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ROTATOR

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CHAPTER I

INTRODUCTION

Preliminary Remarks

The purpose of this dissertation is to present a new method for approximating the energy eigenvalues for the problem of a torque free rigid asymmetric rotator.

The rigid symmetric rotator differs from the asymmetric rotator in that in the former case there are four constants of the motion due to the symmetry involved. These are the Hamiltonian $\hat{H}$, the square of the angular momentum $\hat{P}^2$, the space-fixed $Z$ component of the angular momentum $\hat{P}_Z$ and the rotating body-fixed $z$ component of angular momentum $\hat{P}_z$. The torque free Hamiltonian may be expressed in terms of $\hat{P}^2$ and $\hat{P}_z$ both of which are diagonal operators whose eigenvalues are well known. Thus the energy eigenvalues are readily determined. In the latter or asymmetric case the rotating body-fixed $z$ component of angular momentum is no longer constant and in addition to this, the matrix of the torque free Hamiltonian becomes more complicated through the presence of additional non-diagonal terms.

These two conditions make the case of the asymmetric rotator more complicated than that of the symmetric rotator. The complications are such that the solutions for the eigenvalues involve solving polynomial equations. These solutions are readily obtained for certain values of the total angular momentum quantum number, but cannot be carried out in general for higher values of
In the latter event one has recourse to numerical solutions if he knows the values of the rotational parameters. If, however, one does not have numerical values of these parameters, it is desirable to have approximate solutions which hold for arbitrary values. Thus the primary motivation for this work has been to develop such approximate solutions.

The method utilized involves expanding the asymmetric rotator eigenfunctions in terms of the symmetric rotator eigenfunctions. At this point a set of eigenvalue projection operators as defined by Löwdin are introduced. Following a discussion of their properties these operators are approximated by using the symmetric rotator limits of the asymmetric rotator. The approximations to the projection operators are then used to generate a sequence of approximate eigenvalues. The limit of this sequence is then the correct eigenvalue. The results are such that the symmetric rotator parameters which appear in the Hamiltonian may be held constant and the energy eigenvalues studied as functions of the asymmetry parameter.

The first few pages will serve to introduce certain preliminary information which will be of later use. This information is contained in a review by Nielsen. Since reference to the original articles, which serve as the source of this information, are given by Nielsen, this information will not always be given here.

**Constants of the Motion and Angular Momentum Operators**

The constants of the motion for a rigid asymmetric rotator are the Hamiltonian $\hat{H}$, the square of the angular momentum $\hat{P}^2$ and
the space-fixed Z component of the angular momentum \( \hat{P}_z \). The space-fixed components of angular momentum will be designated as \( \hat{P}_x \), \( \hat{P}_y \) and \( \hat{P}_z \) while the rotating body-fixed components of angular momentum will be designated as \( \hat{P}_x' \), \( \hat{P}_y' \) and \( \hat{P}_z' \). The square of the angular momentum is then given as \( \hat{P}^2 = \hat{P}_x'^2 + \hat{P}_y'^2 + \hat{P}_z'^2 \). The Hamiltonian for a torque free rigid rotator is the kinetic energy operator and is given by

\[
\mathcal{H} = \frac{\mathcal{K}}{2I_x} \hat{P}_x^2 + \frac{\mathcal{K}}{2I_y} \hat{P}_y^2 + \frac{\mathcal{K}}{2I_z} \hat{P}_z^2
\]

where \( I_x \), \( I_y \) and \( I_z \) designate the rotating body-fixed principal axis moments of inertia.

It is usually more convenient to express \( \hat{P}^2 \) and \( \mathcal{H} \) in terms of the raising and lowering operators which are defined by \( \hat{P}_{X\pm} = \hat{P}_X \pm i \hat{P}_Y \) and \( \hat{P}_{X\mp} = \hat{P}_X \mp i \hat{P}_Y \). These raising and lowering operators are discussed at some length in reference 1 and also in section 9 of reference 4. This leads to

\[
\hat{P}^2 = \frac{1}{2}(\hat{P}_{X+}^2 + \hat{P}_{X-}^2) + \hat{P}_Z^2 = \frac{1}{2}(\hat{P}_{X+}^2 + \hat{P}_{X-}^2) + \hat{P}_Z^2 \quad \quad (1.1)
\]

