle$$

$$= -i \langle 0 | [\tilde{\hat{g}}, \tilde{\hat{g}}] | 0 \rangle = \langle 0 | \{ \tilde{\hat{g}}, \tilde{\hat{f}} \} | 0 \rangle$$

using the facts that $[\tilde{\hat{g}}, \tilde{\hat{f}}]$ is a one particle operator and $H_0$ connects no vacuum to one particle states. This means that the correction to $\Theta^{-1}$ is given by
\[ \Theta^{-1} \mathcal{G}^{t}_{t} = -\frac{\langle \mathcal{O}[i A_{xy}, f] | 0 \rangle}{\langle \mathcal{O}[A_{xy}, g] | 0 \rangle} \left\langle \mathcal{O}[i \mathcal{H}, g] | 0 \rangle \right\rangle = -\frac{\langle \mathcal{O}[i A_{xy}, f] | 0 \rangle^{3}}{\langle \mathcal{O}[A_{xy}, g] | 0 \rangle} = \mathcal{S} \tag{5.75} \]

Now invoking the "cranking" approximation of replacing \( \mathcal{H} \) by the H-F Hamiltonian, one gets from equation (69) that

\[ \langle \mathcal{O}[i \mathcal{H}, f + \frac{a}{2} (1 - i \mathcal{O}[E_{x}, y] | 0 \rangle) \mathcal{E}_{xy} | ph \rangle \mathcal{G} (E_{x} - E_{y}) \langle \mathcal{O}[i \mathcal{H}, f + \frac{a}{2} (1 - i \mathcal{O}[E_{x}, y] | 0 \rangle) \mathcal{E}_{xy} | ph \rangle \tag{5.76} \]

\[ = \left( \mathcal{B} (1 - i \mathcal{O}[E_{x}, y] | 0 \rangle \mathcal{A} \mathcal{O}[i \mathcal{H}, f + \frac{a}{2} (1 - i \mathcal{O}[E_{x}, y] | 0 \rangle) \mathcal{E}_{xy} | ph \rangle \right) \langle \mathcal{O}[j | ph \rangle \]

or

\[ \langle \mathcal{O}[f | ph \rangle \mathcal{G} \left( \frac{\mathcal{A}}{(E_{ph} - E_{ph})} \langle \mathcal{O}[j | ph \rangle - C \langle \mathcal{O}[E_{xy} | ph \rangle \tag{5.77} \]

where \( A \) and \( C \) are real constants from the line above and the \( \epsilon \)'s are the H-F energies. With this approximation one has

\[ \langle \mathcal{O}[E_{xy}, f] | 0 \rangle \mathcal{G} \left( \frac{\mathcal{A}}{E_{ph} - E_{ph}} \langle \mathcal{O}[E_{xy} | ph \rangle \langle \mathcal{O}[j | ph \rangle + \text{c.c.} \right) \tag{5.78} \]

Now for highly deformed even nuclei, it is known\(^{(7)}\) that there is an energy gap between the filled and unfilled levels which means that to a good approximation, one may replace the energy denominator here by some average constant value, \( \Delta E \). When this is done, one finds from closure and the fact that \( J \) and \( \Sigma'_{(xy)} \) are single particle operators that

\[ 114 \]
\[
\langle 0| [\Sigma_{xy}, f]| 0 \rangle \sim \frac{i}{\hbar} \left. \frac{\partial}{\partial \mathcal{E}} \langle 0| (\Sigma_{xy}) J + J(\Sigma_{xy}) | 0 \rangle \right|_{\mathcal{E}} = 0
\] (5.79)

using the observation that \((\Sigma_{xy}) J + J(\Sigma_{xy})\) is odd under time reversal, which is a meaningful concept in nuclear physics. Thus, in the limit of large deformations, the correction vanishes. Modifications to this result probably come mostly from the fact that the above closure is only approximate. This means that (79) will be zero only to the order of the ratio of the average level spacing in excited states to the gap spacing.

A simple interpretation can be given to the correction term, \(\mathcal{S}\), by noting that the Thouless-Valatin formula comes from assuming that nuclear rotation can be approximated by a uniform rotation of the axes of the H-F self consistent potential. The present results without the subsidiary condition corresponds to the same approximation in the sense that one considers the H-F axes to always be along the principal quadrupole axes i.e. \(\varphi = 0\) at all times. However, in reality, the motion is not going to be truly uniform or equivalently, the H-F axes are not always the principal axes. Instead, the nuclear distribution "wobbles" about the H-F axes and it is these fluctuations which cause \(\mathcal{S}\) to appear. That this effect goes inversely like the deformation is clear from the
uncertainty principle since the larger the deformation, the smaller the dispersion in angle.

Summing up this section, it appears that the present separation of variables method can be applied to nuclear rotation via the technique of using a redundant basis. The fact that the Thouless-Valatin equations keep appearing is comforting not only because aids in making judgements on the present theory, but also because it indicates that these equations in some sense have a fundamental validity. In otherwords, they are a stationary, derivation independent result. Of course, in the present work, they arrive only after a certain amount of approximation and are somewhat forced into being. However, in a detailed numerical study, these approximations can be studied and appropriate amends made for the particular case in question. It was one of the main purposes here to explicitly enumerate, from a fundamental point of view, what implicit information is contained in the previous theories.

C. Axial Symmetry

As a first example of the application of the separation of variables method to three dimensions, the case of axial symmetry will be treated. This is done not so much because this system is simpler, actually in some respects
it is more difficult, but because axially symmetric systems are more common. The real difficulty in solving the problem for this type of system comes from the fact that the effective moment of inertia for rotations about the symmetry axis is very small. This means that the coupling term for this direction becomes large and thus unsuitable for a perturbation treatment. However, when the intrinsic angular momentum operator is introduced, the strong coupling term can be eliminated by choosing the eigenvalue of the projection of this operator along the symmetry axis appropriately. The corresponding procedure was also employed in the Bohr-Mottelson model where (see Chapter I) it was required to set the eigenvalue difference, \((J_3 - I_3) = (K - \gamma) = 0\). In the present treatment, this condition will also be applied. It will be shown, moreover, that \((J_3 - I_3)\) is a constant of the motion even when the rotation-intrinsic perturbations are included. Thus, this particular choice is conserved to all orders of perturbation theory.

Proceeding with the development, it will be advantageous to employ the Bohr-Mottelson form of the Hamiltonian derived in Chapter II,

\[
H = H_{\text{int}} + \frac{1}{2} \sum_A \frac{1}{J_A} (J_A - I_A)^2
\]  

(5.80)
where

\[ \mathcal{H}_{\text{int}} = \mathcal{H} - \frac{i}{\hbar} \sum_A \mathcal{A}_A (\eta_A)^2 \]  

(5.81)

and \( \mathcal{I}_A \) are the components of the intrinsic angular momentum satisfying

\[ [\mathcal{I}_A, \mathcal{I}_B] \propto i \mathcal{I}_C \]  

(5.82)

Looking back at Chapter II, one sees that for axial symmetry along the \( A=3 \) axis one actually has the exact relations

\[ [\mathcal{I}_1, \mathcal{I}_3] = -i \mathcal{I}_2 \]  

(5.83)

\[ [\mathcal{I}_2, \mathcal{I}_3] = i \mathcal{I}_1 \]  

(5.84)

since the correction terms in equation (82) are proportional to the difference of the values of the quadrupole moments along the \( A \) and \( C \) directions which is zero for axial symmetry. This result allows construction eigenstates in exact analogy with those of the total, real angular momentum component in a particular direction, a result to be exploited later on.

The perturbation separation in this case will be taken as

\[ \hbar = \mathcal{H}_{\text{int}} + \frac{(\mathcal{I}_3 - \mathcal{I}_2)^2}{\hbar^2 \mathcal{I}_3} + \frac{1}{\hbar^2} \left( \mathcal{I}_1^2 + \mathcal{I}_2^2 + \mathcal{J}^2 - \mathcal{J}_3^2 \right) \]  

(5.85)
\[ \nabla = - \frac{1}{\mathcal{L}} ( J_1 \mathcal{L}_1 + J_2 \mathcal{L}_2 ) \quad (5.86) \]

In the above expressions, \( \mathcal{L}_1 \) and \( \mathcal{L}_2 \) were set equal to their expectation value in the appropriate H-F state to be defined below. Since the system is assumed axially symmetric, these values are equal and are denoted by \( \mathcal{L} \). Also note that unlike the two-dimensional examples, the collective parts of the Hamiltonian have not been integrated out yet. This is done for notational purposes as will be seen later.

Associated with the statement that the H-F state describes a system with axial symmetry, is the fact that it is an eigenstate of the \( z \) component of the angular momentum. To make the present formalism useful, there must be some way to interpret this result in terms of the intrinsic angular momentum since the H-F states are taken as a zero order representations of the true intrinsic states. In particular, to provide a consistent interpretation of the operators of the theory, it should be possible to show that \( I_3 \) is at least approximately conserved and its eigenvalues correspond to those of the H-F states. That these properties do indeed hold will now be demonstrated.
First of all, it will be shown that $I_3$ approximately commutes with $h$, the unperturbed Hamiltonian. Since $I_3$ is an intrinsic operator one need not worry about commutator with the $J^A_i$'s. Also, as was shown in Chapter II, the $I^A_i$'s commute with all $Q^A_i$'s and thus these commutators may be dropped. This means that the demonstration is reduced to finding

$$[H_{\text{INT}} + \frac{\mu}{\hbar} (I_1^2 + I_2^2), I_3] \overset{?}{=} 0 \quad (5.87)$$

Now because of the commutation relations of the $I^A_i$'s, one has

$$[\frac{\mu}{\hbar} (I_1^2 + I_2^2), I_3] = \frac{\mu}{\hbar} \{ -I_1 I_2 - I_2 I_1 + I_2 I_1 + I_1 I_2 \} = 0 \quad (5.88)$$

Thus, the only remaining part is

$$[H_{\text{INT}}, I_3] = [H_{\text{INT}}, J_3 - \mathcal{L}_3 \eta_3] \quad (5.89)$$

$$= -[H_{\text{INT}}, \mathcal{L}_3 \eta_3]$$

Now remembering that $\mathcal{L}_3 = \frac{m (Q_2 - Q_1)}{Q_1 + Q_2}$ and that $Q_1$ and $Q_2$ are operators with well defined expectation values with only small fluctuations for the case of pure rotational states, one may replace $\mathcal{L}_3$ by the number

$$J_3 \equiv \frac{m (<Q_2> - <Q_1>)^2}{<Q_1> + <Q_2>} \quad (5.90)$$
The expectation values are with respect to the H-F ground state to be defined later. Since this state is assumed axially symmetric, $\langle Q_1 \rangle = \langle Q_2 \rangle$ and $\mathcal{J}_3 \rightarrow 0$. Before this can be used to set the commutator $[H_{\text{int}}, I_3]$ of equation (89) equal to zero, one must be sure that no singularities of the order $(\langle Q_1 \rangle - \langle Q_2 \rangle)^{-2}$ or greater occur to cancel this zero. This means that one must investigate the properties of $[H_{\text{int}}, \eta_3]$.

The easiest term to look at is

$$\frac{1}{2} \mathcal{J}_3 \left[ \sum_n J_n (\eta_A)^2, \eta_3 \right]$$

since this may be rewritten using the definition of $I_A$, as

$$\frac{1}{2} \mathcal{J}_3 \left[ \sum_n J_n (\eta_A)^2, \eta_3 \right] = \frac{1}{2} \mathcal{J}_3 \left[ \sum_n \frac{J_n - I_A}{J_A}, \frac{J_3 - I_3}{J_3} \right]$$

$$= \frac{1}{2} \mathcal{J}_3 \left\{ (J_1 - I_1)(J_2 - I_2) + (J_2 - I_2)(J_3 - I_3) + h.c. \right\}$$

$$= \frac{1}{2} \mathcal{J}_3 \left\{ (J_1 - I_1)(J_2 - I_2) + (J_2 - I_2)(J_3 - I_3) - h.c. \right\}$$

$$= 0$$

In the above, the approximation of replacing the $J_A$'s by their appropriate average values was used as was the intrinsic character of the $I_A$'s. With this result, one is left with only the term $-\mathcal{J}_3 \left[ H, \eta_3 \right]$, which is unfortunately a bit tedious to calculate. To simplify
things only the most singular terms will be kept and as will be seen, all of the neglected parts vanish in the limit of axial symmetry. Using the expression for \( \eta_3 \) from Chapter II one has to calculate

\[
\mathcal{J}_3 [H, \eta_3] = \frac{Q_1 - Q_2}{2Q_1 + Q_2} \left[ H_j \sum_{\xi \xi_1} \left( e_{\xi} \tilde{t}_{\xi \xi} \epsilon_{\xi_1} + h.c. \right) \right] \tag{5.92}
\]

First of all

\[
[H_j, \tilde{t}_{\xi \xi}] \propto \left[ H_j \frac{P_j}{P_j} + P_j \frac{P_j}{P_j} \right] = -\frac{2\chi^2}{m} \sum_{\xi, \xi_1} \left( x_{\xi} \frac{\partial}{\partial x_{\xi}} + x_{\xi} \frac{\partial}{\partial x_{\xi}} \right) \tag{5.93}
\]

where \( V \) is the two-body potential. None of these terms are singular as \( \langle Q_1 \rangle - \langle Q_2 \rangle \rightarrow 0 \) so they may be dropped.

Next, using the relation

\[
[H_j, \tilde{e}_A] = \frac{i}{2} \left( \eta_\sigma \tilde{e}_c + \tilde{e}_c \eta_\sigma - \eta_c \tilde{e}_\sigma + \tilde{e}_\sigma \eta_c \right) \tag{5.94}
\]

one finds

\[
[H_j, \epsilon_{\xi \xi_1}] = \hat{k} \cdot [H_j, \tilde{e}_i] = -i \eta_3 \epsilon_{\xi \xi_1} + \text{less singular} \tag{5.95}
\]

\[
[H_j, \epsilon_{\xi_1}] = i \eta_3 \epsilon_{\xi_1} + \text{L.S.} \tag{5.96}
\]

These are the most singular terms since \( \eta_3 \propto \frac{1}{Q_1 - Q_2} \)

while all other terms are proportional to \( \eta_1, \eta_2 \) or sums of \( Q_A \)'s none of which has this denominator. Inserting these results into equation (92) gives
\[ \widetilde{\mathcal{Q}}_3 [H, \eta_3] = \frac{\langle Q \rangle - \langle \bar{Q} \rangle}{2\langle Q \rangle + \langle \bar{Q} \rangle} \ i \ \sum_{k} (\eta_3 \epsilon_{k\alpha} T_{\alpha\beta} \epsilon_{k\beta} + \epsilon_{k\alpha} T_{\alpha\beta} \eta_3 \epsilon_{k\beta} + h.c.) \ (5.97) \]

Since \( \eta_3 \)'s denominator cancels the \( \langle Q \rangle - \langle \bar{Q} \rangle \) numerator in this expression, one gets a non-zero result unless the sums vanish. Fortunately, this is the case as they are all of the form

\[ \sum_{k} \epsilon_{k\alpha} T_{\alpha\beta} \epsilon_{k\beta} = i \ \sum_{k} \epsilon_{k\alpha} (H T_{\alpha\beta} - T_{\alpha\beta} H) \epsilon_{k\beta} \]

\[ = i \ \sum_{k} (\epsilon_{k\alpha} \bar{Q} \epsilon_{k\beta} - \epsilon_{k\beta} \bar{Q} \epsilon_{k\alpha}) = i \ \sum_{k} [\epsilon_{k\alpha} \bar{Q} \epsilon_{k\beta}, \bar{Q}] = i \ [H, \bar{Q}] \] (5.98)

where equation (94) was used to get \( \sum_{k} \epsilon_{k\alpha} H \epsilon_{k\beta} = H \bar{D} - \bar{D} C \). Putting this result into (97) gives

\[ \widetilde{\mathcal{Q}}_3 [H, \eta_3] = \frac{\langle Q \rangle - \langle \bar{Q} \rangle}{2\langle Q \rangle + \langle \bar{Q} \rangle} (\eta_3 [H, \bar{Q}_2 - \bar{Q}] + h.c.) \ (5.99) \]

which, according to the approximation that the Q's be replaced by their expectation values, is zero. It should be noted that this approximation essentially ignores the effects of surface vibrations. However, as is well known, in many cases these are not negligible so that even though the Q's are well represented by their average values, their time derivatives may differ significantly from zero. Thus, the present results are not quite general. To rectify this, one must retrace the development with the
approximation $[H, Q_n] \approx 0$ omitted. The only place where this was also used was in equation (92) where $\bar{Q}$ assumed the form of a number as did the $\frac{1}{Q_n - Q_2}$ part of $\eta_3$. However, looking at equation (99) one sees that the

$$\left[ H, \sum_{k=1} \left( \epsilon_{u_k} \hat{T}_{k} \epsilon_{g_k} + h.c. \right) \right]$$

contribution exactly cancels

$$\left[ H, \frac{Q_1 - Q_2}{Q_1 + Q_2} \right]$$

when the limit $Q_1 - Q_2 \to <Q_1> - <Q_2> = 0$ is imposed after taking the commutators, n.b. (99) has

$$[H, Q_2 - Q_1] = - [H, Q_1 - Q_2] \ .$$

Thus, $[H, \eta_3, \eta_3] \approx 0$ in either case noting that all terms neglected as less singular in (95) and (96), have no $(<Q_1> - <Q_2>)^{-1}$ type denominators to cause trouble as $<Q_1> - <Q_2> \to 0$.

The final result of this somewhat lengthy demonstration is that to the degree of accuracy of the approximations used, one has

$$[h, I_3] \approx 0 \quad (5.100)$$

meaning $I_3$ is at least an approximately conserved quantity with respect to the unperturbed Hamiltonian, $h$.

It should be particularly noticed that this result depends strongly on the fact that one has an axially symmetric system so that various terms may be set equal to zero.

This is in line with interpretation of the H-F states as approximately representing the intrinsic states. To
make these states useful for calculations, one must determine how to associate $I_3$ eigenvalues with those of $J_z$ for the H-F states.

Remembering the results of the previous chapter, one sees that by using scalar basis functions constructed from a H-F state with $J_z$ eigenvalue $K$, the correspondence is isomorphic, i.e. $I_3$ has eigenvalue $K$. This fact is crucial in the following developments where one is concerned with eliminating the singular term in the Hamiltonian associated with \( \mathcal{J}_3 \rightarrow 0 \).

Continuing now with the basic problem of finding the energy eigenvalue, keeping the above symmetry property in mind, a variational program will be developed. For the present case, as somewhat complicated procedure is required in order to handle the singular part of the Hamiltonian and yet establish a form useful for numerical treatment. The underlying principle is similar to the one used in two dimensions where the $\mathcal{S}$-functions were abandoned in favor of subsidiary conditions on the variations. However, because of the axial symmetry of the present example, things are not so simple since the subsidiary condition method entails the use of functions which are localized in angle, a situation missing for rotations about the
symmetry axis. Fortunately, this problem can be resolved by a careful examination of matrix elements as will presently be shown.

The first aspect to be considered is the elimination of the terms from the Hamiltonian which diverge as \( J_3 \rightarrow 0 \). To accomplish this, rewrite the Hamiltonian as

\[
H = H_0 + H_3 + V
\]

(5.101)

where

\[
H_0 = H - \frac{i}{2} \mathcal{d} (\eta_i^+ \eta_i^-) - \frac{i}{2} \mathcal{d} (I_i^+ I_i^- + J^+ J^-)
\]

(5.102)

\[
H_3 = \frac{i}{2} \mathcal{d} (I_3 - J_3)^2 - \frac{1}{2} \mathcal{d} (\eta_3)^2
\]

(5.103)

\[
V = -\frac{i}{2} (I_1 J_1 + I_2 J_2)
\]

(5.104)

Here, the notation \( \mathcal{J}_A \) designates the operators which are defined on the D-functions and one can readily check that this expression for \( H \) is indeed identical with the one at the beginning of this section. This form for \( H \) is chosen because as will now be shown, the \( H_3 \) term gives no contribution for low lying rotational bands.

As a prelude to this demonstration, the matrix elements of intrinsic operators in a scalar basis will be

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reviewed. Let $P(\eta)$ be the projection operator which takes H-F states to their scalar form and let $A(\eta)$ be some intrinsic operator. Then according to Chapter III, one has matrix elements of the form

$$\int dr \mathcal{J}(r(r)) \Phi^*_{n_x}(\vec{r}) A(\eta) \Phi_{n_x}(\vec{r}) =$$

$$\int dr \mathcal{J}(r(r)) \left( P(\eta) \Phi^{(v)}_{n_x}(r) \right)^* P(\eta) \left( A(\eta) \Phi_{n_x}(r) \right)$$

where $dr$ means integration over all 3A nucleon coordinates and $\vec{r}$ means the functions are evaluated at a point "rotated" by $\mathcal{R}(r)$. The $A(\eta)$ may be commuted as above because $P$ is purely collective. Now, because of the presence of the $\mathcal{J}$-function, one may set the $P$'s equal to their value at $\nu = 0$ which is 1. Moreover, since the $A$'s usually contain explicit $\mathcal{R}$ terms, one may use the $\mathcal{J}$-function to allow a replacement of $\tilde{A} \equiv A \big|_{\nu = 0}$. This is just what was done in the two-dimensional case and one need not worry about derivative terms in $A$ for the same reasons as given in that case.

Now consider applying this technique to the matrix elements of $H_3$ for states of the form $\mathcal{G}_{m,k}^\eta \Phi_{n_x}(\eta)$. Since the only collectively operating quantity here is $\mathcal{J}_3$, one may immediately do the collective integrations to get
\[ S d\mathcal{V} \left( \mathcal{D}_{m,k}^* \phi_{n\alpha}(\mathcal{V}) \right)^* H_3 \mathcal{D}_{m,k}' \hat{\phi}_{n\alpha}'(\mathcal{V}) = \]

\[ S d\mathcal{V} \mathcal{J}(n(r)) \mathcal{P}_{n\alpha}(\mathcal{V}) \left( \frac{1}{2J_3} (J_3 - \mathfrak{K})^2 - J_3 \hat{\eta}_3^2 - J_3 \hat{\eta}_3^2 \right) \phi_{n\alpha}(\mathcal{V}) \mathcal{J}_3' \mathcal{J}_m' \mathcal{J}_k' = \]

In the last line the tildes mean that all explicit angular dependence is set to zero or equivalently all of the $\mathcal{E}_{KA}'s$ go to $\mathcal{E}_{KA}$. This in particular makes the $J_3$ in $I_3$ go to $J_3$. Now remembering that the $\hat{\phi}'s$ are eigenfunctions of $J_3$, one sees that if $K = \mathfrak{K} = \mathfrak{K}'$, then the above matrix element vanishes. This is just an extension of the results of the previous chapter, i.e. the scalar functions are approximate eigenfunctions of $I_3$. However, in the present instance, because of dividing by $J_3$, one had to be careful with the term previously dropped which was proportional to $J_3$. The reason is, of course, because $\mathcal{J}_3 \eta_3^2$ does not vanish when $\mathcal{J}_3 \to 0$ since $\eta_3^2$ becomes singular to the same order.

With this result, it is apparent that if one is able to show that no matrix elements with $K \neq \mathfrak{K}$ occur in the perturbation program, then $H_3$ can effectively be eliminated from consideration since it always gives zero. This

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can immediately be demonstrated by noting that $V$ connects only states which preserve the $K = \mathcal{J}$ condition. For example,

$$
\int_{\mathcal{A}} \left( \mathcal{J}_{m,k}^{\mathcal{J}} \phi_{n,k}^{(\mathcal{J})} \right)^{K} \left( -\frac{i}{\hbar} \left( \mathcal{J}_{I_1} \mathcal{J}_{I_2} \mathcal{J}_{I_3} \right) \right) \mathcal{J}_{m,k'}^{\mathcal{J}} \phi_{n,k'}^{(\mathcal{J})} = (5.107)
$$

using the known matrix elements of the $\mathcal{J}$'s.\(^{(4)}\) Now since the $\phi^{(\mathcal{J})}$'s are approximate eigenstates of $I_3$ and because

$$
[I_1, \mathcal{J}_{I_2}, I_3] = I_1, -iI_2
$$

one sees that the above integral vanishes unless $\mathcal{J} = K + 1$. Here, because one does not have a $\frac{i}{\hbar} \mathcal{J}_{3}$, the results of the previous Chapter hold, i.e., the $\phi^{(\mathcal{J})}$'s become exact eigenstates when $\mathcal{J}_{3} \to 0$. The above example thus shows that the $K = \mathcal{J}$ condition is preserved by the perturbation which means that to all orders of perturbation theory one need only consider states of $H_0$ instead of $H_0 + H_3$. This corresponds to low lying levels since states with $H_3 \neq 0$ are higher in energy by roughly

$$
\frac{i}{\hbar} \mathcal{J}_{3} (K - \mathcal{J}) > 0
$$

which is, of course, infinite in lowest order.