The Hamiltonian can be expressed as

\[
\mathcal{H} = ac\hat{P}_z^2 + ab\hat{P}_y^2 + ab\hat{P}_z^2 + \frac{ab}{2}(\hat{P}_{X-}^2 + \hat{P}_{X+}^2) \quad \quad (1.2)
\]

where \( ac = \frac{\mathcal{K}}{4}(\frac{1}{x} + \frac{1}{y}) \), \( ab = \frac{\mathcal{K}}{4}(\frac{1}{x} - \frac{1}{y}) \), \( a = \frac{\mathcal{K}}{4}(\frac{2}{z} - \frac{1}{x} - \frac{1}{y}) \)

or \( b = \frac{2}{z} - \frac{1}{x} - \frac{1}{y} \)

\( c = \frac{1}{x} + \frac{1}{y} \)

The constants \( a \) and \( c \) will be referred to as the symmetric rotator parameters while the constant \( b \) will be referred to as the asymmetry parameter. Note that \( \mathcal{K} \) does not appear in the angular momentum
eigenvalues but rather has been absorbed into the rotational parameters. Thus the eigenvalues of $\hat{F}^2$ are given as $J(J+1)$, $\hat{P}_Z$ as $M$ and where it is a good constant of the motion $\hat{P}_Z$ as $K$. These eigenvalues are derived in reference 1 following a procedure similar to that used by Condon and Shortley for the more restrictive eigenvalue problem involving only $\hat{P}^2$ and $\hat{P}_Z$.

At this point it is desirable to discuss the symmetric rotator results. As mentioned earlier there are four constants of the motion $\hat{H}$, $\hat{P}^2$, $\hat{P}_Z$, and $\hat{P}_Z$. The torque free Hamiltonian is given by

$$\hat{H} = \frac{\hbar^2}{2I_x} (\hat{P}^2_x + \hat{P}^2_y) + \frac{\hbar^2}{2I_z} \hat{P}^2_Z = \alpha \hat{P}^2 + \alpha \hat{P}_Z^2$$

where $\alpha = \frac{\hbar^2}{2I_x}$, $\alpha = \frac{\hbar^2}{2I_z}$, $rac{1}{I_z} - \frac{1}{I_x}$

which are the limits of the constants as previously given for the case in which $I_x = I_y \neq I_z$ corresponding to $b = 0$. The eigenvalues of $\hat{P}^2$ are given by $J(J+1)$ where $J$ designates the angular momentum quantum number and those of $\hat{P}_Z^2$ are $K^2$ where $K$ is the rotating body-fixed $z$ component angular momentum quantum number. The space-fixed $Z$ component quantum number is given by $M$. The energy eigenvalues are then given by $E_{ JK}(\alpha, \alpha) = \alpha J(J+1) + \alpha K^2$. They are $2J+1$ fold degenerate in $M$ and twofold degenerate in all non-zero $K$ values or nondegenerate in $K$ for $K = 0$. The eigenfunctions for the symmetric rotator will be designated as $\psi_{JMK}^S$.

At this point one may impose the restriction that $I_x \leq I_y \leq I_z$ which means that $-1 \leq b \leq 0$. One wishes then to study the energy levels as functions of the asymmetry parameter $b$ while $\alpha$ and $\gamma$ remain constant. This can be done by holding one of the body-
fixed moments of inertia constant and allowing the other two to vary. If one defines \( \delta = \frac{\theta}{4} \) and lets \( I_x = \alpha \delta \), \( I_y = \beta \delta \) and \( I_z = \gamma \delta \) then one obtains

\[
a = \frac{\gamma}{\alpha} - \frac{\gamma}{\beta} \quad \text{and} \quad \frac{1}{\alpha} + \frac{1}{\beta} \quad \text{or}
\]

\[
b = \frac{1}{\alpha} - \frac{1}{\beta} \quad \text{and} \quad \frac{1}{\alpha} + \frac{1}{\beta}.
\]