It should be noted here that the commutation of the unperturbed Hamiltonian, $H_0 + H_3$, with $I_3$ was crucial in the above proof since one used states which approximate
simultaneous eigenstates of both operators. Thus, even though nature dictates the \( \frac{1}{\sqrt[3]{3}} \) singularity for axial symmetry, it allows an escape in the form of a conserved quantity which, when used correctly, eliminates the divergence.

Having disposed of the \( \frac{H}{3} \) part of the Hamiltonian, the next step is to formulate a practical procedure for performing the variation-perturbation program. As mentioned before, a practicality prerequisite is the elimination of the \( \hat{\sigma} \)-functions. However, one also wants the simplified forms of the operators i.e. evaluated at \( \sqrt{r}(r)=0 \). The latter is especially crucial here since the unsimplified operators for three dimensions are essentially useless because of their complicated form. To accommodate both requirements, the technique of replacing the \( \hat{\sigma} \)-functions by suitable subsidiary conditions on the variations will be employed. This follows exactly from the two dimensional discussion for directions perpendicular to the symmetry axis since these angles are well defined for the deformed H-F states. Put another way, the expectation value of the square of the angular momentum along one of these directions is large so that the dispersion in the conjugate angle is small via the uncertainty principle. Clearly, the above process is not valid for the angle associated with rotations.
about the symmetry axis since this angle is totally uncertain. Thus, it appears that the $\gamma$-function for that angle must be retained. Fortunately, as will be shown shortly, this is not the case.

Before demonstrating this fact, it is necessary to proceed with the simplification of the operators. According to the simplification prescription, one merely replaces all $\mathbf{E}_{KA}$'s by $\mathbf{S}_{KA}$'s and so one finds directly from Chapter II the following forms.

$$
\tilde{\eta}_1 = \left[ \frac{i}{2} \sum_{kz} \left\{ \mathbf{E}_{kz} \left[ H, T_{kz} \right] \mathbf{E}_{kz} + 2 \leftrightarrow 3 \right\} (\mathbf{Q}_5 - \mathbf{Q}_3)^{-1} \right]_{\mathbf{E}_{sA} \to \mathbf{S}_{sA}} \tag{5.109}
$$

$$
= \frac{1}{2} \left\{ \left[ H, T_{23} \right] + \left[ H, T_{32} \right] \right\} (\mathbf{Q}_5 - \mathbf{Q}_3)^{-1}
$$

$$
= \frac{i}{m} \frac{\sum (\gamma \rho_2 + \gamma \rho_3) \mathbf{Q}_5 (\mathbf{Q}_5 - \mathbf{Q}_3)}{\mathbf{Q}_5 (\mathbf{Q}_5 - \mathbf{Q}_3)}
$$

where the $\mathbf{Q}$'s are the $\mathbf{Q}$'s evaluated at $\mathbf{R}(r) = 0$, which according to Chapter II means that

$$
\mathbf{Q}_A = \left. \sum_{kz} \mathbf{E}_{kz} T_{kA} \mathbf{E}_{kA} \right|_{\mathbf{E} \to \mathbf{S}} = T_{AA} = \mathbf{Q}_A \tag{5.110}
$$

For review, remember that $T_{kA} = \sum_{kz} \mathbf{E}_{kz} V^{(k)} \mathbf{E}_{kA}$ and that $V^k$ commutes with $T_{kA}$, so that the commutators above come just for the kinetic energy. Now with this result for the $\mathbf{Q}$'s one finds

$$
\tilde{\eta}_1 = \frac{i}{m} \frac{\sum (\gamma \rho_2 + \gamma \rho_3) \mathbf{Q}_5 (\mathbf{Q}_5 - \mathbf{Q}_3)}{\mathbf{Q}_5 (\mathbf{Q}_5 - \mathbf{Q}_3)} \tag{5.111}
$$
which is analogous to the form $\frac{M}{\Delta}$ in two dimensions.

Also, in just the same way, one has

$$\vec{\eta}_z = \frac{1}{m} \sum \frac{\Sigma (xP_x zP_z)}{\Sigma (z^2 - x^2)}$$  \hspace{1cm} (5.112)$$

With these facts, one may now write down the simplified form of the Hamiltonian terms.

Before doing this, note that

$$-\frac{\hbar}{2m} \eta_z^2 + \frac{1}{2} \vec{J}_z \cdot \vec{J}_z = -\frac{\hbar}{2m} \eta_z^2 + \frac{1}{2} \eta_1^2 (\vec{J}_1 + \vec{J}_2 \cdot \vec{J}_3)$$  \hspace{1cm} (5.113)$$

$$= -\eta_1 \vec{J}_1 + \frac{\hbar}{2} \vec{J}_1$$

and similarly for the two component. Thus one has

$$\tilde{\mathcal{H}}_0 \equiv \left\{ \mathcal{H} - \eta_1 \vec{J}_1 - \eta_2 \vec{J}_2 + \frac{1}{2} \eta_1 \left( \vec{J}_1 + \vec{J}_2 \cdot \vec{J}_3 \right) \right\} \bigg|_{\epsilon \to \delta}$$  \hspace{1cm} (5.114)$$

$$= \mathcal{H} - \frac{1}{2m} \left\{ \sum \frac{\Sigma (yP_y + zP_z)}{\Sigma (y^2 - x^2)} \vec{J}_2 + \frac{1}{2} \sum \frac{\Sigma (xP_x + zP_z)}{\Sigma (z^2 - x^2)} \vec{J}_2 + h.c. \right\} +$$

$$\frac{1}{2} \bigg\{ \vec{J}_1 \cdot \vec{J}_1 + \vec{J}_2 \cdot \vec{J}_2 - \vec{J}_3 \cdot \vec{J}_3 \bigg\}$$

where, of course, the $\epsilon \to \delta$ condition does not apply for the $\vec{J}_3$ since this operates in a space not governed by the $\delta (\vec{n}(r))$. As a further reduction, make the usual approximations

$$m \Sigma (x^2 + z^2) \approx m \langle \Sigma (x^2 + z^2) \rangle = m \langle \Sigma (y^2 + z^2) \rangle \equiv R$$  \hspace{1cm} (5.115)$$

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\[ m \sum (y^2 - z^2) \leq m \langle \sum (y^2 - z^2) \rangle = m \langle \sum (x^2 - z^2) \rangle \leq \Delta \quad (5.116) \]

\[ m \sum (x^2 - z^2) \leq \Delta \quad (5.117) \]

\[ \frac{\mathcal{R}}{\mathcal{B}} = \frac{\sum (x^2 + z^2)}{m^2 (x^2 - z^2)^2} \leq \frac{\mathcal{R}}{\mathcal{B}^2} \equiv \mathcal{B} \quad (5.118) \]

Also define

\[ M_x \equiv \sum (y \rho_z + z \rho_y) \quad (5.119) \]

\[ M_y \equiv \sum (x \rho_z + z \rho_x) \quad (5.120) \]

Then one gets the approximate form, made up of just one and two body operators,

\[ \tilde{H}_0 \equiv H - \frac{1}{\mathcal{B}} \left\{ M_x J_x + J_x M_x - M_y J_y - J_y M_y \right\} + \frac{1}{\mathcal{B}} \mathcal{B} \left\{ J_x^2 - J_x^2 + J_y^2 - J_y^2 \right\} \quad (5.121) \]

Likewise, the perturbation becomes

\[ \tilde{V} \equiv \left\{ - \frac{\mathcal{R}}{\mathcal{B}} (I_1 J_1 + I_2 J_2) \right\} \mathcal{C}_{\mathcal{A}} = J_{\mathcal{A}} \quad (5.122) \]

\[ \triangleq - \mathcal{B} \left\{ (J_x \mathcal{R} M_x) J_1 + (J_y \mathcal{R} M_y) J_2 \right\} \]

Again demonstrating the results of the previous Chapter that the \( I \)'s are approximately isomorphic to the \( J \)'s
when the scalar basis functions are extended to a redundant space, since $\Delta R = \sim 0.2$.

As one will be dealing with states which have $J_z$ and $J^3_\text{z}$ eigenvalues, it is convenient to rewrite $\hat{\mathbf{V}}$ in the form of raising and lowering operators. To that end define

$$\Lambda_\pm \equiv (J_x - \frac{\Delta}{R} M_x) \pm i (J_y + \frac{\Delta}{R} M_y)$$

(5.123)

Then noting that

$$[J_z, M_x] = [J_z, \Sigma (y \rho_x + z \rho_y)] = -i \Sigma (x \rho_x + z \rho_z)$$

(5.124)

$$= -i M_y$$

and

$$[J_z, M_y] = i M_y$$

(5.125)

one finds

$$[J_z, \Lambda_\pm] = \pm \left( (J - \frac{\Delta}{R} (-M_y)) \pm i (-\Lambda)(J_x + \frac{\Delta}{R} (-M_x)) \right)$$

(5.126)

$$= \pm \left\{ (J_x - \frac{\Delta}{R} M_x) \pm i (J_y + \frac{\Delta}{R} M_y) \right\}$$

$$= \pm \Lambda_\pm$$

Thus the $\Lambda$'s act like raising and lowering operators.

Also introduce
\[ J_\pm = J_1 \mp i J_2 \]  

which according to the body fixed commutation rules, satisfy

\[ [J_3, J_\pm] = \pm J_\pm \]  

Then one finds

\[ \hat{\nabla} \cong -\frac{\alpha}{4} \left\{ (\Lambda_+ + \Lambda_-)(J_+ + J_-) + (\Lambda_+ - \Lambda_-)(J_+ - J_-) \right\} \]
\[ = -\frac{\alpha}{2} \left\{ \Lambda_+ J_+ + \Lambda_- J_- \right\} \]

which, by the way, because the raising and lowering operators are paired, shows why \( H_3 \) remains zero.

Now consider matrix elements of \( \hat{\nabla} \). Clearly, because of the \( K = \eta \) condition, the only non zero ones are of the form, for example,

\[ \int d\hat{r} \hat{\nabla} J_{n_k}(\hat{r}) J_+ B_{m_{\kappa_1}}^{*}(\hat{r}) \int d\hat{r} \hat{\delta}(\hat{r}) \phi_{n_\kappa}^{*}(\hat{r}) \Lambda_+ \phi_{n\kappa'}^{(r)} = \]  

\[ \sqrt{J(J+1)-K(K-1)} \int d\hat{r} \hat{\delta}(\hat{r}) \phi_{n_\kappa}^{*}(\hat{r}) \Lambda_+ \phi_{n\kappa'}^{(r)} \]

where \( \phi \) is the angle of rotation about the symmetry axis, i.e. conjugate to \( J_z \). Now since \( \Lambda_+ \) is a raising operator, \( \Lambda_+ \phi_{n\kappa'}^{(r)} \) is an eigenstate of \( J_z \) with eigenvalue \( K \).

This means that the combination \( \phi_{n_\kappa}^{*}(r) \Lambda_+ \phi_{n\kappa'}^{(r)} \) is independent of \( \phi \) because if one considers a rotation...
about $z$ of $\alpha$, then one finds

$$
\Phi_{n_z}^{(r)} \Lambda \Phi_{n_{z', k}}^{(r)} \rightarrow (e^{-i\omega k_{n_z}} \Phi_{n_z}^{(r)})^* e^{-i\omega k_{n_{z'}}} \Lambda \Phi_{n_{z'}}^{(r')}
\quad (5.131)
$$

$$
\Phi_{n_z}^{(r)} \Lambda \Phi_{n_{z'}}^{(r)'} =
\Phi_{n_{z'}}^{(r)} \Lambda \Phi_{n_z}^{(r)'}
$$

Thus for these matrix elements the $\mathcal{S}(\Psi)$ contributes only a constant independent of the $n$'s and $k$'s. More explicitly, doing the integration without the $\mathcal{S}(\Psi)$ gives only an extra $2\pi$ remembering from Chapter III that $\int d\Psi \mathcal{S}(\Psi)$ gives integration over only intrinsic coordinates.

The other matrix elements which will appear in the perturbation calculation are, of course, those with $\tilde{H}_0$. As will now be shown, these also have the property that $\mathcal{S}(\Psi)$ contributes only a constant factor. This is because

$$
[[J_z, \tilde{H}_0] = [[J_z, \mathcal{H}^{-1/2} \mathcal{J}_z \{M_x J_x - M_y J_y + h.c.\} + \mathcal{B}[J_z, \{J_x J_y J_x J_y\} + \mathcal{B}_0 [J_z, \{J_x J_y J_x J_y\} + h.c.]\]
\quad (5.132)
$$

$$
= -\frac{i}{2\Delta} \left\{ -M_y J_x + M_x J_y \right\} - (M_x J_y - M_y J_x) + h.c.
$$

$$
= 0
$$

using the facts that $\mathcal{H}$ is rotationally invariant and $J_z$ commutes with $J_x, J_y$ as well as the fact that $\mathcal{J}_z$ and the $\tilde{\mathcal{J}}$'s operate in different spaces. Thus, since $\tilde{H}_0$ is diagonal in the $D$-functions and one has the $K=\nu$
condition, the only non zero elements are

\[ \int d^3 r \, \delta^{(4)}(\vec{r}) \left( \mathcal{O}^{(n)}_{m_x} \phi^{(r)}_{n_k} \right) \mathcal{H}_0 \, \mathcal{O}^{(n')}_{m_x'} \phi^{(r)}_{n'_k} \]  

(5.133)

\[ \int d^3 r \, \delta^{(4)}(\vec{r}) \phi^{(r)}_{n_k} \left\{ \mathcal{H} - \frac{i}{2} \mathcal{A} \left( M_x J_x - M_y J_y + h.c. \right) + \frac{i}{2} B \left( J^x - J^x_z + J^x (J^x + i) - K^2 \right) \right\} \phi^{(r)}_{n'_k} \]

Now, because of the above commutation property with \( J_z \), one sees again that the quantity to the right of \( \delta^{(4)}(\vec{r}) \) is \( \psi \) independent. Consequently, dropping \( \delta^{(4)}(\vec{r}) \) involves only a renormalization again.

In review, before solving the perturbation problem, one finds that although axial symmetry gives rise to certain difficulties in the initial formulation, these can be eliminated essentially because one does have axial symmetry and is concerned with low lying states. For the \( \frac{1}{\epsilon_3} \) divergence, the existence of a conserved component of intrinsic angular momentum allowed an elimination of the entire apparently singular term. For the impossibility of dropping \( \delta^{(4)}(\vec{r}) \) on grounds of angular resolution, this same procedure showed that for matrix elements of interest, \( \delta^{(4)}(\vec{r}) \) gives only an overall factor and thus may be eliminated by symmetry arguments. Thus one is left with the very much simplified problem of using \( \mathcal{H}_0 \) and \( \mathcal{V} \) in a restricted variation process, the restriction being the
subsidiary conditions coming from the removal of the \( \mathcal{S} \)-functions.

Proceeding now with the solution of the energy eigen-value problem, the techniques and approximations essentially duplicate the two dimensional case. First, the so far unspecified \( H \rightarrow F \) are chosen as those of \( H \) and it is assumed that the axes of the well are oriented such that

\[
\langle \Sigma x z \rangle = \langle \Sigma y z \rangle = 0 \quad (5.134)
\]

for the ground state. Also, as in two dimension, use the approximations

\[
\langle \phi | J_{(z)}^i \phi \rangle \approx 0 \approx \langle \phi | J_{(z)}^f M_{(z)}^j \phi \rangle 
\quad (5.135)
\]

based on the rough argument given there. It should be again mentioned that in a particular case, this may have to be corrected for by adding these to the perturbation. However, in the lowest order of perturbation theory, as used here, this should not affect the rotational energies since the equations determining the operators giving first order changes in the wavefunctions are linear.

With these preliminaries, the problem can now be stated as finding the best variational solution for

\[
\tilde{H} \equiv \tilde{H}_o + \tilde{V} + \lambda \sum x z + \lambda \sum y z 
\quad (5.136)
\]
to lowest order in the perturbations. Here, the subsidiary conditions are again chosen, on the grounds of simplicity, to be those which guarantee that the average values of \( \Sigma xz \) and \( \Sigma yz \) remain zero. These are, of course, just the conditions for the arguments of the \( \sigma \)-functions, which were dropped, to vanish. It will turn out that the \( \lambda \)'s must be operators in collective, that is \( \mathcal{J} \), space in order that the subsidiary conditions hold for the proper matrix element, i.e. those generated by \( \vec{V} \). As in two dimensions, this is a consistent procedure since \( \Sigma xz \) and \( \Sigma yz \) commute with both \( \vec{H}_0 \) and \( \vec{V} \) as will now be shown. First note that

\[
\left[ J_x, \Sigma xz \right] = -i \sum_y \langle x y \rangle = 0 \tag{5.137}
\]

\[
\left[ J_y, \Sigma xz \right] = -i \sum_y \left( \bar{z} \cdot \bar{x} \right) \sum_y \frac{\Delta}{m} \tag{5.138}
\]

\[
\left[ M_x, \Sigma xz \right] = -i \sum_y \langle y x \rangle = 0 \tag{5.139}
\]

\[
\left[ M_y, \Sigma xz \right] = -i \sum_y \left( \bar{z} \cdot \bar{x} + \bar{x} \cdot \bar{z} \right) \sum_y \frac{\bar{R}}{m} \tag{5.140}
\]

In the above, the usual approximation of replacing summed coordinate pairs was used as well as the axial symmetry property which says \( \Sigma xy \) and \( -\Sigma xy \) occur with equal probability. Besides the commutators, one needs
\[
[H, \sum x \hat{z}] = -\frac{i}{\hbar} \sum \left( \hat{z} p_x + x p_z \right) = -\frac{i}{\hbar} M_y
\] (5.141)

Then, since the $J$'s operate in a different space, one has

\[
[\hat{\mu}_0, \sum x \hat{z}] = -\frac{i}{\hbar} M_y + \frac{i}{\hbar} \left\{ \frac{-\hbar}{\hbar} J_y + M_y (\frac{\hbar}{\hbar}) + B \left\{ (\frac{\hbar}{\hbar}) J_y \right\} \right\}
\] (5.142)

\[
= 0
\]

using the fact that $B = \frac{\hbar}{\hbar}$. Also, the last terms follows from the fact that $J^2 = J_y^2 + J_y^2$. Now the other commutator to be checked is

\[
[\hat{\nu}, \sum x \hat{z}] = -B \left[ J_y + \frac{\hbar}{\hbar} M_y, \sum x \hat{z} \right] J_z
\]

\[
= -i B \left\{ \frac{\hbar}{\hbar} - \frac{\hbar}{\hbar} (\frac{\hbar}{\hbar}) \right\} J_z = 0
\] (5.143)

giving the desired result. Clearly, a similar argument holds for $\sum y \hat{z}$ so that, as stated, the subsidiary conditions are consistent with the diagonalization.

To aid in the formulation of the perturbation solution, introduce the notation

\[
|JmK; nK'\rangle \equiv \mathcal{O}^{m\gamma}_{m\gamma} \phi^{(r)}_{nK'}
\] (5.144)

and reserve $(n,K') = (0,K_0)$ for the ground state which is, of course, the H-F ground state of $H$. Because of the H-F condition that $H$ connect no one particle to vacuum states
and because of the approximations stated by equation (135), one has that

\[ \langle J m \kappa_0 \kappa_0 | \hat{H}_0 | J m \kappa_0 \kappa_0 \rangle = 0 \] (5.145)

for all one particle states, (nK) i.e. one also has an approximate H-F state for \( \hat{H}_0 \). The perturbation-variation program can now be stated as finding the best trial function of the form

\[ |F\rangle \equiv e^{i\mathcal{F}} |J m \kappa_0 \rangle (5.146)\]

to lowest order in the perturbations which are

\[ V_{\text{ext}} = -\frac{B}{2} \left\{ \mathcal{J}_+ \mathcal{J}_+ + \mathcal{J}_- \mathcal{J}_- \right\} + \lambda_1 x^2 + \lambda_2 z^2 \] (5.147)

This form suggests one define

\[ \mathcal{F} = F_+ \mathcal{J}_+ + F_- \mathcal{J}_- + \lambda_1 g_1 + \lambda_2 g_2 \] (5.148)

with the \( F \)'s and \( g \)'s one particle operators. In regard to this, one should note that \( |F\rangle \) is \textbf{not} of the form of a sum of products of D-functions and determinants, since the \( \mathcal{J} \)'s operating on the D's are contrary to Thouless theorem. However, in the first order expansion of the exponential, as used here to find \( F \), the coefficients of the D's are simple determinants and thus trial functions of this type are still useful since the known properties

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of the H-F basis may still be used. The present complications are, of course, due to the more complex nature of the three dimensional rotational problem as reflected in the fact that the "coupling constants", $\mathcal{J}_3$, are operators, i.e. one can not simultaneously diagonalize $\mathcal{J}_\pm$ and $\mathcal{J}_3$.

With this trial function, one can as usual restate the problem in the equivalent form of finding $\mathcal{F}$ such that

$$\hat{\mathcal{H}} = e^{-i\mathcal{F}} (\hat{H}_0 + \hat{V} + \lambda_1 \mathcal{L}_x + \lambda_2 \mathcal{L}_y) e^{i\mathcal{F}}$$

(5.149)

has $|JmK_0;0K_0\rangle$ as a H-F ground state to lowest order in $V_{\text{pert}}$. Thus one requires

$$0 = \langle JmK_0;0K_0 | \hat{\mathcal{H}} | JmK;nk \rangle$$

(5.150)

$$\equiv \langle JmK_0;0K_0 | \hat{H}_0 + i[\hat{H}_0, \mathcal{F}] + \hat{V} + \lambda_1 \mathcal{L}_x + \lambda_2 \mathcal{L}_y | JmK';nK' \rangle$$

for all one particle $n$'s. As shown above, the $H_0$ contribution vanishes for these states. So equating coefficients of each coupling constant to zero gives the following four equations

$$\langle JmK_0;0K_0 | i[\hat{H}_0, \mathcal{F}_2] - B \mathcal{L}_z \mathcal{J}_2 | JmK;nk \rangle = 0$$

(5.151)

$$\langle JmK_0;0K_0 | i[\hat{H}_0, \mathcal{F}_1] + \lambda_1 \mathcal{L}_x \mathcal{J}_1 | JmK;nk \rangle = 0$$

(5.152)

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\[ \langle J m k_0; 0 k_0 | i [\tilde{H}_0, \lambda_z q_2] + \lambda_z \Sigma Y Z | J m k; n k \rangle = 0 \] (5.153)

where the \( \lambda \)'s are kept in the commutators since they are in general operators in D-function space. These are the fundamental equations for the solution of the axial symmetry case.

First consider the equations for the \( F_\pm \). The only part of \( \tilde{H}_0 \) which does not commute with \( J^\pm \) is the term \( -\frac{1}{2} B J_z^2 \). However, in the above matrix elements, one sees that \( k_0 = k_0 + 1 \) so that this term gives \( \frac{1}{2} B (k_z^2 - (k_z')^2) \) which represents a slight contribution from a zero point shift in energy. Since, for rotational states, the energy spacing is much smaller than for intrinsic spacing, this can be ignored. The reason is, of course, because the rest of the \( \tilde{H}_0 \) commutator is essentially the intrinsic spacing, i.e. roughly \( (\langle 0 k_0 | \hat{A}_z | 0 k_0 \rangle - \langle n k | \hat{A}_z | n k \rangle) F_\pm \). Thus one gets the simplification

\[ \langle J m k_0; 0 k_0 | [\hat{A}_z, F_\pm J_z] | J m k; n k \rangle \approx \langle J m k_0; 0 k_0 | [\hat{A}_0, F_\pm J_z] | J m k; n k \rangle \] (5.154)

and

\[ \langle 0 k_0 | i [\hat{A}_0, F_\pm] - \frac{B}{2} \lambda_z | n k, k_0 \pm 1 \rangle = 0 \] (5.155)

Before continuing, it should be noted that since \( \tilde{H}_0 \) commutes with \( J_z \), these equations show that \( F_\pm \) transform
exactly like $\Lambda_{\pm}$ under rotations about $z$ i.e. $e^{-i\hbar J_{z}^*} e^{i\hbar J_{z}}$ are generated by $e^{-i\hbar J_{z}^*} \Lambda_{z} e^{i\hbar J_{z}}$. This fact will be useful later.

Turning now to the $g$'s, it is clear that since the $\lambda$'s must generate collective states connected by $\tilde{V}$, they must be some linear combination of $J_{\pm}$. Thus, the above arguments may also be used here to get

$$\langle \tilde{J}_{mk}; 0, k | (i[H_{o}, g^{(I)}] + (I_{XZ}^{\pm})) (\lambda_{z}^{+}) \tilde{J}_{mk}; n \rangle = 0 \quad (5.156)$$

It will be convenient to take linear combinations of these equations to obtain

$$\langle \tilde{J}_{mk}; 0, k | (i[H_{o}, g^{(I)}] + (I_{XZ}^{\pm})) (\lambda_{-}^{+}) \tilde{J}_{mk}; n \rangle = 0 \quad (5.157)$$

where

$$g_{\pm} = g_{1} \pm i g_{2} \quad (5.158)$$

$$\Sigma_{\pm} = \Sigma_{x\pm} \pm i \Sigma_{y\mp} \quad (5.159)$$

$$\lambda_{\pm} = \lambda_{1} \pm i \lambda_{2} \quad (5.160)$$

The reason is that

$$[J_{z}, \Sigma_{\pm}] = i (\Sigma_{y\mp} \mp i \Sigma_{x\pm}) = \mp \Sigma_{\pm} \quad (5.161)$$

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so that $\sum_\pm$ can connect states only with $K = K_0 + 1$
respectively. This means, then that $\lambda_\pm$ are proportional
to $J_\pm$ respectively and thus one has after integrating
out the collective variables

$$\langle 0_{K_o} \mid i[A_z, g_\pm + \sum_\pm n, k_o \mp \rangle = 0$$

(5.162)

As above, one immediately sees that $g_\pm$ transform like
$\sum_\pm$ under rotations about $Z$.

With these results, one may now proceed to find out
what $\lambda_\pm$ are by applying the subsidiary conditions.

These are

$$\langle F \mid \lambda_\pm \sum_\pm F \rangle = \langle Jm_k_o; o_k_o \mid i[\lambda_\pm \sum_\pm, F] \mid Jm_k_o; o_k_o \rangle = 0$$

(5.163)

where $\lambda$'s are included to insure that one gets the correct
collective states. It is convenient to rewrite the $\lambda$'s
as

$$\lambda_\pm = A_\pm J_\pm$$

(5.164)

Then, inserting $F$ for the $\lambda_+$ equation gives

$$\langle Jm_k_o; o_k_o \mid J_+^2 [\Sigma_+, F_+] + [J_+, J_-] \Sigma_+ F_+ + J_- J_+ [\Sigma_+, F_+] +$$

$$A_+ J_+^2 [\Sigma_+, g_+] + A_- J_- J_+ [\Sigma_+, g_-] + A_- \Sigma_+ g_- [J_+, J_-] \mid Jm_k_o; o_k_o \rangle = 0$$

(5.165)
But the $\mathcal{J}^2_+$ terms are zero since these are diagonal elements in $K_0$. Moreover

$$\{\mathcal{J}_+^+, \mathcal{J}_-\} = [\mathcal{J}_+^+, i\mathcal{J}_z, \mathcal{J}_+^+ + i\mathcal{J}_z] = 2\mathcal{J}_z$$  \hspace{1cm} (5.166)

and

$$\mathcal{J}_+^+ \mathcal{J}_- = \mathcal{J}_+^+ \mathcal{J}_+^+ + \mathcal{J}_z [\mathcal{J}_+, \mathcal{J}_z] = \mathcal{J}_+^2 - \mathcal{J}_z^2 + \mathcal{J}_3$$  \hspace{1cm} (5.167)

Thus, one finds simply

$$\langle 0K_0 | 2K_0 (\Sigma_e F_+ A_+ \Sigma_e g_3) + (J(J+1)) - K_0 (K_0 + 1)(\Sigma_e F_+ A_+ \Sigma_e g_3) \rangle | 0K_0 \rangle = 0$$  \hspace{1cm} (5.168)

giving

$$A_- = \left[ \frac{- (J(J+1) - K_0 (K_0 + 1)) \langle \Sigma_e F_+ \rangle - 2K_0 \langle \Sigma_e F_+ \rangle}{(J(J+1) - K_0 (K_0 + 1)) \langle \Sigma_e g_3 \rangle + 2K_0 \langle \Sigma_e g_3 \rangle} \right]$$  \hspace{1cm} (5.169)

In exactly the same way, one finds

$$A_+ = \left[ \frac{- (J(J+1) - K_0 (K_0 + 1)) \langle \Sigma_e F_+ \rangle + 2K_0 \langle \Sigma_e F_+ \rangle}{(J(J+1) - K_0 (K_0 + 1)) \langle \Sigma_e g_3 \rangle - 2K_0 \langle \Sigma_e g_3 \rangle} \right]$$  \hspace{1cm} (5.170)

and thus giving a complete solution for the Lagrange multipliers.

The only thing left to do is to calculate the energy to second order and thereby obtain the moment of inertia. Because of the particular form of the subsidiary conditions, one has, as in two dimensions,
\[ E = \langle \jmath m k_0; \alpha k_0 | e^{-iF} (\hat{A}_0 + \hat{V}) e^{iF} | \jmath m k_0; \alpha k_0 \rangle \]  \hspace{1cm} (5.171)

\[ = \langle \jmath m k_0; \alpha k_0 | \hat{A}_0 + \hat{V} + i [\hat{A}_0 + \hat{V}, F] - \frac{i}{2} [\hat{A}_0, F] \cdots | \jmath m k_0; \alpha k_0 \rangle \]

\[ = \langle \jmath m k_0; \alpha k_0 | \hat{A}_0 + \frac{i}{2} [\hat{V}, F] | \jmath m k_0; \alpha k_0 \rangle \]

This last form follows from three facts. First, since \( \hat{A}_0 \) can not connect \( | \alpha k_0 \rangle \) to any one particle states and since \( F \) generates only such states, the \( [\hat{A}_0, F] \) term vanishes. Second, equation (150) allows one to infer

\[ \langle \jmath m k_0; \alpha k_0 | [i [\hat{A}_0, F], F] | \jmath m k_0; \alpha k_0 \rangle = - \langle \jmath m k_0; \alpha k_0 | \hat{V} + \lambda \sum x \hat{z} + \lambda, \lambda \hat{z} \hat{z} + \lambda, \lambda \hat{z} \hat{z} \rangle | \jmath m k_0; \alpha k_0 \rangle \]  \hspace{1cm} (5.172)

while the subsidiary conditions give that the last two terms in the commutator on the right vanish. Consequently,

\[ \langle \jmath m k_0; \alpha k_0 | [i [\hat{A}_0, F], F] | \jmath m k_0; \alpha k_0 \rangle = - \langle \jmath m k_0; \alpha k_0 | [\hat{V}, F] | \jmath m k_0; \alpha k_0 \rangle \]  \hspace{1cm} (5.173)

from which part of the last line above follows. Finally, since \( \hat{V} \) contains only \( \mathcal{J}_+ \), it has no diagonal elements.

To extract the rotational energy, insert the explicit forms for the operators above. Then one has

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\[ E = \langle J' m \kappa_0; \sigma \kappa_0 | H - \frac{i}{\hbar} \{ M_x J_x - M_y J_y + h.c. \} + \]
\[ \frac{1}{2} B \{ J^+ - J_- + J'(J'+1) - K^2 \} - \frac{i B}{4} \left[ (\Lambda_+ J_+ + \Lambda_- J_-) \right. \]
\[ \left. (F_+ J_+ + F_- J_- + \frac{i}{2} A_+ J_+ g_+ + \frac{i}{2} A_- J_- g_-) \right] | J' m \kappa_0; \sigma \kappa_0 \rangle \]

Examining the commutator term, using the forms for \([ J_+, J_- ] \)
and \(J_+ J_-\) given above, one gets
\[ -\frac{i B}{4} \langle J' m \kappa_0; \sigma \kappa_0 | \{ \Lambda_+ F_+ + \frac{i}{2} A_- g_- \} J_+ J_- + [ J_-, J_+] \Lambda_+ (F_+ + \frac{i}{2} A_- g_-) + \]
\[ \{ [\Lambda_+ F_+ + \frac{i}{2} A_- g_-] + [\Lambda_- F_+ + \frac{i}{2} A_+ g_+] \}(J'(J'+1) - K^2) + \]
\[ \{ [\Lambda_+ F_+ + \frac{i}{2} A_- g_-] + [\Lambda_- F_+ + \frac{i}{2} A_+ g_+] \} + 2 \Lambda_+ (F_+ + \frac{i}{2} A_- g_-) - \]
\[ 2 \Lambda_- (F_+ + \frac{i}{2} A_+ g_+) \} K_0 \sigma \kappa_0 \rangle \]

At this point the transformation properties of the \(\pm\)
type operators under rotations about \(Z\) developed before
can be used to greatly simplify this expression. Remembering
that \(F_\pm\) transform like \(\Lambda_\pm\) and that \(g_\pm\) transform like \(\Sigma_\pm\) and moreover, that \(\Lambda_\pm\) and \(\Sigma_\pm\) transform identically (i.e., like \(J_\pm\)), one has the following result. Consider any of these operators, say \(O_\pm\). Then under a rotation about \(Z\) of \(-\frac{\pi}{2}\) one has
\[ O_\pm = O_x \pm i O_y \rightarrow -O_y \pm i O_x = \pm i O_\pm \]
(5.176)
Consequently, in the above matrix elements, one has

\[
\langle 0 k_0 | 0, p, | 0 k_0 \rangle = \langle 0 k_0 | e^{-i \frac{p^2}{2}} e^{i \frac{p \cdot q}{2}} (0, p) e^{-i \frac{q^2}{2}} e^{i \frac{q \cdot k_0}{2}} | 0 k_0 \rangle = \langle 0 k_0 | O^- p_+ e^{i \frac{p \cdot k_0}{2}} | 0 k_0 \rangle = \langle 0 k_0 | O^- p_+ | 0 k_0 \rangle
\]

where $O$ and $p$ are representative operators. This means that the matrix element reduces to

\[
- \frac{i B}{\hbar} \langle 0 k_0 | \left\{ 2 [\Lambda_+, F_-] + \left( \frac{A_+ A_-}{2} \right) [\Lambda_+, F_-] \right\} (J'(J'+1) - K_0^2) + \left\{ (\frac{A_+ A_-}{2}) [\Lambda_+, F_-] + 2 \Lambda_+ F_- \right\} | 0 k_0 \rangle
\]

To get the moment of inertia, one must clearly separate off the rotational energy, i.e. that proportional to $J'(J'+1) - K_0^2$. Unfortunately, the $A$'s also depend slightly on this quantity so that in any particular case, one must examine the subsidiary conditions in detail to extract all of the rotational energy.

Looking back at the definition of $A_+$, one sees that if $K_0 = 0$, one can immediately get the moment of inertia since then

\[
A_+ = - \frac{\langle \Sigma_+, F_- \rangle}{\langle \Sigma_+, F_+ \rangle} = A_-
\]

using the facts from above that $\langle [\Sigma_+, F_-] \rangle = \langle [\Sigma_-, F_+] \rangle$ and $[\Sigma_+, g_-] = [\Sigma_-, g_+]$. Considering this special
case, one finds that the matrix element above becomes

\[-\frac{jB}{2} \langle \chi | \{ \Lambda^+, F_+ \} \frac{\langle [\Lambda^+, F_+] \rangle}{2 \langle [\Lambda^+, g] \rangle} | 00 \rangle \langle J' + 1 \rangle \]  

(5.180)

Thus combining this with the unperturbed rotational energy given by equation (174), one readily gets for the inverse moment of inertia

\[ \Theta' = B \{ 1 - j \langle [\Lambda, F] \rangle - \frac{\langle [\Lambda^+, F_+] \rangle \langle [\Lambda^+, g] \rangle}{2 \langle [\Lambda^+, g] \rangle} \} \]  

(5.181)

a form exactly similar to equation (67) for two dimension. To put this result in a more familiar form, introduce the usual approximation of replacing commutators of the \( F \)'s and \( g \)'s by their expectation values. Then equation (155), defining \( F_- \), becomes

\[ \langle 00 | i [H, F_-] - \frac{j}{2} \{ M_x \langle [J_x, F_-] \rangle + J_x \langle [M_x, F_-] \rangle - M_y \langle [J_y, F_-] \rangle - J_y \langle [M_y, F_-] \rangle \} - \frac{jB}{2} \Lambda^- | n, 1 \rangle = 0 \]  

(5.182)

This can be reduced by noting that for both \( M_y \) and \( J_y \) one has

\[ \langle 00 | O_y | n \rangle = \langle 00 | e^{-jF_y} (e^{i\frac{j}{2} J_y} O_y e^{-i\frac{j}{2} J_y}) e^{i\frac{j}{2} J_y} | n \rangle \]  

(5.183)

\[ = i \langle 00 | e^{i\frac{j}{2} J_y} O_y e^{-i\frac{j}{2} J_y} | n \rangle \]

Then looking back at the commutation relations of \( M_y \) and
\( J_y \) with \( J_z \) one sees

\[
e^{-i \frac{\mu}{\hbar} J_z} M_y e^{i \frac{\mu}{\hbar} J_z} = -M_x
\]

(5.184)

and

\[
e^{i \frac{\mu}{\hbar} J_z} J_y e^{-i \frac{\mu}{\hbar} J_z} = J_x
\]

(5.185)

which means one may replace \( M_x \) by \(-i M_x\) and \( J_y \) by \( i J_x\) in the above equation to get

\[
\langle 0| \hat{J}_z \langle H, F, 1 \rangle - \hat{J}_x \{ M_x \langle \hat{J}_x + i \hat{J}_y, F, 1 \rangle + \hat{J}_x \langle [M_x - i M_y, F, 1] \} + \frac{i}{\hbar} \lambda^- | n 1 \} = 0
\]

(5.186)

A very compact final form can now be obtained using the following facts.

\[
\begin{align*}
B(J_x + i J_y) - \frac{i}{\hbar} (M_x - i M_y) &= B \lambda^+ \\
J_x &= \frac{J_+ + J_-}{2} \\
M_x &= i m \left[ H_x, \Sigma_y \Sigma_z \right] ; \quad M_y = i m \left[ H_x, \Sigma_x \Sigma_z \right] \\
\lambda^- &= J_- - \frac{\Delta}{\hbar} (M_x + i M_y) = J_- + \frac{m \Delta}{\hbar} \left[ H_x, \Sigma_- \right] \\
\langle 0|0| \langle H, \Sigma_+ - \Sigma_- | n 1 \} &= \frac{m}{2} \langle 0|0| \langle H, \Sigma_+ - \Sigma_- | n 1 \} = -\frac{m}{2} \langle 0|0| \langle H, \Sigma_- | n 1 \}
\end{align*}
\]

(5.187 - 5.191)
Then, the equation defining $F_-$ becomes

$$
<00| i [H, F_+ + \frac{m}{2\hbar} (\langle \xi_y, F_+ \rangle + i) \Sigma_-] - \frac{\hbar}{2} J_+(1 - i \langle \xi_y, F_+ \rangle) |n\rangle = 0
$$

(5.192)

which upon defining

$$
G_- = \frac{\hbar}{\beta} \left[ \frac{F_- + \frac{m}{2\hbar} (\langle \xi_y, F_+ \rangle + i) \Sigma_-}{1 - i \langle \xi_y, F_+ \rangle} \right]
$$

(5.193)

gives the usual first Thouless-Valatin form

$$
<00| i [H, G_-] |n\rangle = <00| J_- |n\rangle
$$

(5.194)

Trying the second of the pair, one finds

$$
<00| i [J_+, G_-] |00\rangle = \frac{2}{\beta (1 - i \langle \xi_y, F_+ \rangle)} \left( \langle \xi_y, F_+ \rangle + \frac{m}{2\hbar} (\langle \xi_y, F_+ \rangle + i) \langle \xi_y, \Sigma_\uparrow \rangle \right)
$$

(5.195)

$$
= \frac{2}{\beta (1 - i \langle \xi_y, F_+ \rangle)}
$$

using the result

$$
\langle [J_+, \Sigma_\uparrow] \rangle = \langle [J_\uparrow \times J_\downarrow, \Sigma_\uparrow \Sigma_\downarrow - i \Sigma_\uparrow \Sigma_\downarrow] \rangle = \langle \delta (\xi_y + \gamma) + \delta (\xi_y - \gamma) \rangle = -2 \frac{A}{\hbar}
$$

(5.196)

According to the Thouless-Valatin theory, one should get twice the moment of inertia since $J_+$ and $G_-$ contain both $x$ and $y$ parts i.e. the above commutator is really

$$
<00| i ([J_\uparrow, G_\uparrow] + [J_\downarrow, G_\downarrow]) |00\rangle = 2 <00| i [J_\uparrow, G_\uparrow] |00\rangle
$$

owing to axial symmetry. As with the two dimensional case, there is a disagreement due to the subsidiary condition giving
another term in $\theta'$ (see eq. (181)). However, since the present results are practically identical with the two dimensional ones, it is clear that the discussion of the correction exactly parallels that case. In particular, one expects that the Thouless-Valatin equations essentially result for system with large deformations since then the correction term vanishes.

This section, as in two dimensions, can be concluded with the statement that Tomonaga's method plus redundant variables furnishes a convenient and valid framework for discussing nuclear rotation. The criterion for this judgement is, of course, the fact that one gets the Thouless-Valatin equations in some lowest approximation. These should not be considered the fundamental result though. Instead, they should be held as a convenient and familiar starting point from which improvements, via "soup ing up" the approximations involved, may be made. This is especially the case in this three dimensional case where more sources of correction, such as the $J$ dependent of the Lagrange multipliers for $K \neq 0$ systems, are present.

D. **Axially Asymmetric**

To complete the discussion of application of redundant H-F to three dimensions, the case where the nucleus does
not possess axial symmetry will be briefly discussed. This problem will be considered within the framework of ignoring the $\delta$-functions and not using simplified operators, i.e. similar to the first treatment in two dimensions. The reason is that here one is considered mostly with the general structure of the solution and not with applications to real systems. Thus, the approach with the simplest algebraic form is chosen.

The asymmetric case possesses the advantage that in general there exists no zero order moments of inertia which are nearly zero. This is because the three quadrupole eigenvalues, $Q_A$, are usually quite distinct and thus for a stable nuclear shape the $J_A$'s don't just depend on fluctuations as $J_3$ did in the previous case. As a result of this fact, one need not go through a special treatment of the unperturbed problem in order to eliminate terms containing $J_A$ factors. Instead, the Hamiltonian may be split into intrinsic plus rotational parts with a perturbation of the form $\sum_{A}^{3} H_A J_A$.

As for the complications of this case, consider the unperturbed Hamiltonian

$$h = H_0 + \frac{1}{2} \sum_{A}^{3} J_A J_A^2$$  \hspace{1cm} (5.197)
where the original separated form of Chapter II, 
\[ H = H_0 + \sum_A \mathcal{H}_A \mathcal{J}_A + \sum_A \frac{1}{2} \mathcal{J}_A^2 \mathcal{J}_A^2, \]
is used. Note that one need not include any \( P \)'s or \( S \)'s since \( I_3 \) eigenstates are not required. Since the \( \mathcal{J}_A \)'s are in general different the rotational energy won't be diagonalized by a simple function. Instead, one must use a linear combination of the form

\[ S_J = \sum_{k=J}^{J} a_k^m \mathcal{S}^m_{m_k} \]  
(5.198)

where the \( a_k^m \)'s are determined by diagonalizing the matrix

\[ R_{kk'} = \int d\mathcal{J} \mathcal{S}^m_{m_k} \left( \sum_A \frac{1}{2} \mathcal{J}_A^2 \mathcal{J}_A^2 \right) \mathcal{S}^m_{m_k'}, \]  
(5.199)

This is, of course, a complicated algebraic procedure and in most cases no simple expression for the \( a_k^m \)'s exists. Moreover, the spectrum won't exhibit the usual \( J(J+1) \) form but rather some other monotonic progression as a function of \( J \).\(^{14}\)

Assuming that these problems are solved, one still is faced with the tedious task of treating the rotation-intrinsic coupling term. This can be done as before by using a perturbation-variation approach with the H-F states of \( H_0 \). Since in equation (197) the intrinsic and rotational energies commute when one makes the usual approximation of
replacing the $J_A$'s by their expectation values, the
unperturbed function can be taken as a product form

$$|J m_\alpha; \sigma\rangle = S^{(14)}_{J m_\alpha} \phi_0(r)$$

(5.200)

Here $\phi_0$ is the H-F ground state of $H_0$ and $\alpha$ is
an additional quantity necessary to completely specify
$S^{(14)}$ and will be discussed in more detail in the Chapter
on symmetries. For the present it will just be noted
that $\alpha$ takes the place of $K$ which in this case is
not a good quantum number. For the ground state one takes
$J$ in accordance with the known shell model or empirical
value and $\alpha$ in agreement with energetic and symmetry
requirements some of which will be examined in a later
chapter.

With this state one may now construct the first
order trial function

$$|F\rangle \equiv C \hat{J} \cdot \hat{F} |J m_\alpha; \sigma\rangle$$

(5.201)

to take care of the interaction perturbation

$$V = \sum_A H_A J_A$$

(5.202)

The procedure of determining the $F_A$'s by the variational
principle to first order in the perturbation follows
exactly as in the axial symmetry case (except, of course,
3 $F_A$'s now appear). Thus, a direct transcription of the equation (151) may be made to get

$$\langle J m \alpha'; 0 | i [ \hat{h}, F_A \hat{J}_A ] + H_A \hat{J}_A | J m \alpha'; n \rangle = 0$$

(5.203)

where $n$ is a single particle excitation. Note that in this case no $K=\gamma'$ type condition exists so that there is no manifest correlation between $\alpha'$ and $n$. However, from empirical evidence and results of the Bohr-Mottelson model, one expects at least some sort of approximate relationship between these two quantities. This effect will be studied in the chapter on symmetries since it appears that this aspect of the problem determines it.

Solving for the $F_A$'s from equation (203) will in general be quite tedious since the $\hat{J}_A$'s couple many terms in the $S$'s. If one uses the approximation that the intrinsic excitations are much higher than the rotational ones, though, the problem simplifies tremendously. This is because one may then ignore the commutator of $F_A \hat{J}_A$ with the rotational energy and get

$$\langle J m \alpha'; 0 | i [ \hat{h}, F_A ] + H_A \hat{J}_A | J m \alpha'; n \rangle = 0$$

(5.204)

Then, for all $\alpha'$ with $\langle J m \alpha | \hat{J}_A | J m \alpha' \rangle \neq 0$ one may divide out the collective factor to get

$$\langle 0 | i [ \hat{h}, F_A ] + H_A | n(\omega) \rangle = 0$$

(5.205)
where \( n(\alpha') \) was used in light of the fact that \( n \) and \( \alpha' \) may be related.