These may be solved for \( \alpha', \beta \) and \( \gamma \) in terms of \( a, b \) and \( c \) to give

\[
\alpha' = \frac{2}{a(c+b)} \quad \beta = \frac{2}{a(c-b)} \quad \gamma = \frac{2}{a(c+1)}.
\]

If both \( a \) and \( c \) are held constant while \( b \) varies from -1 to 0, one sees that \( \gamma \) remains constant and \( \alpha' \) and \( \beta \) vary in such a way that for \( b = 0 \), \( \alpha' = \beta = \frac{2}{ac} \gamma = \frac{2}{a(c+1)} \). This is satisfied since both \( a \) and \( c \) are < 0. This is referred to as the prolate symmetric rotator limit. When \( b = -1 \) one sees that \( \alpha' = \frac{2}{a(c-1)} \beta = \gamma = \frac{2}{a(c+1)} \) which is referred to as the oblate symmetric rotator limit. Note that \( |c| > 1 \) in order that \( \alpha' \), \( \beta \) and \( \gamma \) all remain finite.

Since the Hamiltonian is expressed by

\[
\hat{H} = ac \hat{P}_z^2 + ab \left( \hat{P}_{x-}^2 + \hat{P}_{x+}^2 \right)
\]

the energies can be given by

\[
E_j(\alpha, b, c) = acJ(J+1) + a \mathcal{E}_{j\gamma}(b) \text{ where } \gamma \text{ is a quantum index that varies from } -J \text{ to } J \text{ and } \mathcal{E}_{j\gamma} \text{ are the eigenvalues of a reduced Hamiltonian } \hat{h} = \hat{P}_z^2 + \frac{b}{2} \left( \hat{P}_{x-}^2 + \hat{P}_{x+}^2 \right). \text{ Both } E_j\gamma \text{ and } \mathcal{E}_{j\gamma} \text{ are } 2J+1 \text{ fold degenerate in the } M \text{ quantum number since the operator } \hat{P}_z \text{ does not appear in the Hamiltonian. In most of what follows the reduced Hamiltonian } \hat{h} \text{ will be used rather than the full Hamiltonian } \hat{H}. \text{ This is defined by } \hat{h} = \frac{1}{a} (\hat{H} - ac \hat{P}_z^2) \text{ and as mentioned above has } \mathcal{E}_{j\gamma}(b) \text{ as its eigenvalues.}
The asymmetric rotator energies become symmetric rotator energies in the prolate and oblate limits referred to above. In the former case the Hamiltonian reduces to $\hat{H} = ac \hat{P}^2 + a \hat{P}_z^2$ and the energies are given by $E_{J\gamma}(a, o, c) = acJ(J+1) + aK^2$. The reduced Hamiltonian is just $\hat{h} = \hat{P}_z^2$ with eigenvalues $\epsilon_{J\gamma}(o) = K^2$.

In the latter or oblate case the Hamiltonian becomes

$$\hat{H} = ac \hat{P}^2 + a \hat{P}_z^2 - a(\hat{P}_x^2 - \hat{P}_y^2) = a(c+1) \hat{P}_x^2 - 2a \hat{P}_x^2,$$

with the energies given by

$$E_{J\gamma}(a, -1, c) = a(c+1) J(J+1) - 2ak^2.$$

The reduced Hamiltonian is then just $\hat{h} = \hat{P}_x^2 - 2\hat{P}_x$ with eigenvalues $\epsilon_{J\gamma}(-1) = J(J+1) - 2K^2$. In both limits the energies become $2(2J+1)$ fold degenerate for non-zero K values and remain $2J+1$ fold degenerate for $K = 0$.

It is useful to express the various angular momentum components in terms of the Eulerian angles and their derivatives. The diagram shows the choice used for these angles. This choice is the same as that of reference 4, and is shown as Figure 1. These component operators, their commutation relations and their eigenvalues are discussed at length in reference 1. Note, however, that the choice of Eulerian angles here is different from reference 1 in that $\psi$ and $\varphi$ are interchanged and conforms instead to the choice of reference 4, section 9.
The operators in terms of these angles and their derivatives are given as follows:

\[
\begin{align*}
\hat{P}_X &= -i \left( -\csc \Theta \cos \frac{2}{3} \phi + \sin \frac{2}{3} \phi + \cot \Theta \cos \frac{2}{3} \phi \right) \\
\hat{P}_Y &= -i \left( \csc \Theta \sin \frac{2}{3} \phi + \cos \frac{2}{3} \phi - \cot \Theta \sin \frac{2}{3} \phi \right) \\
\hat{P}_Z &= -i \frac{2}{3} \phi \\
\hat{P}_X &= \hat{P}_X + i \hat{P}_Y = i \epsilon \pm i \frac{2}{3} \phi \left( -\csc \Theta \cos \frac{2}{3} \phi + i \frac{2}{3} \phi + \cot \Theta \cos \frac{2}{3} \phi \right) \\
\hat{P}_X &= -i \left( \cot \Theta \cos \frac{2}{3} \phi - \sin \frac{2}{3} \phi + \csc \Theta \cos \frac{2}{3} \phi \right) \\
\hat{P}_Y &= -i \left( \cot \Theta \sin \frac{2}{3} \phi + \cos \frac{2}{3} \phi + \csc \Theta \sin \frac{2}{3} \phi \right) \\
\hat{P}_Z &= -i \frac{2}{3} \phi \\
\hat{P}_X &= \hat{P}_X + i \hat{P}_Y = -i \epsilon \pm i \frac{2}{3} \phi \left( -\csc \Theta \cos \frac{2}{3} \phi + i \frac{2}{3} \phi + \cot \Theta \cos \frac{2}{3} \phi \right)
\end{align*}
\]

The commutation rules obeyed by the space-fixed angular momentum components are given by \( [\hat{P}_A, \hat{P}_B] = \epsilon_{ABC} \hat{P}_C \) where \( A, B \) and \( C \) run over \( X, Y \) and \( Z \) and
\[ e_{ABC} = \begin{pmatrix} 1 \\ 0 \\ \end{pmatrix} \text{ when the sequence } A, B, C \text{ is an even permutation of } X, Y, Z. \] 

For the body-fixed components the commutation rules are given by 
\[ [\hat{P}_a, \hat{P}_b] = -i \, e_{abc} \, \hat{P}_c \] 
where \( a, b \) and \( c \) run over \( x, y \) and \( z \) and \( e_{abc} \) is defined in a manner similar to \( e_{ABC} \).

A vector in the space-fixed coordinate system is related to a vector in the rotating body-fixed coordinate system \(^4\) by
\[
\begin{pmatrix} X \\ Y \\ Z \\ \end{pmatrix} = \begin{pmatrix} \lambda_{xX} & \lambda_{xY} & \lambda_{xZ} \\ \lambda_{yX} & \lambda_{yY} & \lambda_{yZ} \\ \lambda_{zX} & \lambda_{zY} & \lambda_{zZ} \\ \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}
\]
where
\[
\begin{pmatrix} \lambda_{Aa} \\ \end{pmatrix} = \begin{pmatrix} \cos \gamma \cos \phi & \sin \gamma \sin \phi & -\cos \gamma \sin \phi & \cos \phi \\ \sin \gamma \cos \phi & \cos \gamma \sin \phi & \sin \gamma \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi & \sin \phi & \cos \phi \\ \end{pmatrix}
\]

This may be used to relate \( \hat{P}_A \) and \( \hat{P}_a \) as follows
\[
\hat{P}_A = \sum_a \lambda_{Aa} \hat{P}_a \quad \text{or} \quad \hat{P}_a = \sum_a \lambda_{Aa} \hat{P}_A
\]

Some additional commutation rules which now follow are
\[
[\hat{P}_A, \lambda_{Ba}] = -i \, e_{ABC} \, \lambda_{Ca} \quad [\hat{P}_a, \lambda_{Ab}] = -i \, e_{abc} \, \lambda_{Ac}
\]
which in turn leads to 
\[
[\hat{P}_A, \hat{P}_a] = 0.
\]

The Eigenfunctions and some of their Properties

The eigenfunctions for the asymmetric rotator will be designated by \( \psi^A_j, \gamma, M \) where \( M \) is space-fixed angular momentum quantum number. The symmetric rotator eigenfunctions will be designated as \( \psi^S_j, K, M \) where \( K \) is the body-fixed angular momentum quantum number.
One may expand the asymmetric rotator eigenfunctions in terms of the symmetric rotator eigenfunctions. This leads to
\[
\psi_{J',\tau',M}^a = \sum_{J'=0}^{\infty} \sum_{K'=J'}^{J'} \sum_{M'=-J'}^{J'} a_{J',\tau',M'} \psi_{J',\tau',M'}^S
\]

where the \( a_{J',\tau',M', J',K',M'} \) are the expansion coefficients.