Once the \( F_A \)'s are found, one may then compute the energy which, in analogy to equation (171) (or eq. (10)) has the value

\[
E_{\alpha J} = \langle J m \alpha; 0 | H_0 + \sum_A \frac{i}{2} j_A J_A^2 + \frac{i}{2} \left[ \sum_A H_A J_A, \sum_B F_B J_B \right] | J m \alpha; 0 \rangle \quad (5.206)
\]

\[
= \langle J m \alpha; 0 | H_0 + \sum_A \left( \frac{i}{2} j_A + \frac{i}{2} \left[ H_A, F_A \right] \right) J_A^2 + \frac{i}{2} \sum_A \left[ H_A J_A, F_B J_B \right] | J m \alpha; 0 \rangle
\]

This shows that the moments of inertia are modified exactly as in axial symmetry except, of course, for the fact no \( \lambda \) conditions occur here. Unfortunately, the \( S \)'s are no longer eigenfunctions for the modified rotational energy so that one must now perform a re-diagonalization of this part. Also, the final commutator terms in \( E_{\alpha J} \) pose no problem because in the symmetries chapter it will be shown that the \( S \)'s may be classified as being either even or odd under rotation by \( \Upsilon \) about one of the principal axes. Thus all combinations of the form \( J_A J_B \neq A \) give zero since rotating by \( \Upsilon \) about, say \( A \), shows that
\[ \langle J^\alpha | J_A J_B | J^\alpha \rangle = \langle J^\alpha e^{-i \pi A} e^{-i \pi B}(J_A J_B) e^{-i \pi A} e^{-i \pi B} | J^\alpha \rangle \] (5.207)

\[ = - \langle J^\alpha | J_A J_B | J^\alpha \rangle = 0 \]

and hence the last sum in \( E_{x^3} \) vanishes.

Completing the treatment of an asymmetric system, one may also employ the technique of simplifying operators according to the \( J \)-function constraints. In this case, one may perform a complete simplification since the H-F functions are localized with respect to all three axes. Then, the Lagrange approximation may be employed throughout, leaving no unwanted \( J \)-functions. This particular aspect of the problem will not be pursued any further here.

Before leaving this case a few comments must be made. First, the problem was only treated cursorily since the case of general asymmetry is not very prevalent at present. A more pertinent problem\(^{(15)}\) is where two moments of inertia are nearly equal and much larger than the third, but where all three moments are sufficiently large so that \( \sum_A H_A J_A \) may still be considered a perturbation. In this case one may proceed as with axial symmetry except not worrying about eliminating the terms with a large \( J \) coefficient. What makes this problem
different from the general case of asymmetry is that one may use $D-$functions for zero order collective functions since the other terms making up $S$ enter with small coefficients and may be neglected to the order of accuracy that the problem is solved. Also, $\alpha$ assumes the asymptotic value $K$.

The other parting comment is that no mention of the intrinsic angular momenta was made because none of its components are conserved for an asymmetric nucleus. These operators were always present in the form $H_A = -\frac{1}{a^2} I_A$, but their explicit identification was never necessary.
VI. SYMMETRIES

A. Introduction

In order to achieve a complete solution of the nuclear rotation problem, one must augment the previous developments by including the symmetry properties of the wavefunctions. Clearly, to do this correctly requires knowing the intrinsic coordinates so that the present formalism is somewhat inadequate. However, by taking the scalar functions constructed from deformed H-F states as an approximation to the intrinsic parts of the eigenfunctions, one may perform a nearly complete analysis of the symmetries. The procedure is similar to using the Born-Oppenheimer approximation in molecular physics in the sense that a zero order framework is employed to extract approximate symmetries. Of course, the molecular case of using axes defined by assumed stationary nuclei to establish a reference point for the electron states is intuitively clearer than using axes defined by a self-consistent potential. Nevertheless, the methods are basically the same.

The symmetry classifications can be divided into two parts. First, there are the global space-time symmetries characteristic of systems of strongly interacting
particles. Some of these, such as angular momentum, have already been included. Inclusion of the others is relatively simple but in turn gives very little in terms of specifying restrictions on the wavefunctions. The second group of symmetries are actually more like boundary conditions. They arise because the set of collective plus intrinsic coordinates is quite unnatural when it comes to spanning a 3A dimensional Euclidean space. In order to affect a unique specification of the system requires in general a complicated set of restrictions on the domains of the coordinates as well as definite branch assignments for multivalued quantities such as angles. Connected with these problems is a set of continuity conditions for the wavefunctions as one passes from one domain to another. These are the second group of symmetry conditions and clearly they are bound to produce severe restrictions on the forms of the wavefunctions.

It will be worthwhile to give a simple example of the second type of symmetry to supplement the somewhat abstract statements made above. The simplest case is a single particle in two dimensions bound by a central potential. By using the usual polar coordinates one does not quite exhibit the nature of the problem since the
symmetries of the radial and angular motions are not coupled. Instead use the pseudo polar coordinates

\[ \varphi = \tan^{-1}\left( \frac{y}{x} \right) ; \quad \rho = \frac{x}{i\pi} \sqrt{x^2 + y^2} \]  

(6.1)

To affect a unique mapping \((x,y) \leftrightarrow (\varphi,\rho)\), one must impose certain conditions on this set. These are chosen as

\[ \varphi = \tan^{-1}\left( \frac{y}{x} \right) = \text{princ. value} \]  

(6.2)

or equivalently

\[ -\frac{\pi}{2} < \varphi < \frac{\pi}{2} \]  

(6.3)

and

\[ -\infty < \rho < \infty \]  

(6.4)

With these variables, the Schrödinger equation is separable in the regions

\[ + = \begin{cases} x > 0 \\ -\frac{\pi}{2} < \varphi < \frac{\pi}{2} \end{cases} \quad \text{and} \quad - = \begin{cases} x < 0 \\ -\frac{\pi}{2} < \varphi < \frac{\pi}{2} \end{cases} \]  

(6.5)

and one obtains solutions of the form

\[ \psi_{\pm}(\varphi) = e^{\pm i\sqrt{k} \varphi} f_{\pm}(\rho) \]  

(6.6)

At this point the \(k\)'s are not specified as being integers. To complete the solution in the angular variable, one must impose the conditions of continuity of \(\psi\) and \(\frac{\partial \psi}{\partial \varphi}\).
at the boundaries \( \varphi = \pm \frac{\pi}{2} \). This gives rise to
the set of equations
\[
\begin{align*}
\mathcal{E} \mathcal{E}^{\pm i \frac{\pi}{2} k^+} f_+(\rho) &= \mathcal{E}^{\pm i \frac{\pi}{2} k^-} f_-(\rho) \\
\pm i k_+ \mathcal{E}^{\pm i \frac{\pi}{2} k^+} f_+(\rho) &= \pm i k_- \mathcal{E}^{\pm i \frac{\pi}{2} k^-} f_-(\rho)
\end{align*}
\] (6.7)
The ratio of the first two equations gives
\[
\mathcal{E}^{i \pi (k_+ + k_-)} = 1 \quad \Rightarrow k_+ + k_- = 2n \quad (n \text{ an integer})
\] (6.8)
The ratio of the first and third equation gives
\[
k_+ = k_- \equiv k
\] (6.9)
and thus using equation (8) one finds \( K = n \) an integer
as expected. This example of how to solve an easy problem
the hard was used to show a case where boundary con-
ditions depend on continuity of the functions evaluated
at completely different values of all the variables, e.g.
\[
\psi_+(\rho, \frac{\pi}{2}) = \psi_-(\rho, -\frac{\pi}{2})
\]

Returning now to the nuclear rotation case, one sees
that it is necessary to impose sets of conditions of the
form
\[
\psi_{jm}(\rho, \eta)_n \mid_{\eta_0} = \psi_{jm}(\rho, \eta)_n \mid_{\eta_0}
\] (6.10)
and similarly for derivatives. In this equation \( \eta_0, \eta_0 \)

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and \((\mathcal{A}_1, \eta_1)\) describe the same point at the boundary connecting two domains. However, in many cases a direct specification of the boundaries is not feasible; in particular, for the present case it is not even possible since the \(\eta\)'s are not known. Clearly, to proceed, another equivalent set of conditions are required. These can be obtained by noting that in general, the specification of the domains of definition of the coordinates is quite arbitrary so that continuity equations such as (10) could just as well have been applied at a different point in space. For example, equation (7) could also assume the form, \(\Psi(\rho, \alpha + \frac{\pi}{2}) = \Psi(-\rho, \alpha - \frac{\pi}{2})\) etc. if one chooses the branch \(-\frac{\pi}{2} < \varphi < \alpha + \frac{\pi}{2}\). Of course, in this particular case, \(\alpha = 0\) is the most natural choice since it defines also the regions of separability of the Schrödinger equations, but this is a special case. Thus, to complete the alternative scheme, one need only note that the complicated process of specifying boundaries and boundary condition may be replaced by the somewhat simpler procedure of allowing the coordinates to vary freely and using the conditions

\[
\Psi_j^*(\mathcal{A}, \eta) = \Psi_j^*(\mathcal{A}', \eta')
\]  

(6.11)
and similarly for derivatives. Here \( (\eta, \xi) \) and \( (\eta', \xi') \) describe the same point in space. These are very similar to the conditions used by Bohr\(^2\) in the unified model where the intrinsic coordinates were characterized by the shape parameters \( \beta \) and \( \gamma' \). In that application, the sets giving identical space points were quite easy to find; however, even with the severe approximation of using only two intrinsic coordinates, the qualitative predictions resulting from symmetries like equation (11) gave excellent agreement with experiment. For the present formulation of the problem, these conditions can not be applied directly since \( \{\eta\} \) is not known. Nevertheless, a knowledge of the transformation properties of the approximate intrinsic parts of the wavefunctions will allow conditions of the form of equation (11) to be enforced. Of course, one must still determine which sets describe the same point or equivalently what transformations leave the wavefunctions invariant. It will be seen that by using scalar projections of H-F states, this can be done at least approximately.

B. **Axial Symmetry**

The case of axial symmetry will be considered in some detail as this represents the most commonly observed
situation. Fortunately, for the ground state rotational band, this case requires very little empirical input to carry out the symmetry classification. The reason is that the $K = \neq$ condition, which in itself is a dynamical symmetry, excludes most of the levels. In the present discussion of symmetries, only the classifications for the unperturbed systems will be considered. As long as the perturbation program is applicable, this is sufficient since one will still have good approximate symmetries.

To begin the discussion recall that in Chapter V the lowest order state is taken as

$$| JmK; 0K \rangle = \mathcal{D}_{mK}^{(J)} \phi_{0K}^{(F)}$$  \hspace{1cm} (6.12)

where $\phi_{0K}^{(F)}$ is the scalar projection of the axially symmetric H-F state $\phi^{(F)}_{0K}$. Consider the rotational part of the energy,

$$\frac{l}{2J} (J^2 - J_3^2) | JmK; 0K \rangle = \frac{l}{2J} (J(J+1) - K^2) | JmK; 0K \rangle$$  \hspace{1cm} (6.13)

Clearly, this is degenerate with respect to $\pm K$. Likewise, one knows that $\phi^{(F)}_{0K}$ and $\phi^{(F)}_{0-K}$ are degenerate H-F states since they are both determinants and

$$E_{-K} = \langle 0K | e^{-\pi \frac{\pi}{2} \tau_{y}} H_{int} e^{\pi \frac{\pi}{2} \tau_{y}} | 0K \rangle = \langle 0K | H_{int} | 0K \rangle = E_{K}$$  \hspace{1cm} (6.14)
recalling that \( H_{\text{int}} = H - \frac{1}{2} \sum_A \mathcal{J}_A \mathcal{N}_A \) is purely intrinsic. Thus, one sees that \(|JmK;0\rangle\) and \(|JmK;0\rangle\) are degenerate since according to the previous chapter,

\[
\phi_{\sigma_k}(v) = e^{i\pi J_L} \phi_{\sigma_k}(v) \Rightarrow \phi_{\sigma_k}(v) = e^{i\pi \mathcal{I}_z} \phi_{\sigma_k}(v)
\]

(6.15)
i.e. the projection does not ruin the degeneracy. It will be convenient now to classify these according to their space-time symmetries, other than angular momentum which is already included.

First consider the parity transformation. Since the \( \mathcal{E}_A \)'s were required to satisfy \( \mathcal{E}_A \times \mathcal{E}_B = \mathcal{E}_C \), it is clear that they must be pseudo-vectors if this result is covariant under parity. Thus, the \( \mathcal{E}_A \)'s are unaffected and consequently the Euler angles in the \( O \)-functions remain unchanged under parity. As for the intrinsic parts of the wavefunction, note that \( \mathbf{r}_A = \mathcal{E}_A \cdot \mathbf{r} \) means that the \( \mathbf{r}_A \) change sign under parity. Hence one gets

\[
\phi_{\sigma_k}(\mathbf{r}) \rightarrow \phi_{\sigma_k}(-\mathbf{r}) = (-1)^P \phi_{\sigma_k}(\mathbf{r})
\]

(6.16)
where \((-1)^P\) is the parity of the H-F state. This means that the states given by equation (12) have the parity of the H-F ground state.
Besides parity, one should also consider the time reversal properties of the wavefunctions. However, since this does not result in any quantum numbers or restrictive conditions on the states, it will not be discussed.

There remains one more symmetry of the unperturbed Hamiltonian which is a combined collective-intrinsic operation. This consists of the "rotation", \( e^{i\pi(I_x - I_y)} \), as can be seen by remembering that the complete unperturbed system is described by

\[
\mathcal{H} = \mathcal{H}_{\text{int}} + \frac{1}{\alpha^2} (J_x^2 - J_y^2) + \frac{1}{\beta} (J_y - I_3) \tag{6.17}
\]

The last term here is responsible for the fact that one must employ a combined transformation since the first two terms are invariant under the individual collective and intrinsic parts. It should be noted that the invariance of \( \mathcal{H}_{\text{int}} \) under \( e^{-i\pi I_x} \) is actually only approximate to the degree that \( I_2 \) and \( J_y \) are only isomorphic to order \( \beta \approx 0.1 \) as shown in the previous chapter.

Accompanying this fact is, of course, the implicit restriction that one is working in a basis of H-F states so that the above correspondence holds. Aside from this, one may construct states which are even or odd under combined rotation by noting that (4)
\[ e^{-i\pi J_z} \mathcal{D}_{m_k}^{x'}^{y'}(\alpha, \beta, \gamma) = \mathcal{D}_{m_k}^{x'}^{y'}(\pi + \alpha, \pi - \beta, \pi - \gamma) \]
\[ = e^{i\pi (J-K)} \mathcal{D}_{m-k}^{x'}^{y'}(\alpha, \beta, \gamma) \]  

where \((\alpha, \beta, \gamma)\) are the Euler angles. So by constructing the states

\[ |Jm|k, \lambda \rangle \equiv |Jm_k; 0 \rangle + e^{i\pi (J-K+\lambda)} |J_{m-k}; 0, -k \rangle \]  

with \(\lambda = 0\) or \(1\), one has

\[ e^{i\pi (J_z - J_L)} |Jm|k, \lambda \rangle = e^{i\pi (J-k)} |Jm_k; 0, -k + e^{i\pi (J+2m)} e^{i\pi \lambda} |Jm_k; 0 \rangle \]  

\[ = e^{i\pi \lambda} |Jm|k, \lambda \rangle \]

as desired. In this derivation, the \(e^{i\pi}\) were used instead of (-1)'s because one is considering both integer and half integer \(J\)'s. For the latter, one must be careful with regard to phases since half integral spin requires rotation by \(4\pi\) to get back to the original orientation. Also, in conjunction with this was used the fact

\[ e^{i\pi J_z} \phi_{\alpha k}(\varphi) = e^{i\pi J_z} \phi_{\alpha k}(\varphi) = e^{i\pi \kappa \varphi} \phi_{\alpha k}(\varphi) \]

(6.21)

With the classification of states according to sign under \(e^{i\pi (J_z - J_L)}\) one has a convenient basis for examining the boundary condition symmetries. The reason
is that this operation is one which sends a point in space back into itself. To show this, recall the results of Chapter IV where it was demonstrated that to order $\beta$, the operation of $I_2$ on $\phi(r)$ was the same as $J_Y$ on $\phi(r)$. This means that

$$C^{-\frac{\pi I_2}{2}}\phi_{\alpha}(\vec{r}, \vec{r}_1, \vec{r}_3) = \phi_{\alpha}(\vec{r}, \vec{r}_2, -\vec{r}_3)$$  \hspace{1cm} (6.22)

i.e., the $r$'s are "rotated" by $\Psi$ about the two axis.

But, $C^{-i\Psi J_z}$ just rotates the two axis by $\Psi$ so that the combination of these two operations leaves the $\vec{r}$'s unaffected. Another way of seeing this is that since the $\vec{r}_A$'s form a complete Euclidean set, one may invert the definition of the $\vec{r}$'s to get

$$\vec{r}^{(j)} = \sum_{A=1}^{3} \vec{\xi}_A \vec{r}_A^{(j)}$$ \hspace{1cm} j=1 \ldots A \hspace{1cm} (6.23)

Now,

$$C^{-\frac{\pi I_2}{2}} \vec{r}_A^{(j)} C^{-\frac{\pi I_2}{2}} = (-1)^A \vec{r}_A^{(j)} + O(\beta^2)$$  \hspace{1cm} (6.24)

as will now be shown. To demonstrate this, use the result

$$[I_2, \vec{r}_A^{(j)}] = [J_z - \delta_{\alpha_\beta}, \vec{r}_A^{(j)}] = -\delta_{\alpha_\beta} [\eta_{\alpha_\beta} \vec{\xi}_A \vec{r}^{(j)}]$$  \hspace{1cm} (6.25)

$$= \delta_{\alpha_\beta} \vec{\xi}_A \vec{r}^{(j)} - \frac{\delta_{\alpha_\beta}}{2(\alpha_\beta - \alpha_\beta)} \vec{\xi}_A \cdot \left( \sum_{i=1}^3 \left[ \epsilon_{\alpha_3} \left[ \sum_{j=1}^3 \epsilon_{\alpha_2} \left[ \sum_{i=1}^3 \left( \frac{\alpha_j - \alpha_i}{\alpha_3 + \alpha_i} \right) \epsilon_{\alpha_3} \vec{r}_i^{(j)} \vec{r}_3^{(i)} \right] \right] \right] \right)$$

$$= \delta_{\alpha_\beta} \vec{\xi}_A \vec{r}^{(j)} + \frac{\epsilon_{\alpha_3} \epsilon_{\alpha_2} \epsilon_{\alpha_3} \epsilon_{\alpha}}{2(\alpha_3 + \alpha_i)} \vec{r}_i^{(j)} \vec{r}_3^{(i)} \vec{\xi}_A \cdot \vec{\xi}_A$$

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where the facts $\tilde{r}_A$ are intrinsic and $[\hat{J}, \hat{E}_A] = [\hat{J}_{\alpha}, \hat{E}_A]$ were employed. This means that, for example,

$$e^{i \pi I_z} \tilde{r}_I e^{-i \pi I_z} = \tilde{r}_I - i \pi [\tilde{r}_I, I_z] - \frac{\pi^2}{2} [[\tilde{r}_I, I_z], I_z] + \cdots$$  \hspace{1cm} (6.26)

$$= \tilde{r}_I + \pi (1-\beta) \tilde{r}_I - \frac{\pi^2}{2} (1-\beta^2) \tilde{r}_I - \frac{\pi^2}{6} (1-\beta)(1-\beta^2) \tilde{r}_I + \cdots$$

$$= \tilde{r}_I \cos (\pi (1-\beta)) + \frac{\sqrt{1-\beta^2}}{1+\beta} \tilde{r}_I \sin (\pi (1-\beta)) = -\tilde{r}_I + O(\beta^2)$$

with $\beta = \frac{Q_3 - Q_1}{Q_3 + Q_1} \geq \frac{<Q_3> - <Q_1>}{<Q_3> + <Q_1>}$ as desired.

Now

$$e^{-i \pi I_z} \hat{E}_A e^{i \pi I_z} = (-1)^A \hat{E}_A$$  \hspace{1cm} (6.27)

and so

$$e^{i \pi (L_z - \tilde{J}_z)} \tilde{r}_I e^{-i \pi (L_z - \tilde{J}_z)} = \tilde{r}_I^{(j)} + O(\beta^2)$$  \hspace{1cm} (6.28)

thus showing that to order $\beta^2 << 1$, one does indeed get back to the same point. In fact, by a simple rescaling of a few of the operators this result can be made exact. This however adds new terms to the Hamiltonian which, though not crucial, are not very easy to interpret. Thus, it seems better to keep the simpler Hamiltonian and put up with the slight inaccuracy of the above transformation. With this boundary condition, one now sees
that only the \( \lambda = 0 \) state is allowed, a result in perfect agreement with the unified model and consequently with observed spectra.

Of particular interest is the case where \( K=0 \) since this includes the most common case of even nuclei. It also represents a special case since no degeneracy of the form \( \pm K \) exists. In this type of system one has

\[
\mathcal{E}^{\pi I_z} \phi_{oo}^{(r)} = \pm \phi_{oo}^{(r)}
\]

(6.29)

where the sign depends on the structure of \( \phi_{oo} \). Thus, one finds

\[
\mathcal{E}^{\pi (I_z - J_z)} |Jm\sigma; oo\rangle = \pm \mathcal{E}^{\pi J} |Jm\sigma; oo\rangle
\]

(6.30)

and so if the boundary condition above is to hold, one needs \( \mathcal{E}^{\pi J} \) to be equal to sign of equation (29).

This is, of course, the well known result that for \( K=0 \) nuclei only entirely even or odd rotational bands exist. To know which type results one needs to know how \( \mathcal{E}^{\pi J} \) acts on the deformed H-F state, \( \phi_{oo}(r) \). Generally, one observes ground state \( K=0 \) bands. For these, the H-F function is formed by including single particle states with both the plus and minus values of \( J_z \) i.e. if \( \psi_{nK}(\vec{r}) \) is in the determinant so is \( \psi_{n-K}(\vec{r}) \). This
gives a plus sign in (29) and thus, as observed, only even \(J\)'s arise. However, for excited state rotational bands, this pairing off may not occur. A particular example is the odd parity band in \(0^{16}\) which has only odd \(\lambda^{(15)}\) indicating a \(K=0\) intrinsic state but with a more complicated structure exemplified by a minus sign in equation (29).

Before indicating how the use of the states with correct symmetry properties affect the results of Chapter IV, a few comments on the above procedure should be made. First of all, the fact that boundary condition symmetry was only approximate is not a severe defect since as long as \(\beta^2 \ll 1\), the transformation \(e^{i\eta(x_r-J_r)}\) will send a point of space into a very near neighbor. As the boundary condition applies for all points of the 3A dimensional space, it is impossible for the wavefunction to change sign every time this transformation is performed, i.e. it would have a large number of nodes if this were the case. Thus, in equation (19), \(\lambda = 1\) can never occur because this approximation was employed. The second point to be made, is that in conjunction with this fact is the observation that these symmetry properties are inapplicable to most molecular systems since \(\beta^2 \ll 1\) is severely
violated. In other words, the present analysis pertains only to slightly deformed systems such as nuclei. This seems to be a fairly significant point not mentioned in any previous treatment of nuclear rotation, though implicitly assumed in the unified model of Bohr and Mottelson. A final point is that since the perturbation is of the form \( I_1 \mathcal{J}_1 + I_2 \mathcal{J}_2 \), all of the symmetries derived are also true for the total system.

Turning now to the use of the symmetrized states in the perturbation program one sees that by forbidding \( \lambda = 1 \) one has removed the degeneracy of the \( + K \) form. This is important since the work of Chapter V tacitly assumed non-degenerate states. Now using unperturbed states of the form

\[
|Jm|k\rangle \equiv \mathcal{S}^J_{\lambda \bar{\lambda}}^{(\pm)} \phi^{(r)}_{\lambda k} + (-1)^{J-S} \mathcal{S}^{J}_{\bar{\lambda} \lambda}^{(\mp)} \phi^{(r)}_{\bar{\lambda} -\lambda k}
\]  

(6.31)

where the \( \phi \)'s are H-F states for \( H \) as in the previous chapter, one may proceed in exactly the same manner as before in doing the variation-perturbation treatment of the coupling. To see this, note that \( |JM|K\rangle \) is a generalized form of a H-F state in the sense that it is stationary under variations of either or both of the \( \phi \)'s. As a proof, remember that

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\[ \langle \phi_{0, \pm k} | H | \rho \rangle = 0 \quad (6.32) \]

by the definition of the \( \phi \)'s. Thus one has

\[ \langle Jm | H | \phi_{0, \pm k} \rangle = \langle Jm | H | \phi_{0, \pm k} \rangle + \langle Jm | H | \phi_{0, \pm k} \rangle = 0 \quad (6.33) \]

where the ket states are one particle excitations. The crucial point is that the D-functions partition the problem into two independent ones. This will also carry over into the perturbation program as long as \( \vec{V} \) does not connect states differing by the sign of \( K \). Since \( \vec{V} \) contains only \( J^1 \) and \( J^2 \), it is clear that only for \( |K| = 1/2 \) can this occur, this of course being the well known decoupling effect of the unified model. Thus, except for this case, the entire work of Chapter V is also valid here. The only change is that by using a trial function of the form (ignoring subsidiary conditions here)

\[ |F\rangle = e^{i(J_x F_x + J_z F_z)} |Jm|K\rangle \quad (6.34) \]

one gets a defining equation for \( F_\pm \), (see previous chapter),
\[ \langle \vec{\partial}_{m_k} \phi_{0_k} \mid i [\hat{H}_0, F_z J_z] - \frac{\theta}{2} \vec{\Lambda} \cdot \vec{J} \mid \vec{\partial}_{n_{-k},+} \phi_{n_{-k},+} \rangle + \]

\[ (-1)^{-J_k} \langle \vec{\partial}_{m_{-k}} \phi_{0_{-k}} \mid i [\hat{H}_0, F_z J_z] - \frac{\theta}{2} \vec{\Lambda} \cdot \vec{J} \mid \vec{\partial}_{m_{-k}} \phi_{n_{-k},+} \rangle = 0 \]

by the usual variational method. This is slightly more complicated than the previous result, however they are equivalent since (35) must be true for all one particle excited states \( n' \) and \( n'' \). As these are independent variations, each term above must be zero and hence \( F_z \) is defined just by

\[ O = \langle \vec{\partial}_{m_k} \phi_{0_k} \mid i [\hat{H}_0, F_z J_z] - \frac{\theta}{2} \vec{\Lambda} \cdot \vec{J} \mid \vec{\partial}_{n_{+k},+} \phi_{n_{+k},+} \rangle \]

as usual. Thus the moment of inertia and perturbation program are unaffected by including the symmetry properties.

For the \( K = 1/2 \) case, the moment of inertia calculation will carry through as usual. However, besides the usual intrinsic and rotational energies, one gets an additional contribution of

\[ E = \langle \mathcal{J} m \mid \hat{\mathcal{H}} \mid \mathcal{J} m \rangle \]

\[ = - (\mathcal{J}^{1/2}) (-1)^{-J_k} \langle \vec{\partial}_{m_k} \phi_{0_k} \mid \frac{\theta}{2} (\Lambda_+ J_+ + \Lambda_- J_-) \mid \vec{\partial}_{m_{-k}} \phi_{0_{-k}} \rangle + C.C. \]

\[ = - \frac{(-1)^{J_k+1}}{2} \left\{ \langle \phi_{0_{+}} \mid \Lambda_+ \phi_{0_{-k}} \rangle + \langle \phi_{0_{-k}} \mid \Lambda_- \phi_{0_{+}} \rangle \right\} (J + \frac{1}{2}) \]
this last line following from a simple evaluation of the
collective matrix elements and by inserting the definition
of \( B \). Thus one gets for the decoupling parameter, \( a \),
defined by
\[
\epsilon = \frac{1}{Z} ( -1 )^{J+\frac{1}{2}} ( J+\frac{1}{2} ) \alpha
\]
in the unified model,
\[
\alpha = \langle \phi_{0\frac{1}{2}} | J_+ - \frac{1}{K} ( m_x - i m_y ) | \phi_{0\frac{1}{2}} \rangle + c.c.
\]  \( (6.38) \)

This is similar to the result found using the Peierls-
Yoccoz projection method. \( (12) \) The only difference is
that in that result there are no \( M \) terms i.e., it is
just
\[
a = \langle \phi_{0\frac{1}{2}} | J_+ | \phi_{0\frac{1}{2}} \rangle + c.c.
\]
This is not too signif-
ificant though numerically since \( \frac{\alpha}{K} \sim 0.1-0.3 \) and thus
the \( M \) terms contribute only slightly.

At the present, no more symmetries or effects of
using them are apparent. This is not to say that more do
not exist but just that the ones presented here seem
sufficient to account for most of the observed facts.
Certainly, if one were able to study \( |K| > 1/2 \) nuclei
in sufficient detail, higher order corrections to the
energy would most likely need contributions from decoupling.
These come, of course, from higher order terms in the
perturbation expansion, an aspect of the problem out of
the range of the present thesis.
C. Axial Asymmetry

As was mentioned in Chapter IV, most asymmetric nuclei are sufficiently close to axial symmetry that a trivial extrapolation of the results for that case are all this is required. However, for completeness and possibly future reference, the symmetries of nuclei with three significantly different moments of inertia will be examined. Because the $K = \pi$ condition is inapplicable here, the analysis will be a bit more tedious. It is quite possible that similar conditions will hold for coupling of other sets of intrinsic and collective quantities. However, within the framework of the present formalism, it is impossible to identify them.

The symmetries of the rotational part of the Hamiltonian are just those of the rigid asymmetric rotor\(^{(13)}\) as long as one makes the usual approximation of replacing the quadrupole moments by their average values. Then

\[
H_R = \sum_{A=1}^{J} \frac{J}{2} \mathcal{J}_A \mathcal{J}_A^\dagger
\]  \hspace{1cm} (6.39)

with $\mathcal{J}_A \neq \mathcal{J}_B$ for all $A \neq B$. The first thing to note here is that this is invariant under the operations

\[
R_A = e^{i \pi \mathcal{J}_A}
\]  \hspace{1cm} (6.40)
since all angular momenta appear quadratically. Thus, if

\[ S_{jm} = \sum_{\kappa=\pm} C_{j\kappa m} \mathcal{Q}_{j\kappa m} \]  \hspace{1cm} (6.41)

is any eigenfunction of \( H_\mathcal{R} \), so is \( R_A S_{jm} \). Now note that

\[ e^{i \frac{\pi}{4} J_A} e^{-i \frac{\pi}{4} J_A} = J_B + i \frac{\pi}{2} [J_A, J_B] + \cdots \]  \hspace{1cm} (6.42)

\[ = J_B + \frac{\pi}{2} J_C + \cdots \]

\[ = J_B \cos \frac{\pi}{4} + J_C \sin \frac{\pi}{4} = \overline{J_C} \quad (AB \in \{c, c, \overline{c}\}) \]

Therefore

\[ R_A R_B = e^{i \frac{\pi}{4} J_A} (e^{i \frac{\pi}{4} J_A} e^{i \pi J_B} e^{-i \frac{\pi}{4} J_A}) e^{i \frac{\pi}{4} J_A} \]  \hspace{1cm} (6.43)

\[ = e^{-i \frac{\pi}{4} J_A} e^{i \pi J_C} e^{i \frac{\pi}{4} J_A} \]

and since in a similar manner to equation (42) one can show that

\[ e^{-i \pi J_C} J_A e^{i \pi J_C} = -J_A \]  \hspace{1cm} (6.44)

one gets the result

\[ R_A R_B = e^{i \pi J_C} (e^{-i \pi J_C} e^{i \frac{\pi}{4} J_A} e^{i \pi J_C} e^{-i \frac{\pi}{4} J_A}) e^{i \frac{\pi}{4} J_A} \]  \hspace{1cm} (6.45)

\[ = e^{i \pi J_C} = R_C \]

For the present, assume that one has an even A nucleus so that

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or \( R_A = R_A^{-1} \). With these results, it is clear that \( R_1, R_2, R_3 \) and 1 form a group of order four and thus that the wavefunctions may be classified according to its irreducible representations. From elementary group theory, one knows that the sum of the squares of the dimensions of the irreducible representations equals the order of the group. Also, each group has the trivial representative of all 1's. Thus, for the four group, one obviously has four one dimensional irreducible representations which can be taken as

\[
\begin{array}{cccc}
1 & R_1 & R_2 & R_3 \\
1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 \\
\end{array}
\]  

(6.47)

Since \( R_2 R_3 = R_1 \), it is clear that the wavefunctions are specified by the values of \( R_2 \) and \( R_3 \) called \( \lambda \) and \( \alpha \) respectively.

With the above facts, one may write the eigenfunctions of \( H_R \) as

\[
S_{Jm}^{N\pi\lambda} = \sum_{k=-J}^{J} C_{Jm k}^{N\pi\lambda} \zeta_{m k}^J
\]  

(6.48)
where the index $N$ is included since in general $\lambda$ and $\alpha$ are not sufficient to completely specify the state. To see what conditions are placed on the $C$'s by the present classification, note that

$$R_3 \mathcal{C}^{\nu \kappa \lambda}_{m,k} = e^{i \pi J_3} \mathcal{C}^{\nu \kappa \lambda}_{m,k} = (-1)^K \mathcal{C}^{\nu \kappa \lambda}_{m,k}$$

(6.49)

and

$$R_2 \mathcal{C}^{\nu \kappa \lambda}_{m,k} = e^{i \pi J_2} \mathcal{C}^{\nu \kappa \lambda}_{m,k} = (-1)^{J-k} \mathcal{C}^{\nu \kappa \lambda}_{m,k}$$

(6.50)

From the first relation one sees that if

$$R_3 S^{\nu \omega \lambda}_{J,m} = (-1)^K S^{\nu \omega \lambda}_{J,m} \quad \alpha = 0 \text{ or } 1$$

(6.51)

then

$$C^{\nu \omega \lambda}_{J,m,k} = 0$$

(6.52)

for $(-1)^K \neq (-1)^{J-k}$ or equivalently the expansion, equation (48), contains only even or only odd $K$'s depending on the value of $\alpha$. The second relation above shows that if

$$R_2 S^{\nu \omega \lambda}_{J,m} = (-1)^\lambda S^{\nu \omega \lambda}_{J,m} \quad \lambda = 0 \text{ or } 1$$

(6.53)

then

$$C^{\nu \omega \lambda}_{J,m,k} = (-1)^{J-k+\lambda} C^{\nu \omega \lambda}_{J,m-k}$$

(6.54)
Thus, one may incorporate both conditions by writing

$$S_{Jm}^{N\alpha\lambda} = \sum_{k \geq 0} \frac{1}{k} (1 + (-1)^k) C_{Jm}^{N\alpha\lambda} \left( \mathcal{O}_{nk}^{k\lambda} + (-1)^{J-k}\mathcal{O}_{Jm-k}^{k\lambda} \right)$$

(6.55)

Now this represents the major symmetry classification due to purely collective transformations. To continue, one must consider intrinsic as well as combined collective-intrinsic properties. For the former, one examines the invariances of

$$H_o = H + \sum_A j_A \bar{A}_A + \sum_A \frac{1}{2} \sum_j \bar{J}_A$$

(6.56)

which is, of course, just the intrinsic Hamiltonian of Chapter II. In this asymmetric case, none of the components of the intrinsic angular momentum are conserved so their eigenvalues cannot be used to classify the states. Also, one expects that in general, the intrinsic ground state is non-degenerate except of course for instances of accidental degeneracies or "hidden" symmetries. Consequently, for the unperturbed ground state of $h = H_0 + H_R$, one may write

$$\psi_{Jm}^{N\alpha\lambda} = \phi_0(\gamma) S_{Jm}^{N\alpha\lambda}(\gamma)$$

(6.57)

where $\phi_0(\gamma)$ is the H-F ground state for $H_0$ and
\( \phi_0(\overline{r}) \) is its scalar projection. Assuming that the nucleus is only slightly deformed, i.e. the \( \beta \)'s are \( \ll 1 \), one still has the approximate symmetry that \( e^{i \pi (I_A - J_A)} \) sends a point into itself and thus under this operation the wavefunctions are invariant. With this result, one is able to discover not only symmetries of (57) but also those for \( \phi_0(\overline{r}) \). The reason is that since \( H = H_0 + H_A - \sum_{A} I_A J_A \) is invariant under \( e^{i \pi (I_A - J_A)} \), and since \( H_A \) and \( \sum_{A} I_A J_A \) are also, one has

\[
e^{i \pi (I_A - J_A)} e^{-i \pi (I_A - J_A)} = e^{i \pi I_A} e^{-i \pi I_A} = H_0
\]

Thus, an analysis similar to that for the \( S \)'s may be applied to the intrinsic wave functions and the results should at least approximately hold for \( \phi_0(\overline{r}) \). In particular, one would expect

\[
e^{i \pi I_A} \phi_0(\overline{r}) \approx \pm \phi_0(\overline{r})
\]

where, of course, at the present level of development no clear cut prescription for predicting the sign is possible. Defining in analogy to the previous case, the eigenvalues of \( e^{i \pi I_A} \) and \( e^{i \pi I_A} \) as \((-1)^{\alpha'}\) and \((-1)^{\lambda'}\) respectively, one finds that

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\[ C(\pi(I_3 - I_2)) \psi_{jm}^{N_{\lambda \lambda'}} = (-1)^{\lambda + \lambda'} \psi_{jm}^{N_{\lambda \lambda'}} \]  
(6.60)

and

\[ C(\pi(I_3 - I_3)) \psi_{jm}^{N_{\alpha \alpha'}} = (-1)^{\alpha + \alpha'} \psi_{jm}^{N_{\alpha \alpha'}} \]  
(6.61)

To satisfy the uniqueness boundary condition, only those states with 
\((-1)^{\lambda + \lambda'}\) and 
\((-1)^{\alpha + \alpha'}\) equal to one are allowed or equivalently \(\lambda = \lambda'\) and \(\alpha = \alpha'\). Thus one again finds a coupling of symmetries similar to the \(K=\nu\) condition for axial symmetry.

With the above results, one is able to affect at least a partial symmetry classification for the ground state, though generalization to excited states is straightforward. The extent to which these are sufficient to allow a complete specification of the nuclear system depends on \(J\). This is because for each value of \((Jm)\), there are \(2J+1\) different \(S\)'s coming from the diagonalization of \(H_R\). Thus for \(J < 2\), the present analysis can be used to classify states, but for larger values a more detailed study must be made or empirical information must be included. As this will depend on the particular system in question, the problem will be left open at this point.
Besides the boundary condition symmetries presented here, there are, of course, the space-time symmetries. However, as in the case of axial symmetry these give no further information about the classification of states except in the event one were able to relate the sign of equation (59) to one of these symmetries. Again, this is out of the domain of the present treatment.

The final aspect of this section is naturally the application of the properly symmetrized wavefunctions to the perturbation programs of Chapter IV. Since it was assumed there that these symmetry conditions existed, nothing much can be added beyond the statement that these so far undefined symmetries may be at least partially identified. In particular it was mentioned during the perturbation treatment of the asymmetric system that even though the \( K=\mathcal{R} \) condition was lost, certain intrinsic-collective symmetry couplings still existed. These can now be seen in the form of \( \lambda=\lambda' \) and \( \alpha=\alpha' \) requirements.
VII. TENSOR OPERATORS

A. Separation Method

Besides being used to decompose the Hamiltonian into a convenient form, Tomonaga's method may also be applied to other operators of physical interest. These can be classified according to their rotational properties, a fact which will later allow a considerable simplification when one must separate out the collective and intrinsic parts. Examples of the operators which can occur are magnetic moments, electric quadrupole moments, and various multipole contributions to transition amplitudes. In general, the entire class of operators, called tensor operators, can be classified by the following scheme: (4)

\[ T_K^q \] is the qth component of a tensor of rank K if

\[ [J_z, T_K^q] = q T_K^q \] \hspace{1cm} (7.1)

and

\[ [J_x \pm i J_y, T_K^q] = \sqrt{(k+q)(k+q+1)} T_K^{q \pm 1} \] \hspace{1cm} (7.2)

Clearly, according to the second equation, a tensor of rank K has 2K+1 components.

For the present formulation, this form of the tensors is inconvenient. The reason is that in order to transform
them to a body fixed system, one must generalize the \( \hat{e}_A \)'s for higher order tensors. Instead of trying to find this generalization, one need only note that any tensor of rank \( K \) may be written as a linear combination of cartesian tensors of rank \( K \). That is

\[
T_k = \sum_{i_1 \ldots i_k} C_{i_1 \ldots i_k}^{i_1 \cdot i_2 \cdot i_k} \mathbf{T}_{i_1 \ldots i_k}
\]

(7.3)

where the \( C \)'s are numerical constants and the \( \mathbf{T} \)'s are cartesian tensors, i.e., each component \( j_n \), transforms under rotations like a component of \( \mathbf{T} \). For example, for \( K=1 \), vectors, one has the well known result

\[
\begin{bmatrix}
T'_{i_1} \\
T'_{i_2} \\
T'_{i_3}
\end{bmatrix} =
\begin{bmatrix}
-\frac{1}{i_1}(\mathbf{T}_{i_1 + 1} \mathbf{T}_{i_1}) \\
\mathbf{T}_{i_2} \\
\frac{1}{i_3}(\mathbf{T}_{i_3 - 1} \mathbf{T}_{i_3})
\end{bmatrix}
\]

(7.4)

and for higher order tensors one can find the \( C \)'s from equations (1) and (2) or more simply by noting that these are the same as the coefficients in the representation of spherical harmonics in terms of \( x, y, \) and \( z \). The reason cartesian tensors are convenient is that they are transformed by the \( \hat{e}_A \)'s according to the rule

\[
\mathbf{T}_{i_1 \ldots i_k} = \sum_{j_1 \ldots j_k} \varepsilon_{j_1 \ldots j_k} \mathbf{T}_{i_1 \ldots i_k}
\]

(7.5)

where as usual \( \varepsilon_{jA} = \hat{e}_A \cdot \hat{j} \), \( \hat{j} \) a space fixed unit vector.
All of the concern for the transformation properties of the tensors stems from the following fact. If the \( \hat{e}_A \)'s specify a body fixed system, that is they obey the commutation relations with \( \hat{J} \) presented in Chapter II, then the \( \hat{\tau}_{A_1...A_k} \)'s are scalars, i.e. commute with \( \hat{J} \). The proof of this depends on the basic fact

\[
[\hat{J}_i, \hat{\tau}_{j_1...j_k}]=\hat{\epsilon}_{ij_1j_2...j_k} \hat{\tau}_{i_1...i_k}+ \hat{\tau}_{j_1...j_k} \hat{\epsilon}_{i_1i_2...i_k} = \hat{\epsilon}_{ij_1j_2...j_k} \hat{\tau}_{i_1...i_k} + \hat{\tau}_{j_1...j_k} \hat{\epsilon}_{i_1i_2...i_k}
\]  \hspace{.5in} (7.6)

where the \((i \times j)\) means the component is \((\hat{i} \times \hat{j})\) and \(\hat{\tau}_k=-\hat{\tau}_{-k}\). Also, for reference, remember that

\[
[\hat{J}_i, \hat{\epsilon}_{j_1j_2...j_k}] = \hat{i} \hat{\epsilon}_{ij_1j_2...j_k}
\]  \hspace{.5in} (7.7)

Then, one finds that

\[
[\hat{J}_i, \hat{\tau}_{A_1...A_k}]=\hat{i} \hat{\epsilon}_{i_1i_2...i_k} \{\hat{\tau}_{i_1...i_k} \hat{\epsilon}_{A_1A_2...A_k} + \hat{\tau}_{j_1...j_k} \hat{\epsilon}_{A_1A_2...A_k} \hat{\epsilon}_{i_1i_2...i_k} \hat{\tau}_{j_1...j_k} + \text{same for all other components}\}
\]  \hspace{.5in} (7.8)

By changing the summation variable in the second term to \(j_1\) and using \(\hat{\tau}_1 = -(\hat{i} \times \hat{\tau}_1)^1 = -\hat{i} \times (\hat{i} \times \hat{\tau}_1)\), one easily sees that this is the negative of the first term. Using exactly the same procedure for the remaining terms, one finds as desired that \([\hat{J}_i, \hat{\tau}_{A_1...A_k}] = 0\). Note, though, that in general \(\hat{\tau}_{A_1...A_k}\) is not intrinsic since in most cases \([\hat{\tau}_{A_1...A_k}, \hat{e}_A] \neq 0\).
To fit naturally into the present formulation of the nuclear rotation problem, the various tensor operators must be separated with respect to collective and intrinsic dynamics just as was done with the Hamiltonian. This is a trivial task since, according to the previous argument, the $\Gamma_{A_1 \cdots A_n}$ are scalars and thus may be decomposed via Tomonaga's method just like the energy. In other words, one may write (dropping $A$ subscripts)

$$\Gamma = \Gamma^{(o)} + \sum_C \Gamma^{(c)} J_C + \cdots$$  \hspace{1cm} (7.9)

where the $J_C$ are body fixed angular momenta and the $\Gamma^{(c)}$ are intrinsic operators which may be calculated in the usual way in terms commutators with $\varepsilon$'s. The convergence of this series depends on the nature of the tensor involved, but in the physically interesting cases, the first few terms usually suffice.

Assuming that this is the case for $\Gamma$, one has according to the rules of Chapter II

$$\Gamma^{(o)} = \Gamma - \frac{i}{\hbar} \sum_C \left\{ \left[ \Gamma, \varepsilon_A \right] \cdot \varepsilon_B - \left[ \Gamma, \varepsilon_B \right] \cdot \varepsilon_A \right\} J_C + \cdots$$  \hspace{1cm} (7.10)

$$\Gamma^{(c)} = \frac{i}{\hbar} \left\{ \left[ \Gamma, \varepsilon_A \right] \cdot \varepsilon_B - \left[ \Gamma, \varepsilon_B \right] \cdot \varepsilon_A \right\} + \cdots$$  \hspace{1cm} (7.11)
where ABC are cyclic. These operators can be shown to be intrinsic to the order of accuracy represented by equation (9), i.e. assuming all coefficients of higher powers of $J$ vanish. The proof of this is identical to that given for the various operators in the decomposition of $H$ since it should be noted there that no specific properties were used except the scalar nature of $H$. In particular, assumptions about the potential and form of the $\hat{e}$'s were used only to establish a convenient termination of the series, not the intrinsic properties of the coefficients of the $J$'s.

Once this decomposition has been performed, one has a clear picture as to what effects are attributable to collective or intrinsic properties of the system. Using the separated form of the wavefunction from the previous chapters,

$$\psi_{jm}^n = \sum_k \mathcal{S}^{(n)}_{mk} \phi_k^{(n)}(\eta)$$

one may readily evaluate pertinent matrix elements of the tensors and put the results in such a form that effectively isolates the effects of the two types of motion. In a practical calculation, of course, one must resort to an approximate form for $\phi_k$ such as found in the previous chapter.
For the present work, the more important tensor operators will be studied. These are, of course, magnetic moments, electric quadrupole moments and some of the low order multipole transition amplitudes. After the operators have been decomposed, the problem of calculating matrix elements using the wavefunctions of the previous chapters will be studied and carried out as far as is possible without resorting to numerical methods.

B. Magnetic Moments

The magnetic moment operator is a tensor of rank one and may be written as

$$\vec{\mu} = \sum_i (g^i_l \vec{\ell}^i + g^i_s \vec{s}^i)$$  \hspace{1cm} (7.13)

where $\vec{\ell}^i$ and $\vec{s}^i$ are the orbital and spin angular momenta of particle $i$ and the $g$'s are the usual $g$ factors, i.e. $(g^i_l, g^i_s)$ equals (0, -3.8) for neutrons and (1, 5.6) for protons in units of nuclear magnetons. Thus, one has the scalars

$$\mu_A = \sum_i (g^i_l \ell_A^i + g^i_s s_A^i)$$  \hspace{1cm} (7.14)

where $\ell_A = \vec{e}_A \cdot \vec{\ell}$ and $s_A = \vec{e}_A \cdot \vec{s}$, to which must be applied the decomposition.