The summation may be reduced to a single sum over \( K' \) by making use of the properties of the diagonal operators \( \hat{P}_Z^2 \) and \( \hat{P}_Z \).

If one operates on both sides of the expansion with \( \hat{P}_Z \) one sees that

\[
\hat{P}_Z \psi_{J',\tau',M}^a = M \psi_{J',\tau',M}^a = \sum_{J',K',M'} M a_{J',\tau',M', J',K',M'} \psi_{J',\tau',M'}^S
\]

If one now multiplies both sides of this equation by \( \psi_{J'',K'',M''}^S \) and integrates over configuration space the result is

\[
\int \psi_{J'',K'',M''}^S \hat{P}_Z \psi_{J',\tau',M}^a \, d-\mathcal{L} = M \int \psi_{J'',K'',M''}^S \psi_{J',\tau',M}^a \, d-\mathcal{L} = M \sum_{M'} a_{J',\tau',M', J',K',M'} \int \psi_{J'',K'',M''}^S \, d-\mathcal{L}
\]

Therefore \((M - M'') a_{J',\tau',M', J'',K'',M''} = 0\)

and \( a_{J',\tau',M', J',K',M'} \neq 0 \) if \( M' = M \)

or \( a_{J',\tau',M', J',K',M'} = 0 \) if \( M' \neq M \).

The summation then reduces to

\[
\psi_{J',\tau',M}^a = \sum_{J',K'} a_{J',\tau',M', J',K',M} \psi_{J',\tau',M'}^S
\]

The sum over \( J' \) can be seen to drop out by operating on both sides of the last equation with \( \hat{P}_Z^2 \). This gives
Multiplying by $\psi_{J',K',M}^{S*}$ and integrating over configuration space gives

$$\int \psi_{J',K',M}^{S*} \hat{p}^2 \psi_{J,\tau,M} \, d\Lambda = J(J+1) \int \psi_{J',K',M}^{S*} \psi_{J,\tau,M} \, d\Lambda = J(J+1) \ a_{J,\tau,M;J',K',M}$$

Thus \( (J(J+1) = J'(J'+1) \) \( \ a_{J,\tau,M;J',K',M} = 0 \)

and \( \ a_{J,\tau,M;J',K',M} \neq 0 \) if \( J' = J \)

or \( \ a_{J,\tau,M;J',K',M} = 0 \) if \( J' \neq J \)

From this one sees that the expansion in $\psi_{J',K',M}^S$ becomes

$$\psi_{J,\tau,M}^a = \sum_{K=-J}^J \ a_{J,\tau,M;J,K,M} \psi_{J,K,M}^S \quad (1.4)$$

As mentioned earlier the eigenvalues are \( 2J+1 \) fold degenerate in the \( M \) quantum number. Once the eigenfunction for that \( M \) value is known the \( 2J \) functions which are degenerate with it can be found by means of the \( M \) raising and lowering operators $\hat{P}_{X^m}^\pm$.

It is convenient from the standpoint of symmetry considerations to define a set of symmetrized symmetric rotator eigenfunctions as follows $\varphi_{J,0,0}^S = \psi_{J,0}^S$.
\[ \phi^{S}_{J,K,Y} = \frac{1}{\sqrt{2}} \left( (-1)^Y \psi^{S}_{J,K} + \psi^{S}_{J,-K} \right) \]

Note that there is a phase difference between the manner of defining these here and in reference 4, section 24.