For the present analysis, the $\vec{e}$'s specifying the
orientation of the quadrupole axes will be used. Then, remembering that these are spin and momentum independent one finds

$$[\mu_A, \vec{e}_B] = \sum_{i} g_i [\ell_A^i, \vec{e}_B^i] = \sum_{\text{protons}} [\ell_A, \vec{e}_B]$$  \hspace{1cm} (7.15)$$

and since $\lambda$ is linear in momentum this commutator is momentum independent which means all higher commutators with $\vec{e}'s$ vanish and thus the series (equation (9)) terminates at $J$. This means that one has the exact result

$$M_A = (\mu_A - \frac{i}{2} \sum_{\text{protons}} (\ell_A \cdot \hat{c}_c \cdot \hat{e}_c - \ell_A \cdot \hat{e}_c \cdot \hat{e}_c) J_{\beta c}) + \frac{i}{2} \sum_{\text{protons}} (\ell_A \cdot \hat{e}_c \cdot \hat{e}_c - \ell_A \cdot \hat{e}_c \cdot \hat{e}_c) J_{\beta c}$$  \hspace{1cm} (7.16)$$

where the first term and coefficients of $J_{\beta c}'s$ are exactly intrinsic. It will be convenient to write this as

$$M_A = M_A^* + \sum g_{AB} J_B$$  \hspace{1cm} (7.17)$$

where

$$g_{AB} = \frac{i}{2} \sum_{\text{protons}} (\ell_A \cdot \hat{c}_c \cdot \hat{e}_c - \ell_A \cdot \hat{e}_c \cdot \hat{e}_c)$$  \hspace{1cm} (7.18)$$

and

$$M_A^* = M_A - \sum g_{AB} J_B$$  \hspace{1cm} (7.19)$$
are both intrinsic.

To evaluate matrix elements of \( \hat{\mu} \), use the "vector model" result of the Wigner-Eckart theorem \((4)\)

\[
\langle n J m | \hat{\mu} | n' J m' \rangle = \frac{\langle n J m | \hat{\mathcal{J}} | n' J m' \rangle}{\mathcal{J}(J+1)} \langle J m | \hat{\mathcal{J}} | J m' \rangle
\]

(7.20)

where the \( | n J m \rangle \) are the \( \psi \)'s of equation (12). By the magnetic moment, one usually means the expectation value of \( \mu_z \) in the state with \( m=J \) or in other words

\[
\mu = \langle n J J | \mu_z | n J J \rangle = \frac{1}{(2J+1)} \langle n J J | \hat{\mathcal{J}} \cdot \hat{\mathcal{J}} | n J J \rangle
\]

(7.21)

Now since \( \hat{\mu} \cdot \hat{\mathcal{J}} \) may be written as \( \sum_A (\mu_A \mathcal{J}_A) \) and one knows how to decompose \( \mu_A \) into collective and intrinsic parts, one may insert the form of equation (12) in the above matrix element to get

\[
\mu = \frac{1}{(2J+1)} \sum_{k, k'} \langle \mathcal{S}_{k}^{(n)} | \mathcal{J}_A | \mathcal{S}_{k'}^{(n)} \rangle \langle \mu_A | \mathcal{J}_A + \sum_{c} \mathcal{J}_A | \mathcal{J}_c | \mathcal{J}_c \rangle \langle \phi_{k}^{(n)} | \phi_{k'}^{(n)} \rangle
\]

(7.22)

\[
= \frac{1}{(2J+1)} \sum_{k, k'} \left\{ \langle \mathcal{S}_{k}^{(n)} | \mathcal{J}_A | \mathcal{S}_{k'}^{(n)} \rangle \langle \phi_{k}^{(n)} | \phi_{k'}^{(n)} \rangle + \right. \\
\left. \frac{1}{2} \langle \sum_c \mathcal{J}_A | \mathcal{J}_A | \mathcal{J}_c | \mathcal{J}_c \rangle \langle \phi_{k}^{(n)} | \phi_{k'}^{(n)} \rangle \right\}
\]

For a lowest order axial symmetry calculation, that ignoring collective-intrinsic coupling, only one value of \( | k \rangle \) occurs and \( \psi \) has the form from Chapter VI

\[
\psi_{J M K}^{(n)} = \frac{1}{\sqrt{2}} \left( \mathcal{S}_{k}^{(n)} \phi_{k}^{(n)} | \mathcal{J}_A \rangle + (-1)^{j-k} \mathcal{S}_{k'}^{(n)} \phi_{k'}^{(n)} | \mathcal{J}_A \rangle \right)
\]

(7.23)
except for \( K=0 \) which must be considered separately.

Also, for simplicity, assume that the neutron and proton distributions are identical so that one may write

\[
\sum_{\hat{p}_A} [\hat{l}_{\hat{A}}, \hat{e}_{\hat{B}}] = \frac{\hat{z}}{A} \sum_{\hat{p}_A} [\hat{l}_{\hat{A}}, \hat{e}_{\hat{B}}] = \frac{\hat{z}}{A} [\hat{l}_{\hat{A}}, \hat{e}_{\hat{B}}] = -\frac{\hat{z}}{A} \hat{e}_{\hat{C}} \tag{7.24}
\]

where, of course, \( z \) and \( A \) are the proton and nucleon numbers and \( \hat{L}_A \) is the total orbital angular momentum.

The final form above comes from the relation \([\hat{J}_A, \hat{e}_B] = -i \hat{e}_C\) noting that the \( \hat{e} \)'s are spin independent. Now with this result one finds

\[
\mathcal{Q}_{AC} = \frac{\hat{z}}{A} \mathcal{S}_{AC} \tag{7.25}
\]

and

\[
\mu_A = \mu_A - \frac{\hat{z}}{A} \hat{J}_A \tag{7.26}
\]

Combining these facts, the lowest order value of \( \mu \) for \( K \not\in \frac{1}{2} \) is

\[
\mu = \frac{1}{2(z+1)} \left\{ k \langle \phi_k^{(m)} | \mu_A^0 | \phi_k^{(n)} \rangle - \langle \phi_k^{(m)} | \mu_A^0 | \phi_k^{(n)} \rangle + \frac{2z}{A} \hat{J}(z+1) \right\} \tag{7.27}
\]

Specializing to the ground state, one may employ the H-F states from Chapter V for the \( \phi \)'s. Then, remembering that for these functions one has a localization in angle such that the symmetry axis and \( z \) axis are nearly
parallel or equivalently that \( \epsilon_{k3} \approx \delta_{k3} \), one finds

\[
\langle \phi_k | \mu^z_3 | \phi_k \rangle = \langle \phi_k | \sum_{j=x}^{\frac{3}{2}} \left( \mu_j - \frac{\hbar}{A} j \right) \epsilon_{k3} | \phi_k \rangle
\]

\[
= \langle \phi_k | \left( \mu_z - \frac{\hbar}{A} J^z \right) | \phi_k \rangle
\]

Now defining, as in the unified model, an intrinsic g-factor by

\[
\langle \phi_k | \mu^z | \phi_k \rangle \equiv K g_k
\]

one gets the final result

\[
\mu \approx (g_k - \frac{\hbar}{A}) \left( \frac{k^z}{c m} \right) \rho + \frac{\hbar}{A} J
\]

This is in exact agreement with the Bohr-Mottelson answer, noting that there they have \( g_R \), the rotational g-factor, instead of \( \frac{Z}{A} \), but that within their model \( \frac{Z}{A} \) is the lowest order estimate for \( g_R \).

The above calculation of \( \mu \) represents a very crude approximation since first the neutron and proton distributions will generally be different and second the collective-intrinsic coupling will alter the wavefunctions giving correction terms to (27). From shell model experience, one knows that many times this latter effect can have a profound influence. Thus, in general one
should refine the calculations by at least including the effects of coupling.

The procedure for handling this latter problem will now be sketched. For the present, ignore the symmetry properties and subsidiary conditions, and write the corrected wavefunction as

$$\lvert F \rangle = e^{i(F_x J_x + F_y J_y)} \lvert JJK; OK \rangle$$

(7.31)

using the notation of Chapter V. Then one finds that instead of equation (22), the result is

$$\mu = \frac{i}{\langle JJK; OK \rangle} \sum_{\alpha} \langle JJK; OK \rangle \mu_0 J_{\alpha} + \sum_{\alpha} \alpha g_{\alpha c} J_{\alpha} J_{\alpha} +$$

$$i \left[ \mu_0 J_{\alpha} + \sum_{\alpha} \alpha g_{\alpha c} J_{\alpha} J_{\alpha} , F_x J_x + F_y J_y \right] JJK; OK \rangle$$

(7.32)

The first two terms of course represent the contribution to \( \mu \) found before while the commutator is the correction. This latter quantity may be simplified somewhat by eliminating the \( J \)'s as will now be shown. First, use the uniform distribution approximation as above to write

$$\mu_0 = \left( \mu_0 - \frac{3}{5} J_A \right) + \frac{8}{7} J_A$$

(7.33)

$$= \mu_0^{\circ} + \frac{8}{7} J_A$$

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Then, the correction term becomes

$$\mu_{\text{cor}} = \frac{i}{r^{(3/2)}} \langle JJK; 0K | \left[ M^2 \mathcal{J} + \frac{3}{2} \mathcal{J}^2, \mathcal{F}_+ \mathcal{J}_+ + \mathcal{F}_- \mathcal{J}_- \right] | JJK; 0K \rangle \quad (7.34)$$

Next, note that neither $\mathcal{J}_3$ nor $\mathcal{J}^2$ can connect states generated by $\mathcal{J}_\pm$ so that one has

$$\mu_{\text{cor}} = \frac{i}{r^{(3/2)}} \langle JJK; 0K | \left[ M^0 \mathcal{J}_+ + M^0 \mathcal{J}_-, \mathcal{F}_+ \mathcal{J}_+ + \mathcal{F}_- \mathcal{J}_- \right] | JJK; 0K \rangle \quad (7.35)$$

$$= \frac{i}{2r^{(3/2)}} \langle JJK; 0K | \left[ M^0 \mathcal{J}_+ + M^0 \mathcal{J}_-, \mathcal{F}_+ \mathcal{J}_+ + \mathcal{F}_- \mathcal{J}_- \right] | JJK; 0K \rangle$$

where, of course

$$M^0 = M^0 \pm i \mu^0 \quad (7.36)$$

The collective parts may now be eliminated by using the formulas

$$\langle JJK | \mathcal{J}_\pm \mathcal{J}_\mp | JJK \rangle = J(J+1) - K(K-1) \quad (7.37)$$

$$\langle JJK | [\mathcal{J}_+, \mathcal{J}_-] | JJK \rangle = 2 \langle JJK | \mathcal{J}_y | JJK \rangle = 2K \quad (7.38)$$

which when inserted into (35) gives

$$\mu_{\text{cor}} = \frac{i}{2r^{(3/2)}} \langle 0K | (E \mathcal{F}_+ \mathcal{F}_- + E \mathcal{F}_- \mathcal{F}_+) (J(J+1) - K(K-1)) + 2K (M^0 \mathcal{F}_+ - M^0 \mathcal{F}_-) | 0K \rangle \quad (7.39)$$

$$= \frac{i}{2r^{(3/2)}} \langle 0K | (E \mathcal{F}_+ \mathcal{F}_- + E \mathcal{F}_- \mathcal{F}_+) \mathcal{J} + 2K (M^0 \mathcal{F}_+ - M^0 \mathcal{F}_-) | 0K \rangle$$

$$= \frac{i}{2r^{(3/2)}} \langle 0K | (E \mathcal{F}_+ \mathcal{F}_- + E \mathcal{F}_- \mathcal{F}_+) + 2K (M^0 \mathcal{F}_+ - M^0 \mathcal{F}_-) | 0K \rangle$$

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Now comparing this with equation (30), one sees that it is possible to interpret these results in terms of corrections to $g_K$ and $g_R$ (the $\frac{Z}{A}$ in (30)). This gives the first order results.

$$g_R = \frac{g}{A} + \frac{1}{2} \langle \Omega K | \mu^0, F^\perp + \mu^0, F^\parallel | Ok \rangle$$  \hspace{1cm} (7.40)

and

$$g_K = \langle \Omega K | \mu^0, F^\parallel | Ok \rangle + \frac{1}{2} \langle \Omega K | \mu^0, F^- - \mu^0, F^+ - h.c. | Ok \rangle$$  \hspace{1cm} (7.41)

which are used in

$$\mu = (g_K - g_R) \frac{\epsilon^2}{\epsilon - \nu} + g_R \Gamma$$  \hspace{1cm} (7.42)

To complete the above calculation, one must find $F^\perp$. The obvious procedure of referring to Chapter V and using some approximate form may be employed if the $\mu^0$'s are put in their simplified forms. This latter step is necessary if one wants consistent results since mixing of intrinsic and simplified intrinsic operators can lead to trouble. Assuming equal neutron and proton distributions, one may use equation (26) to perform the simplification since this will just entail replacing 1 and 2 by $x$ and $y$ in the subscripts, i.e., $\gamma = 0$ means $\epsilon_k A \rightarrow \delta_k A$.  

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With the reduced $\mu$'s, one may then use the $F_+$ of the previous chapter to get the correction terms above. Of particular interest is the term for $g_R$ since $\frac{Z}{A}$ is known to be valid only on the average. To get an estimate of the correction, employ the cranking and closure approximations as used in Chapter V in the discussion of the size of the added term in the moment of inertia due to a subsidiary condition. Then, omitting the algebra one finds

$$Q^2 \approx \frac{3}{4} - \frac{1}{2} \epsilon \Theta \langle \epsilon \rangle \left[ (\mu_x - i \mu_y - \frac{3}{2} J) J_x + J_x (\mu_x - i \mu_y - \frac{3}{2} J) + \epsilon \right] \rho_0^2 (7.43)$$

where $\Theta$ is the moment of inertia and $\epsilon$ is the average particle-hole spacing, $\langle \epsilon_{\sigma \epsilon} - \epsilon_{\rho \sigma \epsilon} \rangle \approx \epsilon_{CAP}$. Since $\Theta \approx \frac{2 \langle j^2 \rangle}{\epsilon}$, it is clear that the correction term here need not be small.

All of the present discussion has been concerned with axial symmetry and $K \neq \frac{1}{2}$. At present this covers the bulk of important cases. For $K = \frac{1}{2}$, which is not uncommon, one need only include the $\frac{1}{2}$, $-\frac{1}{2}$ coupling to make the result correct. However, for an asymmetric system, one is faced with a much more difficult algebraic problem which won't be considered here.
C. **Electric Quadrupole Moment**

The electric quadrupole operator is a rank two tensor constructed from the cartesian tensors

\[
\mathcal{T}_{ij} = \sum_{\alpha} q_\alpha \mathcal{R}_i^{\alpha} \mathcal{R}_j^{\alpha}
\]  

(7.44)

where \( q_\alpha \) is the charge of particle \( \alpha \), i.e., (44) is a sum over protons only. One usually defines the quadrupole moment by

\[
Q = \langle n J J | T_2^0 | n J J \rangle
\]  

(7.45)

where \( T_2^0 \) is given by

\[
T_2^0 = \frac{1}{2} (\mathcal{E} \mathcal{T}_{zz} - \sum_{i} \mathcal{T}_{ii})
\]  

(7.46)

i.e. just the Legendre polynomial, \( P_2 \).

Now, to affect a decomposition into collective and intrinsic parts one needs to transform to the body fixed system via

\[
\mathcal{T}_{AB} = \sum_{ij} \epsilon_{iA} \epsilon_{jB} \mathcal{T}_{ij}
\]  

(7.47)

For this particular operator, one has the fortunate circumstance that it does not depend on momenta and thus is automatically intrinsic. Consequently, equation (46) may be rewritten as
\[ T_2^0 = \frac{1}{2} \left( 3 \sum_{AB} \epsilon_{j_A} \epsilon_{j_B} \Gamma_{AB} - \sum_j \sum_{AB} \epsilon_{j_B} \epsilon_{j_B} \Gamma_{AB} \right) \tag{7.48} \]

\[ = \frac{1}{2} \sum_{AB} \left( 3 \epsilon_{j_A} \epsilon_{j_B} - \sum_j \epsilon_{j_B} \epsilon_{j_B} \right) \Gamma_{AB} \]

\[ \equiv \sum_{AB} R_{AB} \Gamma_{AB} \]

Here, all of the collective behavior resides in \( R \) while \( \Gamma \) contains only intrinsic information. For purposes of illustration, the electric quadrupole moment for the ground state of an axially symmetric system will be calculated in lowest order, i.e., with \( \psi \) given by equation (23). To simplify things, again assume that the neutron and proton distributions are identical so that

\[ \Gamma_{j} = \frac{2}{A} \sum_{4i \alpha} s_{j}^{\alpha} s_{j}^{\alpha} \tag{7.49} \]

Then, remembering that the \( \epsilon \)'s are eigenvectors for

\[ \sum_{4i} s_{j}^{\alpha} s_{j}^{\alpha} \]

one gets immediately

\[ \Gamma_{AB} = \frac{2}{A} Q_A \delta_{AB} = \frac{\Gamma_A}{A} \delta_{AB} \tag{7.50} \]

where the \( Q_A \)'s are the mass quadrupole moments defined in Chapter II and for axial symmetry \( \langle Q_1 \rangle = \langle Q_2 \rangle \). This may now be incorporated into (48) to give using also the the completeness of the \( \epsilon_{j_A} \)'s

\[ T_2^0 = \sum_A R_{AA} \Gamma_A = \frac{1}{2} \sum_A (3 \epsilon_{j_A}^z - 1) \Gamma_A \tag{7.51} \]

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and finally

\[ Q = \frac{1}{2} \langle Q^{x^y}_k | \phi_k \rangle + (-1)^{J_{-k}} \langle Q^{x^y}_k | \phi_k \rangle + \sum_A R_{AA} \langle Q^{x^y}_k | \phi_k \rangle + (-1)^{J_{-k}} \langle Q^{x^y}_k | \phi_k \rangle \]  \hspace{1cm} (7.52)

\[ = \frac{1}{2} \sum_A \left\{ \langle Q^{x^y}_k | R_{AA} | Q^{x^y}_k \rangle \langle \phi_k | \tau_A | \phi_k \rangle + (\kappa \rightarrow -\kappa) + (-1)^{J_{-k}} \langle Q^{x^y}_{-k} | R_{AA} | Q^{x^y}_k \rangle \langle \phi_{-k} | \tau_A | \phi_k \rangle + \text{c.c.} \right\} \]

Now, the last term is zero since the \( \phi_K \)'s are eigenvalues of \( I_3 \) and, as was shown in Chapter II, the \( Q_A \)'s commute with all of the \( I_A \)'s. Consequently, noting that \( \tau_A \) is proportional to \( Q_A \), it cannot connect states of different \( K \). Allied with this result is the fact that since \( \phi_{-K} \) is gotten from \( \phi_K \) by the transformation \( e^{i\pi J_z} \), the expectation value of \( \tau_A \) is the same for \( K \) and \(-K\).

Then also noting that \( Q^{x^y}_{J_{-k}} \) is found from \( Q^{x^y}_{J_k} \) using \( e^{i\pi J_z} \) (see previous chapter) and that \( R_{AA} \) is invariant under this operation (i.e., \( e^{-i\pi J_z} e^{i\pi J_z} = \pm e^{i\pi A} \)), one gets

\[ Q = \sum_A \langle Q^{x^y}_k | R_{AA} | Q^{x^y}_k \rangle \langle \phi_k | \tau_A | \phi_k \rangle \]  \hspace{1cm} (7.53)

Up to this point, the \( \phi_K \)'s have not been explicitly defined except for the fact that they are \( I_3 \) eigenstates. To proceed one must provide more detail. As usual, this will be done in the form of using the redundant H-F states.
introduced in Chapter V since these are the zero order functions used in the perturbation program. Remembering that the system has axial symmetry, one finds, denoting the H-F state by $|0k\rangle$,

$$Q = \sum_A \langle \mathcal{O}^*_{jk} | R_{AA} | \mathcal{O}^*_{jk} \rangle |0k\rangle + \langle 0k | \tau_3 - \tau_1 | 0k \rangle \langle \mathcal{O}^*_{jk} | R_{33} | \mathcal{O}^*_{jk} \rangle$$

(7.54)

However

$$\sum_A \langle \mathcal{O}^*_{jk} | R_{AA} | \mathcal{O}^*_{jk} \rangle = \frac{1}{2} \sum_A \langle \mathcal{O}^*_{jk} | \{ 3 \epsilon_{zA}^2 - 1 \} | \mathcal{O}^*_{jk} \rangle = 0$$

(7.55)

using the completeness of the $\epsilon_A$'s to get $\sum_A \epsilon_{zA}^2 = 2 = 1$. Thus,

$$Q = \langle 0k | \tau_3 - \tau_1 | 0k \rangle \langle \mathcal{O}^*_{jk} | R_{33} | \mathcal{O}^*_{jk} \rangle$$

(7.56)

and one is left with only one collective matrix element to get the final answer. This can be found by noting that $\epsilon_{zA}$ is the cosine of the angle between $z$ and $e_A$ which is just $\theta$ in the Euler angle specification. Thus

$$\langle \mathcal{O}^*_{jk} | R_{33} | \mathcal{O}^*_{jk} \rangle = \langle \mathcal{O}^*_{jk} | \frac{1}{2} (\cos^2 \theta - 1) | \mathcal{O}^*_{jk} \rangle$$

(7.57)

$$= \langle \mathcal{O}^*_{jk} | P_2 (\cos \theta) | \mathcal{O}^*_{jk} \rangle$$

and for the present normalization of the $D$-functions (to $l$ not $\frac{\pi l}{2l+1}$) one has

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\[ P_2(\cos \beta) = \sqrt{\frac{8\pi}{5}} D_{20}^2(\beta) \]  

Now using the usual formula (16) for the integral of three \( D \)'s, one finds

\[ \langle D_{jk}^* R_{33}^* D_{jk} \rangle = \langle J_2 0 | J 0 | J J \rangle \]

where the \( \langle J_1 J_2 m_1 m_2 | J m \rangle \) are the usual Clebsch-Gordan coefficients. This expression can be readily evaluated using the fact (16)

\[ \langle J 2 m 0 | J m \rangle = \frac{3 m^2 - J(J+1)}{[J(J+1)(2J+1)]^{1/4}} \]

in which case one gets the final result

\[ Q = \langle 0 k | T_0 - T, 0 k \rangle \left( \frac{3 k - J(J+1)}{[J(J+1)(2J+1)]} \right) \]

\[ = \frac{2 e}{A} \langle 0 k | (Q_3 - Q_1) | 0 k \rangle \left( \frac{3 k - J(J+1)}{[J(J+1)(2J+1)]} \right) \]

Of particular interest is, of course, the "intrinsic" quadrupole moment, \( \frac{2 e}{A} \langle Q_3 - Q_1 \rangle \), which can be compared to the Bohr-Mottelson result

\[ Q_{em} = \frac{3}{8\pi} Ze R_0^2 \langle \beta \cos \gamma' \rangle \]

where \( R_0 \) is the average nuclear radius and \( \beta \) and \( \gamma' \) are deformation parameters defined in Chapter I. For axial symmetry, \( \gamma' \) is 0 or \( \pi \) and assumed constant, i.e. no vibrations. To make a comparison of these two answers
note that one has

\[ \langle 0k | Q_s + \bar{Q}_s, 10k \rangle = \frac{2}{3} \langle 0k | Q_s, 10k \rangle \langle \frac{2}{3} A R_0^2 \]  

(7.63)

assuming a small deformation as well as \[ \langle \frac{2}{3} \bar{V}_1 \rangle \approx \frac{2}{3} A R_0^2 \]

i.e. a uniform distribution of particles. Using also the fact that

\[ \beta \approx \frac{1}{2} \frac{\langle 0k | Q_s - \bar{Q}_s, 10k \rangle}{\langle 0k | Q_s + \bar{Q}_s, 10k \rangle} \]  

(7.64)

found by comparing the Bohr-Mottelson moment of inertia from Chapter I with the zero order result here of

\[ m \frac{\langle Q_s - \bar{Q}_s \rangle^2}{\langle Q_s + \bar{Q}_s \rangle} \]  

one gets

\[ \frac{2}{3} \frac{\langle 0k | Q_s + \bar{Q}_s, 10k \rangle}{\langle 0k | Q_s - \bar{Q}_s, 10k \rangle} \approx \frac{2}{3} \frac{\langle 0k | Q_s, 10k \rangle}{\langle 0k | Q_s + \bar{Q}_s, 10k \rangle} \]  

(7.65)

\[ \approx \frac{4}{3} \frac{\varepsilon A}{A} R_0^2 \sim Q_{bm} \]

Thus, at least roughly, the intrinsic moment of inertia calculated here and the Bohr-Mottelson value compare.