These 2J+1 functions may be used in place of the \( \psi^{S}_{J,K} \) for an arbitrary M value. Inverting these one gets \( \psi^{S}_{J,0} = \phi^{S}_{J,0,0} \).

\[ \psi^{S}_{J,K} = \frac{1}{\sqrt{2}} \left( \phi^{S}_{J,K,0} + \phi^{S}_{J,K,1} \right) \quad K = 1, 2, \ldots, J. \]

If these are substituted into the expansion for the eigenfunctions one obtains

\[ \psi^{a}_{J,\tau} = \sum_{Y=0}^{J} \sum_{K=0}^{J} b^{a}_{J,\tau,K,Y} \phi^{S}_{J,K,Y} \quad \text{(where } b^{a}_{J,\tau,0,1} = 0) \]

and \( b^{a}_{J,\tau,0,0} = a^{a}_{J,\tau ; J,0} \), \( Y = 0, 1 \) \( K = 1, 2, \ldots, J. \)

\[ b^{a}_{J,\tau,K,Y} = \frac{1}{\sqrt{2}} \left( (-1)^Y a^{a}_{J,\tau ; J,K} + a^{a}_{J,\tau ; J,-K} \right) \quad (1.5) \]

Symmetry conditions can now be used to show that not all 2J+1 of the \( b^{a}_{J,\tau,K,Y} \) associated with a given J and \( \tau \) are nonvanishing.

To bring about this further reduction of the expansion it is convenient to introduce the group of the constants of the motion. It has been mentioned that the energies \( E_{J,\tau} \) are 2J+1 fold degenerate in the M quantum number. This is due to the invariance of the three constants of the motion with respect to the three dimensional rotation group and will always be true for a system which does not interact with its surroundings. However, this is not the full symmetry group of the problem. The constants of the motion are also invariant to the Klein Four Group\(^6,7\) which is defined as follows:
1 = Identity
$C_x$ = Rotation by 90° about the body-fixed $x$ axis
$C_y$ = Rotation by 90° about the body-fixed $y$ axis
$C_z$ = Rotation by 90° about the body-fixed $z$ axis

The group multiplication table is readily seen to be:

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>$C_x$</th>
<th>$C_y$</th>
<th>$C_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>I</td>
<td>$C_x$</td>
<td>$C_y$</td>
<td>$C_z$</td>
</tr>
<tr>
<td>$C_x$</td>
<td>$C_x$</td>
<td>I</td>
<td>$C_z$</td>
<td>$C_y$</td>
</tr>
<tr>
<td>$C_y$</td>
<td>$C_y$</td>
<td>$C_z$</td>
<td>I</td>
<td>$C_x$</td>
</tr>
<tr>
<td>$C_z$</td>
<td>$C_z$</td>
<td>$C_y$</td>
<td>$C_x$</td>
<td>I</td>
</tr>
</tbody>
</table>

**TABLE 1**

**THE FOUR GROUP MULTIPLICATION TABLE**

Thus the group is Abelian so that each element constitutes a class by itself. There are then four irreducible representations given by Table 2:

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>$C_x$</th>
<th>$C_y$</th>
<th>$C_z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>I</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$B_x$</td>
<td>1</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_y$</td>
<td>1</td>
<td>-1</td>
<td>1</td>
<td>-1</td>
</tr>
<tr>
<td>$B_z$</td>
<td>1</td>
<td>-1</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>

**TABLE 2**

**THE IRREDUCIBLE REPRESENTATIONS OF THE FOUR GROUP**
Since the constants of the motion are invariant with respect to this group as well as the three dimensional rotation group, the eigenfunctions must transform according to these irreducible representations when acted upon by the four group elements. The consequences of this are seen by considering the effect of these group operations successively on the Eulerian angles $\varphi$, $\theta$ and $\psi$, the symmetric rotator eigenfunctions $\psi_{S}^{J,K}$ and the symmetrized symmetric rotator eigenfunctions $\phi_{S}^{J,K,Y}$. 