The above results indicate what the quadrupole moment looks like to lowest order. Again, to increase the accuracy, one should drop the \( \Gamma_A \approx \frac{2e}{A} Q_A \) approximation as well as include corrections to the wavefunctions because of coupling. However, for this and all electric multipoles, these are not expected to give rise to significant changes. In particular, in the spirit of replacing
the $Q$'s by their expectation values, corrections resulting from using first order wavefunctions are small since they occur in the form $\langle [Q,F] \rangle$ where $F$ is of course the operator generating the first order wavefunction correction. Consequently, higher order terms won't be considered here.

D. Transition Rates

As a final application of the present formalism, the problem of electromagnetic transition rates will be considered. Following the conventional procedure, this will be discussed on the basis of a multipole expansion in the long wavelength, non-relativistic approximation. The transition probability per unit time for a multipolarity, $L$, is then given by (16)

$$\Gamma(L) = 8\pi \frac{e^2}{k} \frac{L_{Lm+n}}{L_{Lm+n+1}} \frac{R_{Lm+n}}{R_{Lm+n+1}} B(L)$$ (7.66)

where $k = \frac{\omega}{c} \ll \frac{1}{R_0}$ and $B(L)$ is the so-called reduced transition rate and will be defined shortly. This latter quantity, of course, contains all of the detailed information about the radiating system.

Using standard perturbation theory and assuming the nucleons have point charge distributions, one may determine the $B(L)$'s which come in two varieties, electric.
and magnetic. For the electric multipole transitions from a state \( \psi_{nJm} \) to a state \( \psi_{n'J'm'} \), one has

\[
BE(L) = |< \psi_{nJm}, | \frac{1}{\varepsilon} \sum_{j} q_j \gamma_j^L \mathcal{Y}^L_m(\theta_j, \phi_j) | \psi_{n'J'm'} >|^2
\]  

(7.67)

where \( q_j \) is the charge of particle \( j \). The operator appearing in the matrix element is a tensor of rank \( L \) and may readily be written in terms of cartesian tensors, to conform to the present treatment, by just looking up the corresponding \( \mathcal{Y}^L_m \). Moreover, since this operator is independent of momenta, its body fixed components are automatically intrinsic, i.e. they commute with both \( \vec{J} \) and the \( \vec{e}'s \). Consequently, by writing it in the basis of the body fixed unit vectors, one has accomplished a complete separation into collective and intrinsic parts and may thus immediately evaluate the matrix element in \( BE(L) \). This will be done later for some cases particularly interesting for nuclear rotational systems.

The magnetic multipoles have the slightly more complicated form, \( (16) \)

\[
BM(L) = |< \psi_{nJm}, | \mathcal{L} \{ \sum_j \gamma_j \mathcal{L} \mathcal{Y}_{m, L}^{\ell} (\theta_j, \phi_j) [\frac{1}{2} g_s \gamma_j \vec{g}_j + \frac{1}{2} g_s \vec{g}_j \gamma_j ] | \psi_{n'J'm'} >|^2
\]  

(7.68)

where the \( g's \) are the g-factors introduced before and
it should be noted that the "grad" operates only on the $r^L_Y^L$ part. This can be rewritten in various forms by using the machinery of tensor algebra, but for the present purposes the above form is satisfactory. Now, in the above matrix element, one sees that the operator here is the product of a tensor of rank $L-1$ with one of rank 1 remembering that $r^L_Y^L_{(m',m)}$ is a homogeneous polynomial of degree $L$ in the $(x, y, z)$'s and that grad reduces this degree by one. Thus by using $L$ of the $\hat{e}$'s one may transform to the body fixed system as usual. However, this does not generate intrinsic operators since the $\hat{\mathbf{r}}$'s contain derivatives. Instead one must perform the Tomonaga decomposition to complete the separation into collective and intrinsic parts. This follows the magnetic moment case exactly since the $L-1$ rank tensor acts just like a constant with respect to taking commutators of the $\hat{e}$'s. In other words, schematically, for this case

$$[T_{\mathbf{r}}', T', \hat{e}] = T_{\mathbf{r}}' [T', \hat{e}]$$ (7.69)

since the $T^{L-1}$ tensor contains no derivative operators i.e. the grad does not operate on the $\Psi$'s. Consequently, one simply decomposes the second factor in (68) just like the magnetic moment and then multiplies by the body fixed components of $T^{L-1}$ i.e.
\[ T_{k_{1},\ldots,k_{n}}^{L_{1}} = \sum_{A_{1} \cdots A_{n}} \epsilon_{A_{1}A_{1}} \cdots \epsilon_{A_{n}A_{n}} T_{A_{1},\ldots,A_{n}}^{L_{1}} \left( T_{A_{1},\ldots,A_{n}}^{L_{1}^{(0)}} + \sum_{\beta} T_{A_{1},\ldots,A_{n}}^{L_{1}^{(\beta)}} \mathcal{J}_{\beta} \right) \]

where, of course, the subscripts refer to cartesian components and the \( T_{A_{1}}^{L_{1}^{(0)}} \) and \( T_{A_{1},B}^{L_{1}^{(1)}} \) are analogies of \( \mu_{A_{1}}^{0} \) and \( g_{A_{1},B}^{0} \) for the magnetic moment. The examples given next will exhibit this procedure in more detail.

In the problem of nuclear rotation, the transitions of particular interest are those from one level of a band to another. The most favorable transitions are between adjacent levels since this entails the minimum change in angular momentum and thus the lowest multipolarity.

These are the cases which will be illustrated here. Now noting that the levels progress in integer steps of \( J \), except for \( K=0 \) bands where the steps are by two, and that all levels within the band have the same parity, that of the intrinsic state, one sees that the important multipoles are the \( ml \) and \( E2 \). Fortunately, these cases almost parallel the magnetic and electric quadrupole moment calculations so much of the work has already been done.

For the \( E2 \) transitions, as with all cases, one need only consider the \( m'=m \) reduced transition rate since
all others are related to it via the Wigner-Eckart theorem. Thus, the tensor under consideration is

$$\frac{1}{\varepsilon} \sum_{j_{0}} \tilde{q}_{j_{0}} \tilde{r}_{j_{0}}^{2} \psi_{j_{0}}^{*}(\Theta_{j}, \Phi_{j}) = \frac{1}{\varepsilon} \sum_{j_{0}} \tilde{q}_{j_{0}} \sqrt{\frac{8}{6\pi}} (3z_{j_{0}}^{*} - r_{j_{0}}^{*})$$

$$= \frac{1}{\varepsilon} \sqrt{\frac{5}{6\pi}} T_{2}^{0}$$

where $T_{2}^{0}$ is given by equation (46). With this form, one may now just refer to the quadrupole moment calculation noting that the only difference is that BE(2) has $J' \neq J$. Consequently, in analogy to equation (56), one has, at least for the ground state band

$$BE(2) = |<\psi_{J' m_{J'}} | \frac{1}{\varepsilon} \sqrt{\frac{5}{6\pi}} T_{2}^{0} | \psi_{J m_{J}}>|^{2}$$

$$= \frac{5}{4\pi\varepsilon^{2}} |<\psi_{J' m_{J'}} | \frac{\hat{r}_{0}}{1-\Theta_{J' m_{J'}}} R_{33} | \hat{G}^{*}_{m_{J' m}}>|^{2}$$

Again, the collective integration can be done using the formula for the product of three D-functions. In this case one finds

$$<\hat{G}^{*}_{m_{J' m}} | R_{33} | \hat{G}^{*}_{m_{J' m}} > = \frac{2\pi}{2z_{J' m_{J' m}}^{*}} <J_{2} k 0 | J' k' <J_{2} m_{0} | J' m_{0}>$$

and so defining the intrinsic quadrupole moment as

$$Q_{o} = <\hat{r}_{0} | \hat{r}_{0} - \Theta_{J' m_{J' m}}>$$

one gets for a $J' \rightarrow J$ transition

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\[ B(E2) = \frac{5}{16\pi e^2} Q_0^2 \langle \frac{2J'+1}{2J+1} \rangle \langle J_2 k_0 | J' k \rangle \langle J_2 m_0 | J' m \rangle \]  \tag{7.75}

The most prevalent case is of course the \( K=0 \) band in which case \( J'=J+2 \), and which requires looking up \( J=J+1 \), and using the fact \( J=J+1 \)

\[ \langle J_2 m_0 | J+1, m \rangle = m \left[ \frac{3 (J-m+1)(J+m+1)}{J(2J+1)(J+2)} \right]^{1/2} \]  \tag{7.78}

thus, for this situation

\[ B(E2) = \frac{5}{16\pi e^2} Q_0^2 \left[ \frac{3 (J-m+2)(J-m+1)(J+m+2)(J+m+1)}{(2J+5)(2J+1)(2J+3)^2} \right] \]  \tag{7.77}

with \( K \neq 0 \), one may have \( J'=J+1 \) and using the fact \( J=J+1 \)

obtain

\[ B(E2) = \frac{45}{16\pi e^2} Q_0^2 \left[ \frac{m^2 k^2(J-k+1)(J-k+1)(J-m+1)(J+m+1)}{(2J+3)(2J+3) [J(J+1)(J+2)]^2} \right] \]  \tag{7.79}

The most important aspect of these results is, of course, the fact that the transition probabilities are proportional to \( Q_0^2 \) and thus, since \( Q_0 \) is much larger than the single particle value, the transitions are enhanced. Moreover, a measurement of the \( E2 \) transition rate affords a direct determination of \( Q_0 \). These are all well known results.
coming directly from the unified model to which the
present level of approximation is equivalent. Corrections
induced by going to a higher order are generally small
for the reasons given in the quadrupole moment discussion
and thus won't be discussed here.

Turning now to the M1 transitions, one has

\[ B_M(l) = |\langle \psi_{n' m'} | \sum_i [y_{2ad}(r_i, \psi_i, \eta_i)] \cdot \left[ g_s (g_1^i \vec{J}_1 + g_2^i \vec{S}_2) \right] | \psi_{n m} \rangle |^2 \]  \hspace{1cm} (7.80)

and since \( \psi_0^1 = \sqrt{4\pi} \frac{2}{p} \), this reduces to

\[ B_M(l) = \frac{3}{4\pi} e^2 |\langle \psi_{n' m'} | \sum_i \left( g_1^i \vec{J}_1 + g_2^i \vec{S}_2 \right) | \psi_{n m} \rangle |^2 \] \hspace{1cm} (7.81)

The operator appearing here is just the magnetic moment
operator for which the decomposition has already been
performed. Consequently, one may transpose the results
directly with the only change being one considers off
diagonal matrix elements here. So, assuming identical
neutron and proton distributions, one has from equations
(7), (25), and (26)

\[ \mathcal{M}_Z = \sum_{\alpha = i}^{A} c_{z \alpha} \left\{ (\mu_\alpha - \frac{z}{A} J_\alpha) + \frac{z}{A} J_\alpha \right\} \]  \hspace{1cm} (7.82)

This may now be inserted into equation (81). For the
present illustration, consider intra-band transitions for
the ground state band. Also, assume \( K = 0 \) so that decoupling
effects do not arise. Then using the zero order states, i.e. without coupling corrections, as exemplified by equation (23) one has

$$B M(l) = \frac{3}{8\pi e^2} \left| \langle \mathcal{Q}_{m^L}^{J^\prime} | \mathcal{L}^{x^7}_{m^L} \phi_k | \mu_1 \mathcal{L}^{x^7}_{m^L} \phi_k \rangle + (-1)^{J^\prime - J} (k \leftrightarrow -k) \right|^2$$

(7.83)

where the $\phi_k$'s are the H-F states of Chapter V. With the decomposed form given by equation (82) one sees that

$$\langle \mathcal{Q}_{m^L}^{J^\prime} \phi_k | \mu_1 \mathcal{L}^{x^7}_{m^L} \phi_k \rangle = \frac{3}{8\pi} \left[ \langle \mathcal{Q}_{m^L}^{J^\prime} \cdot \epsilon_{2A} \mathcal{S}_{m^L}^{x^7} \phi_k | \mu_1 \mathcal{L}^{x^7}_{m^L} \phi_k \rangle + \left( \frac{\mathcal{Q}_{m^L}^{J^\prime}}{2} \right) \langle \epsilon_{2A} \mathcal{J}_A | \mathcal{S}_{m^L}^{x^7} \rangle \right]$$

(7.84)

Now, the second term vanishes since $\sum_A \epsilon_{2A} \mathcal{J}_A = \mathcal{J}_2$, can not connect states with different $J$. Also, because $[\epsilon_{2A}, \mathcal{J}_3] = -i \epsilon_{2A} \epsilon_{A3}$, one sees that only $\epsilon_{23}$ has a non-zero diagonal matrix element in $k$. This can be easily found from the fact that $\epsilon_{23}$ is just $\cos \theta$ or merely $\sqrt{\frac{2}{3}} \mathcal{Q}_{m^L}^{J^\prime}$. Thus, using the formula for the integral of three D-functions again, one finds

$$\langle \mathcal{Q}_{m^L}^{J^\prime} | \epsilon_{2A} \mathcal{S}_{m^L}^{x^7} \rangle = \sqrt{\frac{2}{3}} \langle J^\prime | \epsilon_{J^\prime} | J^\prime \rangle \langle J^\prime | m_10 | Jm \rangle \langle J^\prime | k_10 | k \rangle$$

(7.85)

An exactly analogous result holds for $-k$ and so one gets
\[ \mathcal{B} M(l) = \frac{3}{16 \pi^2} \left( \frac{2J+1}{2J'+1} \right) \left\langle J'\ell 0 \mid J m \right\rangle^2. \] (7.86)

To put this in its final form, remember that transitions between adjacent rotational levels have \( J' = J + 1 \) which means one uses (16)

\[ \left\langle J+1, m 0 \mid J m \right\rangle = -\sqrt{\frac{(J+m)(J+1+m)}{(J+1)(2J+1)}} \] (7.87)

Also, use the approximations and definitions from equations (28) and (29) to get

\[ \left\langle \phi_e \mid \mu_g - \frac{2}{A} J_3 \mid \phi_k \right\rangle = (g_k - \frac{2}{A}) \kappa = -\left\langle \phi_k \mid \mu_g - \frac{2}{A} J_3 \mid \phi_e \right\rangle \] (7.88)

Then equation (86) reduces to

\[ \mathcal{B} M(l) = \frac{3K^2}{4 \pi^2} \left( \frac{2J+1}{2J'+1} \right) \left[ \frac{(J+m)(J+1+m)(J+1+k)(J+1+k)}{(J+1)^2 (2J+1)^2} \right] \left| g_k - \frac{2}{A} \right|^2 \] (7.89)

It should be noted that this is proportional to the square intrinsic magnetic moment, \( (g_k - \frac{Z}{A}) \frac{K^2}{(J+1)} \), and that the collective part gives no contribution to these M1 transitions. This is true in general and stems from the fact that the rotational part of the magnetic moment is proportional to \( J \) which can never connect states of different \( J \). It can, of course, connect different bands, values of \( n \), where the initial and final states have the same \( J \) but
these transitions are usually highly attenuated due to the fact that they require a change of the internal structure.

The reduced transition rate just calculated for $M_1$ transitions will generally be inadequate for comparison with experimental data since coupling corrections to the wavefunctions were not included. These are handled exactly as was done for the magnetic moment. As this adds nothing to the present illustration of transition rates, it won't be performed here.

In summary, it appears that the present formalism allows a very simple and natural framework in discussing the various tensors of physical interest. The separation into collective and intrinsic parts is performed in a clear and unambiguous manner and calculations of matrix elements with the wavefunctions derived in the main body of the thesis is straightforward. Finally, since the rotation-intrinsic coupling can be considered, correction terms to the Bohr-Mottelson results are readily obtained.
VIII. ALTERNATIVE METHODS OF SOLUTION

Besides the perturbative solutions utilized in the previous chapters, one may also inquire if there are any other ways to eliminate or at least reduce the effects of the rotation-intrinsic coupling. In this chapter, two methods will be outlined which are based on the fact that the angle variables exhibit a certain amount of freedom in their definitions. Using this property and a few assumptions about the nature of the angles, it will be shown that one can quite easily obtain the Thouless-Valatin type of moment of inertia. The real weakness of this type of approach is the fact that the assumptions about the angles can not be verified and thus these methods are just "one shot" and do not lead to well defined systematic improvements. However, the relative ease with which the answers are obtained warrants a brief exposition.

For the sake of simplicity, only the two dimensional case will be considered. Recalling the results of Chapter II, it is seen that in general the Hamiltonian is decomposed in an infinite series in $J$. Only when one requires $\varphi$ to be a function of just the coordinates does the simplification that this series terminate at $J^2$ occur. Now in
the present chapter, this requirement can not be imposed
since one will be trying to find a $\varphi$ which satisfies
certain conditions with respect to eliminating the coupling
term. In general, this operator will contain momenta
and hence one must contend with the problem of convergence
of the terms in the decomposed Hamiltonian. However, it
will be assumed that the momentum dependence is weak
enough so the series, at least asymptotically for deformed
nuclei, is sufficiently accurate through order $J^2$. In
other words, all commutators of the form $[[H, \varphi], \ldots \varphi]$ vanish for more than two $\varphi$'s and so one has the usual
form

$$H_k = (H - \hat{\varphi} J + \frac{1}{2} Q J^2) + (\hat{\varphi} - Q J) K + \frac{1}{2} Q K^2 + \ldots$$

(8.1)

$$\cong H_0 + H_1 K + \frac{1}{2} Q K^2$$

Here the notation of Chapter II is used and, of course, $K$
is just a number.

Now the obvious way to eliminate coupling is to
choose

$$\varphi = Q J$$

(8.2)

However, this equation is formidable and it is doubtful
whether a solution for $\varphi$ even exists. So instead of imposing this stringent requirement on $\varphi$, it will be more appropriate to develop an approximate program. Keeping with the philosophy of the thesis, it is natural to base this on an underlying H-F scheme. Thus, the first method of solution will be to require equation (2) to hold for an appropriate set of matrix elements of a H-F basis. The obvious choice for this basis is the one for $H_0$. In other words, let $|\phi\rangle$ be the H-F ground state for $H_0$ and thus for $H_0 + \frac{1}{2} Qk^2$ as long as $Q$ can be considered constant. This means that

$$\langle 0 | H_0 + \frac{1}{2} Qk^2 | \phi \rangle = 0$$

(8.3)

for all one particle-hole states, $|\phi\rangle$. Then, by defining $\varphi$ such that these are also H-F states for $H_K$, one finds

$$\langle 0 | H_0 + H_1 k + \frac{1}{2} Qk^2 | \phi \rangle = 0$$

(8.4)

$$= k \langle 0 | H_1 | \phi \rangle$$

or

$$\langle 0 | \varphi | \phi \rangle = \mathcal{J} \langle 0 | [H, \varphi] | \phi \rangle = Q \langle 0 | J | \phi \rangle$$

(8.5)
With this $\Psi$, $\frac{1}{Q}$ is clearly the true moment of inertia and as will now be shown, is the Thouless-Valatin value. First, define

$$G = \frac{\Psi}{Q}$$  \hspace{1cm} (8.6)

then equation (5) gives

$$i\langle 0| [H, G]|\psi\rangle = \langle 0| J|\psi\rangle$$  \hspace{1cm} (8.7)

while the conjugate properties of $\Psi$ and $J$ give

$$i\langle 0| [J, G]|\psi\rangle = \frac{i}{\alpha} \langle 0| [J, \Psi]|\psi\rangle = \frac{1}{\alpha}$$  \hspace{1cm} (8.8)

Clearly (7) and (8) are of the Thouless-Valatin form though the fact $\Psi$ won't in general be a one body operator represents a slight disparity. Noting that for $G \rightarrow G+f(J)$ one gets the same equations, since $[H, J] = 0$, this latter discrepancy can be softened and possibly eliminated by the proper choice of $f$. Also note that, as opposed to equation (2), (5) represents a matrix equation which can in principle be solved in conjunction with the canonical commutation relations.

The second alternative method is actually not entirely unrelated to the use of perturbation theory. This consists of noting that for the ground state
rotational band, one gets a perturbation result for the inverse moment of inertia of

$$\Theta^{-1} = Q - \sum_{\alpha} \frac{2|\langle 0 | H_{\alpha} | \psi_b \rangle |^2}{\epsilon_\alpha - \epsilon_{\psi b}}$$

(8.9)

$$= \langle 0 | -[\pi H, \psi] + [[H_\psi, f], f] | 0 \rangle$$

where $f$ is the one particle operator generating the first order correction to the wavefunctions. This indicates that no matter what choice is made for $\psi$, the renormalized value of $\Theta$ is always greater than $\frac{1}{Q}$ i.e. $(\epsilon_\alpha - \epsilon_{\psi b}) < 0$ for all $\alpha$. There is, of course, the reservation that the moment of inertia remain positive, a necessity for what is usually called a rotational spectrum. With the above fact, it is clear that one may possibly be able to define the problem for the moment of inertia as a variational one on $\psi$. That is, choose $\psi$ such that $\langle 0 | \psi | 0 \rangle$ is minimized.

To show that this is a valid procedure, one must examine equation (9) and see if it can be put in the form

$$\Theta^{-1} = -\langle 0 | [[H, \psi + g], \psi + g] | 0 \rangle$$

(8.10)

where $g$ is an operator which commutes with $J$ so that if one defines $\psi' = \psi + g$, then $\psi'$ is also conjugate to $J$. This can be made plausible by assuming, as was
done in Chapter V, that $[\dot{\psi}, f]$ is constant and $f$ is intrinsic. Neither of these is expected to be exact, but as was argued in Chapter V, the redundancy of the problem allows them to be enforced approximately. Then, using the fact that

$$\lambda <0| [H, \psi + f]|\rho h> = \frac{i}{\hbar} <0| J|\rho h> \tag{8.11}$$

and assuming that $2\rho h$, $3\rho h$, etc., matrix elements of $[H, \psi + f]$ are small, one finds

$$<0|[H, \psi + f]|0> \approx -\frac{i}{\hbar} <0| J|0> = -\frac{i}{\hbar} \tag{8.12}$$

as required by equation (10). Thus, by this crude plausibility argument, one can indeed prescribe a variational principle for $\Theta$.

It will now be shown that to a lowest order approximation one again arrives at a Thouless-Valatin form. First of all, it is necessary to define the variational principle for an operator. This will be taken as the usual functional variation defined by

$$\delta_A <0| f(A)|0> = <0| f(A+\delta A)|0> - <0| f(A)|0> \tag{8.13}$$

where $A$ is an operator and $\delta A$ is an arbitrary small operator. In the present case, however, one must be
certain that \( \psi \) remain conjugate to \( J \), i.e. keep
\[ [\psi, J] = i. \] This can be done using Lagrange multipliers
and in general must be enforced for all matrix elements
of \( [\psi, J] \). As a lowest approximation though, this will
be required only for the vacuum expectation value.
Associated with this is the fact that one should only
perform single particle variations, i.e. \( \delta \psi \) a one
particle operator. The reason for this is that \( J \) is
a one particle operator so that \( \langle 0 | [\psi, J] | 0 \rangle = i \) insures
only that the one particle part of \( \psi \) remains consistent
with the canonical commutation relations. Thus, a one
particle variation will keep \( \psi \) conjugate to \( J \) but, of
course, is only a subset of the possible \( \delta \psi \)'s. The
variational program can now be written as
\[
\delta \psi \langle 0 | -[[H, \psi], \psi] + i \lambda [J, \psi] | 0 \rangle = 0
\] (8.14)
where for the present case take \( | 0 \rangle \) as the H-F
ground state for \( H \) and not \( H_0 \). This is for convenience
since one really needs states of \( H_0 \); however, the results
are essentially equivalent since \( H_0 \triangleq H - \frac{i}{\lambda} \frac{1}{\lambda} J^2 \) and
the \( \frac{i}{\lambda} J^2 \) term is a small perturbation. Now writing
out the variation, one finds
\[
\langle 0 | -2 [\epsilon H, \psi], \delta \psi] + i \lambda [J, \delta \psi] - [\psi, \delta \psi], H | 0 \rangle = 0
\] (8.15)
The last term is approximately zero since $\delta \psi$ is a one particle operator and $H$ does not connect any one particle states by the Brillouin theorem. Then, if $\psi$ were strictly one particle, $[\psi, \delta \psi]$ would also be and thus this term would vanish. Since $\psi$ may have two or more particle parts, this is only approximate but valid as long as the H-F program is accurate since only the off diagonal two body part of $H$ will couple with $[\psi, \delta \psi]$. So,

$$<0|(-2[H, \psi] + i \lambda J), \delta \psi|0> \approx 0$$  \hspace{1cm} (8.16)

or equivalently

$$<0| -2[H, \psi] + i \lambda J, \rho\psi|0> = 0$$  \hspace{1cm} (8.17)

for all one particle states, $\rho\psi$. Now $\lambda$ is determined by requiring

$$<0|i[J, \psi]|0> = 1$$  \hspace{1cm} (8.18)

which according to equation (17) means

$$<0|2[H, \psi], \psi|0> = \lambda$$  \hspace{1cm} (8.19)

But, since $<0|-[H, \psi], \psi|0> = \frac{1}{\rho}$, one sees that

$$\lambda = -\frac{2}{\rho}$$  \hspace{1cm} (8.20)
The Thouless-Valatin form is evident if one defines

$$G = \frac{-\lambda}{\lambda}$$  \hspace{1cm} (8.21)

because then (17) and (18) give

$$\langle 0 | \hat{\mathcal{L}} [H, \mathcal{G}] | \rho \rangle = \langle 0 | \hat{J} | \rho \rangle$$  \hspace{1cm} (8.22)

and

$$\langle 0 | \hat{\mathcal{L}} [J, \mathcal{G}] | 0 \rangle = -\frac{\lambda}{\lambda} \langle 0 | \hat{\mathcal{L}} [J, \Psi] | 0 \rangle = -\frac{\lambda}{\lambda} = \Theta$$  \hspace{1cm} (8.23)

as desired.
IX. CONCLUSION

As the present thesis is an examination of the nuclear rotation problem from a more fundamental or rigorous viewpoint than the previous modelistic and semi-classical theories, it seems that the most effective conclusion is a summary of results along with their relation to the previous works. In this way the basics of the various theories become evident as well as their limitations. Moreover, this approach allows one to see how the new results derived in the present work may be incorporated into the existing practical calculations and thus alleviate the necessity of duplicating results already established.

In summary, then, this thesis has presented a separation method whereby the Hamiltonian is given in a form which is very convenient for discussing nuclear rotation. The essence of the method is that the dependence of the Hamiltonian on the total angular momentum is explicitly exhibited. This is crucial since the rotational bands are characterized by a well defined progression in terms of the total angular momentum. And since this is also a conserved quantity, one can treat this part of the motion
exactly leaving only intrinsic, non-rotational, dynamics to approximation. The real merit of the present means of separation, Tomonaga's method, is that the operators associated with the intrinsic motion are expressed in terms of the variables describing the total system. This circumvents the problem of explicitly finding the variables required to specify the intrinsic problem. Moreover, it allows a solution scheme based on using Hartree-Fock theory in a redundant space.

Applying this separation method to the nuclear Hamiltonian, produced a form which is directly interpretable in terms of the Bohr-Mottelson unified model. In particular, the, so far poorly defined, concept of an intrinsic angular momentum emerged in a natural and clearly defined way. Operators for this quantity were exhibited and were shown to be intrinsic, that is, independent of the total rotational motion. Moreover, in the limit of small deformation (to order $\beta^2$), these operators were seen to obey the commutation relations of space fixed angular momentum as stipulated in the unified model. An important consequence of obtaining a precise form for the intrinsic angular momentum is that one may determine the exact form for the coupling between the collective and intrinsic
motions. This allows one to calculate corrections to
the moment of inertia, a procedure ignored in the unified
model.

With the Hamiltonian transformed exactly into the
Bohr-Mottelson form a basic formalism for studying nuclear
rotation was established. The much more difficult problem
of obtaining solutions with this Hamiltonian still had
to be considered. Using conservation of angular momentum,
it has been possible to reduce the problem to purely an
intrinsic one. In order to proceed it was necessary to
employ the technique of redundant variables and base the
solutions on the H-F approximation. This process is
neither new to many body physics nor to nuclear rotation
in particular. In fact, though usually implicit, the
use of redundant variables actually was extensive in the
Bohr-Mottelson model. Now in the present work, one was
able to extend to a redundant space via certain $S$-functions
which appeared in matrix elements. The price paid was
that one was forced into using an over complete set of
functions as well as into using a non-orthogonal basis.
In practical applications, though, it is unlikely that
these technical problems will give any trouble.

Once the redundant variables scheme was introduced,
one was still faced with alternative means of solution.
The crudest approach was to eliminate the $\delta$-functions which appeared in the matrix elements. Then by performing a perturbation-variation program, one was able to extract a fairly simple solution to the rotational problem with coupling included. Using a few approximations, it was demonstrated that the resulting form for the moment of inertia was in agreement with that found by Thouless and Valatin. This was encouraging since the latter appears to correlate well with experimental values, at least in its simplified cranking model form.

A somewhat better approach to the intrinsic problem was obtained by using the $\delta$-functions to eliminate certain explicit dependences of the intrinsic operators on the angle variables. To obtain a practical form, the $\delta$-functions were dropped in favor of a subsidiary condition on the variational principle. This is clearly an approximate procedure; however, arguments were presented, based on the fact that deformed H-F states are used, to substantiate the approximation. With the operators in their simplified form, a perturbation solution was obtained which essentially again agreed with the Thouless-Valatin results. There is a correction term due to the subsidiary condition, but it was shown to be small for highly
deformed nuclei. This fact is in agreement with the basic assumption of previous theories that the nuclear rotation in lowest order is simulated by a uniform classical rotation of the H-F axes.

In applying the method to axially symmetric systems, certain difficulties arose due to the fact that the moment of inertia about the symmetry axis tends to zero. The main problem was that some parts of the Hamiltonian became singular. However, in this type of system, it was shown that the component of the intrinsic angular momentum along the symmetry axis was conserved and by judicious choice of its eigenvalue, the divergence could be eliminated. This is what was also done in the Bohr-Mottelson model. In the present case, though, it was possible to show that the choice was conserved to all orders of perturbation theory.

Once the basic solutions were obtained, the problem of determining their symmetries was attacked. The main consequence of this investigation was that the symmetries of the unified model were essentially correct in the sense of being verified by a fundamental theory. Of particular importance was the result that K=0 bands
may have only even or only odd rotational levels depending on the time reversal properties of the intrinsic, i.e. H-F, states.

The procedure for determining the symmetries in the present work was based on the observation that the same space point was expressible in terms of more than one set of collective plus intrinsic coordinates. This meant that certain symmetries or more accurately boundary conditions, must hold in order to achieve a single valued wavefunction. In contrast, the usual modelistic results are based on arguments about the intrinsic "shape" and are probably more empirical than derivable.

To complete the study of rotational systems, the properties of the various physically interesting tensors were considered. Again the separation method proved very fruitful in exhibiting the explicit collective and intrinsic dependences of the pertinent operators. In particular, the intrinsic and rotational g-factors appearing in the magnetic moments arose in a very natural way. Moreover, by considering the unperturbed states of the previous chapters, it was shown that the magnetic moments, as well as the electric quadrupole moment, had
exactly the values stipulated by the Bohr-Mottelson model. When the first order corrections were included in the magnetic moment calculation, it was shown that appreciable changes resulted as expected. Hopefully, more detailed numerical work will verify that these are indeed significant corrections.

Besides the static moments, the off-diagonal matrix elements of the tensor operators were treated in the context of transition amplitudes. With the present formulation, the contributions to radiative processes from collective and intrinsic properties were clearly identified. For purposes of illustration, the two most important cases, M1 and E2, were worked out in lowest order.

As a final, aesthetic, sideline, the results of the two dimensional work were derived by two alternative methods. These were terse and non-perturbative, but suffered from the defect of being not entirely justifiable or systematic. The first method was based on the fact that one had considerable latitude in defining the conjugate angle. By choosing it so as to eliminate the coupling term in a H-F program, the Thouless-Valatin equations readily emerged. The second method used the observation that in lowest order perturbation, the
renormalized moment of inertia was always larger than the unperturbed value. This led to a variational procedure in which one minimized the inverse moment of inertia with respect to changes in the angle variable. Again, Thouless-Valatin results.

To complete the Conclusion, as well as tie up a loose end, a brief discussion of the validity of the perturbation expansion will be given. This will be done for two dimensions where from Chapter V one finds that the lowest order energy shift is

$$\Delta E = \frac{k^2}{2} \langle 0 \mid i \chi (H_1, f) \mid 0 \rangle$$  \hspace{1cm} (9.1)

Remembering that $f$ may be related to the $G$ of Thouless-Valatin theory by

$$f = \frac{G}{\Theta} - \varphi$$  \hspace{1cm} (9.2)

where $\Theta$ is the "true" moment of inertia one finds

$$\Delta E \approx \frac{i k^2}{2 \Theta} \langle 0 \mid [H_1, G] \mid 0 \rangle$$ \hspace{1cm} (9.3)

using the intrinsic nature of $H_1$. Now considering only lowest order in $\beta$, one has

$$H_1 = -\frac{1}{\beta} \mathbf{J} + O(\beta)$$  \hspace{1cm} (9.4)
where $\mathcal{J}$ is the unperturbed (i.e., Bohr-Mottelson) moment of inertia. Also, from the cranking model, one knows

$$
\langle 0 | \mathcal{J} | \rho \rangle \cong i \frac{\langle 0 | \mathcal{J} | \rho \rangle}{\varepsilon_\mu - \varepsilon_\sigma}
$$

so that

$$
\Delta E \cong \frac{k^2}{\mathcal{J}} \Delta \varepsilon \frac{\sum | \langle 0 | \mathcal{J} | \rho \rangle |^2}{\varepsilon_\sigma - \varepsilon_\mu}
$$

(9.6)

To simplify this further, use the fact that one has an energy gap so that $\varepsilon_\mu - \varepsilon_\sigma$ may be replaced by some average value, $-\Delta \varepsilon$, of the order of the gap. Then

$$
\Delta E \cong \frac{k^2 \langle \mathcal{J} \rangle}{\mathcal{J} \Delta \varepsilon}
$$

(9.7)

Now for a valid expansion, this shift must be less than the distance to the nearest excited intrinsic level. This latter is, of course, just the gap width so that one requires

$$
\frac{k^2 \langle \mathcal{J} \rangle}{\mathcal{J} \Delta \varepsilon} \leq \varepsilon_{\text{gap}} \Delta \varepsilon
$$

(9.8)

Thus there exists a critical value,

$$
k_c \Delta \varepsilon \leq \sqrt{\frac{\mathcal{J}}{2\pi k^2}}
$$

(9.9)

beyond which the perturbation expansion breaks down. A
manifestation of this result is the somewhat abrupt
disappearance of the rotational band.

As an example to see what \( K_c \) is, consider the region \( A \sim 150 \). Here one has the typical numbers

\[
\epsilon \sim 1.5 \text{ mev} \tag{9.10}
\]

\[
\Theta \sim 5 \text{ fm} \sim 100 \text{ mev}^{-1} \tag{9.11}
\]

\[
\sqrt{\langle r^2 \rangle} \sim 5 \tag{9.12}
\]

and thus

\[
K_c \sim 13 \tag{9.13}
\]

This is consistent with observed facts that the rotational levels begin to deviate from a strict rotational sequence
at \( K \sim 8 - 10 \) and seem to disappear around \( K \sim 12 - 16 \).
APPENDIX A

In this Appendix, the commutator from Chapter II,

\[ \mathcal{J}_{AB} \equiv [\mathbf{\eta}_A, \mathbf{\eta}_B] = -i \left\{ \frac{1}{1 + \omega_0 \omega_0} \mathbf{\eta}_A \cdot \mathbf{\eta}_B \right\} \mathbf{\eta}_C + \frac{2}{1 + \omega_0 \omega_0} \mathbf{\eta}_A \cdot \mathbf{\eta}_C \mathbf{\eta}_A \mathbf{\eta}_C \right\} \quad (A.1) \]

will be derived. To do this, recall from that chapter that

\[ \mathbf{\eta}_A = \frac{i}{2} \sum_{k \ell} \left\{ \mathbf{\varepsilon}_{k \ell} \cdot \left[ H_j, \mathbf{T}_{k \ell} \right] \right\} \mathbf{\varepsilon}_{l \ell} + \mathbf{\varepsilon}_{l \ell} \right\} (\mathbf{Q}_B - \mathbf{Q}_C)^{-1} \quad (A.2) \]

Then, since \( \mathbf{T}_{k \ell} = \sum_{x=1}^{4} r_x^i \cdot r_x^j \) and \( V \) commutes with the \( r \)'s one finds

\[ \left[ H_j, \mathbf{T}_{k \ell} \right] = \frac{i}{2m} \sum_{k \ell} \left\{ \mathbf{\rho}_k \cdot r_k^i + \mathbf{\rho}_k \cdot r_k^j + h.c. \right\} \quad (A.3) \]

which when coupled with the orthogonality of the \( \mathbf{\varepsilon} \)'s gives

\[ \mathbf{\eta}_A = \frac{i}{2m} \sum_{k \ell} \left\{ \mathbf{\varepsilon}_{k \ell} \cdot \left[ \frac{1}{2} \left( \mathbf{\rho}_k \cdot r_k^i + \mathbf{\rho}_k \cdot r_k^j \right) \right] \mathbf{\varepsilon}_{l \ell} + \mathbf{\varepsilon}_{l \ell} \right\} (\mathbf{Q}_B - \mathbf{Q}_C)^{-1} \quad (A.4) \]

\[ = \frac{i}{2m} \sum_{k \ell} \left\{ \mathbf{\varepsilon}_{k \ell} \cdot \mathbf{\varepsilon}_{l \ell} \cdot \left[ \frac{1}{2} \left( \mathbf{\rho}_k \cdot r_k^i + \mathbf{\rho}_k \cdot r_k^j \right) \right] + h.c. \right\} (\mathbf{Q}_B - \mathbf{Q}_C)^{-1} \]

Now defining

\[ r^i_A = \sum_k \mathbf{\varepsilon}_{kA} r_k^i \quad (A.5) \]

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and

\[ p^j_A = \sum_k \epsilon_{kA} \rho_k^j \quad (A.6) \]

this can be simplified to

\[ \eta_A = \frac{1}{2m} \sum_k \left\{ \rho_{\theta}^i r_{\theta}^i + \rho_{\alpha}^i r_{\alpha}^i + h.c. \right\} (Q_{\theta} - Q_{\theta})^{-1} \quad (A.7) \]

\[ \equiv \frac{1}{2m} \left( N_A + N_A^+ \right) (Q_{\theta} - Q_{\theta})^{-1} \]

Then, since the \( \eta \)'s commute with the \( Q \)'s, one sees that

\[ J_A J_B [\eta_A, \eta_B] = J_A J_B \left( \frac{\eta_A}{\eta_B} \right) (Q_{\theta} - Q_{\theta}) (Q_{\theta} - Q_{\theta})^{-1} \left[ N_A + N_A^+, N_B + N_B^+ \right] \quad (A.8) \]

\[ = \frac{1}{4} \left( \frac{Q_{\theta} - Q_{\theta}}{Q + Q} \right) \left( \frac{Q_{\theta} - Q_{\theta}}{Q + Q} \right) \left[ N_A + N_A^+, N_B + N_B^+ \right] \]

so that the problem reduces to showing that

\[ \frac{1}{4} \left[ N_A + N_A^+, N_B + N_B^+ \right] = i \left\{ L_{\theta} - \frac{Q_{\theta} - Q_{\theta}}{2Q_{\theta} - Q_{\theta}} (Q_{\theta} - Q_{\theta}) \left( N_C + N_C^+ \right) \right\} \quad (A.9) \]

As a prelude to this demonstration, several pertinent commutators will be derived. Remembering the eigenvalue problem

\[ \sum_{k, \ell} \epsilon_{kA} T_{k\ell} \epsilon_{\ell B} = Q_A S_{AB} \quad (A.10) \]

one has for \( A \neq B \) upon taking \( \frac{\partial}{\partial \epsilon_{\ell B}} \).
\[ \sum_k \frac{\partial \varepsilon_k}{\partial r_k^i} \varepsilon_{kB} + \omega \varepsilon_{kA} \frac{\partial \varepsilon_{kB}}{\partial r_k^i} + \frac{\partial}{\partial r_k^i} \left( \varepsilon_{kA} (r_k^i r_k^i + r_k^i \dot{r}_k^i) \varepsilon_{kB} \right) = 0 \] (A.11)

But noting that
\[ \sum_k \varepsilon_{kA} \frac{\partial \varepsilon_{kA}}{\partial r_k^i} = \frac{1}{2} \frac{\partial}{\partial r_k^i} \left( \sum_k \varepsilon_{kA} \varepsilon_{kA} \right) = 0 \] (A.12)

one finds
\[ \sum_k \varepsilon_{kA} \frac{\partial \varepsilon_{kA}}{\partial r_k^i} = \frac{r_k^i \varepsilon_{kB} + \dot{r}_k^i \varepsilon_{kA}}{Q_A - Q_B} \] (A.13)

Moreover,
\[ \sum_k \varepsilon_{kA} \frac{\partial \varepsilon_{kA}}{\partial r_k^i} = \frac{1}{2} \frac{\partial}{\partial r_k^i} \left( \sum_k \varepsilon_{kA} \varepsilon_{kA} \right) = 0 \] (A.14)

and since \[ \sum_{k'} \varepsilon_{kA} \varepsilon_{k'A} = \delta_{kk'} \], one gets
\[ \frac{\partial \varepsilon_{kA}}{\partial r_k^i} = \sum_{k+A} \left( \frac{r_k^i \varepsilon_{kB} + \dot{r}_k^i \varepsilon_{kA}}{Q_A - Q_B} \right) \varepsilon_{kB} \] (A.15)

With this result one may now prove
\[ [p_k^i, p_k^j] = \sum_{k'} \left[ \varepsilon_{kA} p_k^i, \varepsilon_{kA} p_k^j \right] = \sum_{k'} \left( \varepsilon_{kA} [p_k^i, p_k^j] + \varepsilon_{kA} \varepsilon_{kA} [p_k^i, \varepsilon_{kA}] \rho_k^i \right) \] (A.16)

\[ = \lambda \left\{ \left( 1 - 2 \chi_{AB} \right) r_k^i r_k^j + \rho_k^i r_k^j \right\} \varepsilon_{kA} \varepsilon_{kA} + \varepsilon_{kA} \varepsilon_{kA} \left( \frac{\rho_k^i r_k^j}{Q_A - Q_B} + \frac{\rho_k^i r_k^j}{Q_B - Q_A} \right) \} \]

omitting some of the algebra. Likewise, one has
\[ [\rho_A^i, r_B^j] = \sum_{k} \left[ \left[ p_k^i, r_k^j \right] \varepsilon_{kA} \varepsilon_{kB} + r_k^i \varepsilon_{kA} \varepsilon_{kA} \varepsilon_{kB} \right] \] (A.17)

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\[-i \left\{ (\iota - \delta_{AB}) \frac{\hat{r}^2_r \hat{r}^2_e}{\hat{a}_e - \hat{a}_A} + \delta_{AB} \left( \delta^{i_1}_{\hat{a}_i} + \sum_{\hat{a}_i = \hat{a}_i} \frac{\hat{r}^2_r \hat{r}^2_e}{\hat{a}_e - \hat{a}_c} \right) \right\} \]

Equipped with these commutators, one may proceed with the calculation of (A.9). The first thing to note is that because of the eigenvalue problem condition
\[\sum_{\hat{a}_i} r^A_{\hat{a}_i} r^B_{\hat{a}_i} = 0 \quad \text{for } A \neq B, \text{ one gets} \]
\[\sum_{\hat{a}_i} r^A_{\hat{a}_i} r^B_{\hat{a}_i} = \sum_{\hat{a}_i} (r^A_{\hat{a}_i} r^B_{\hat{a}_i} - i \frac{\hat{r}^2_r \hat{r}^2_e}{\hat{a}_e - \hat{a}_A}) = \sum_{\hat{a}_i} r^A_{\hat{a}_i} r^B_{\hat{a}_i} \quad (A \neq B) \quad (A.18) \]
This means that \( N_A = N_A^+ \) so that the calculation reduces to just \( [N_A, N_B] \). To shorten things, only the non-zero terms in the commutator will be listed. The remaining ones vanish either because the \( r \)'s commute or as a result of the above eigenvalue condition. One finds, then,
\[[N_A, N_B] = \sum_{\hat{a}_i} \left\{ [r^A_{\hat{a}_i}, r^B_{\hat{a}_i}] r^A_{\hat{a}_i} r^B_{\hat{a}_i} + \rho^A_{\hat{a}_i} [r^B_{\hat{a}_i}, r^A_{\hat{a}_i}] r^A_{\hat{a}_i} r^B_{\hat{a}_i} + \rho^A_{\hat{a}_i} [r^B_{\hat{a}_i}, r^A_{\hat{a}_i}] r^A_{\hat{a}_i} r^B_{\hat{a}_i} + \rho^A_{\hat{a}_i} [r^B_{\hat{a}_i}, r^A_{\hat{a}_i}] r^A_{\hat{a}_i} r^B_{\hat{a}_i} \right\} \quad (A.19) \]
Numbering the terms consecutively and calculating the first one explicitly one has
\[1 = i \sum_{\hat{a}_i} (\rho^A_{\hat{a}_i} r^B_{\hat{a}_i} + \rho^B_{\hat{a}_i} r^A_{\hat{a}_i}) r^A_{\hat{a}_i} r^B_{\hat{a}_i} = i \sum_{\hat{a}_i} \rho^A_{\hat{a}_i} r^A_{\hat{a}_i} \frac{\hat{a}_e}{\hat{a}_e - \hat{a}_c} \quad (A.20) \]
Rembering that \( \sum_{\hat{a}_i} r^A_{\hat{a}_i} r^B_{\hat{a}_i} = Q_c \). Also,
\begin{align}
2 &= i \sum_j \rho^i_\theta \alpha^i_A \frac{\alpha_c}{\alpha_c - \alpha_A} \quad \text{(A.21)} \\
3 &= 2 \\
4 &= -i \sum_j \rho^i_\alpha \alpha^i_\theta \frac{\alpha_c}{\alpha_c - \alpha_\theta} \quad \text{(A.23)} \\
5 &= i \sum_i \rho^i_\alpha \alpha^i_\theta \frac{\alpha_c}{\alpha_c - \alpha_A} \quad \text{(A.24)} \\
6 &= 4 \\
7 &= i \sum_j \rho^i_\theta \alpha^i_\theta \frac{\alpha_c}{\alpha_c - \alpha_\theta} + i \sum_i \rho^i_\alpha \alpha^i_\theta \frac{\alpha_c}{\alpha_c - \alpha_A} \quad \text{(A.26)} \\
\end{align}

Now collecting all of these gives

\[
[N_\alpha, N_\theta] = i \sum_j \left\{ \rho^i_\theta \alpha^i_\alpha \frac{\alpha_c + \alpha_\theta}{\alpha_\theta - \alpha_c} + \rho^i_\alpha \alpha^i_\theta \frac{\alpha_c + \alpha_A}{\alpha_A - \alpha_c} + \rho^i_\alpha \alpha^i_\theta \frac{2 \alpha_c}{(\alpha_\theta - \alpha_c)(\alpha_A - \alpha_c)} \right\} \quad \text{(A.27)}
\]

That this is the desired result follows from the definition of \( N_c/2 \) as well as the fact

\[
L_c = \bar{C}_c \sum_i \left( \vec{r}_i \times \vec{p}_i \right) = (\bar{C}_\alpha \times \bar{C}_\theta) \sum_i \left( \vec{r}_i \times \vec{p}_i \right) = \sum_i \left( \vec{r}_i \rho^i_\alpha - \rho^i_\alpha \vec{p}_i \right)
\quad \text{(A.28)}
\]

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