Referring to Figure 1 which shows the choice used for the Eulerian angles one sees that

$$
\begin{align*}
I \begin{pmatrix} 
\varphi \\
\theta \\
\psi 
\end{pmatrix} &= \begin{pmatrix} 
\varphi \\
\theta \\
\psi 
\end{pmatrix} , \\
C_{2}^{\pi} \begin{pmatrix} 
\varphi \\
\theta \\
\psi 
\end{pmatrix} &= \begin{pmatrix} 
\mp \varphi \\
\pm \theta \\
\mp \psi 
\end{pmatrix} \\
C_{2}^{\pi} \begin{pmatrix} 
\varphi \\
\theta \\
\psi 
\end{pmatrix} &= \begin{pmatrix} 
\mp \varphi \\
\pm \theta \\
\mp \psi 
\end{pmatrix} \\
C_{2}^{\pi} \begin{pmatrix} 
\varphi \\
\theta \\
\psi 
\end{pmatrix} &= \begin{pmatrix} 
\mp \varphi \\
\pm \theta \\
\mp \psi 
\end{pmatrix}
\end{align*}
$$

In order to see how the symmetric rotator eigenfunctions $\psi_{S}^{J,K,M}$ and the symmetrized symmetric rotator eigenfunctions $\phi_{S}^{J,K,M,Y}$ transform under these operations, it is probably simplest to use the fact that the $\psi_{S}^{J,K,M}$ are simply related to the elements of the irreducible representations $\Gamma_{J}$ of the three dimensional rotation group. As Wigner has shown

$$
\psi_{S}^{J,K,M} = \left( \frac{2J+1}{\delta J^2} \right)^{1/2} \psi_{-M}^{J,K}
$$

The matrix elements of the irreducible representations can be expressed as
\[
D^J_{M,K}(\psi, \Theta, \varphi) = \left[ \frac{(J+M)! (J-M)!}{(J+K)! (J-K)!} \right]^{1/2} e^{iM\psi} (\cos \frac{\Theta}{2})^{M+K} (\sin \frac{\Theta}{2})^{M-K} e^{iK\varphi} P_{J-M}(\cos \Theta)
\]

where \( P_{J-M}(\cos \Theta) \) is a Legendre polynomial.

\[
\begin{align*}
&= \frac{(-1)^J}{2^{J-M}(J-M)!} (1-\cos \Theta)^{-M+K} (1+\cos \Theta)^{-M-K} \frac{d^J_{J-M}}{d(\cos \Theta)}^J_{J-M} \\
&\times \left[ (1-\cos \Theta)^{-J-K}(1+\cos \Theta)^{J+K} \right].
\end{align*}
\]

The identity operator when acting on \( D^J_{M,K} \) gives \( D^J_{M,K} \) back again and hence has no effect on \( \psi^S_{J,K,M} \) or \( \varphi^S_{J,K,M,\gamma} \). If one next considers the effect of \( C_2^X \) on \( D^J_{M,K} \) one sees that

\[
C_2^X D^J_{M,K}(\psi, \Theta, \varphi) = D^J_{M,K}(\psi+\Theta, \psi-\Theta, 2 \psi - \varphi)
\]

\[
= \left[ \frac{(J+M)! (J-M)!}{(J+K)! (J-K)!} \right]^{1/2} e^{iM(\psi+\Theta)} \cos(\frac{\varphi-\Theta}{2})^{M+K} \sin(\frac{\varphi-\Theta}{2})^{M-K}
\]

Now \( \cos \left( \frac{\varphi-\Theta}{2} \right) = \sin \frac{\Theta}{2}, \sin \left( \frac{\varphi-\Theta}{2} \right) = \cos \frac{\Theta}{2}, \cos \left( \varphi - \Theta \right) = -\cos \Theta \).

Therefore

\[
C_2^X D^J_{M,K} = (-1)^J D^J_{M,-K}
\]

or

\[
C_2^X \psi^S_{J,K,M} = (-1)^J \psi^S_{J,-K,M}
\]

From this one sees that

\[
C_2^X \varphi^S_{J,K,M,\gamma} = C_2^X \frac{1}{\sqrt{2}} \left( (-1)^{\gamma} \psi^S_{J,K,M} + \psi^S_{J,-K,M} \right)
\]

\[
= (-1)^{J+\gamma} \frac{1}{\sqrt{2}} \left( \psi^S_{J,-K,M} + (-1)^{\gamma} \varphi^S_{J,K,M,\gamma} \right) = (-1)^{J+\gamma} \varphi^S_{J,K,M,\gamma}
\]

The effect of \( C_2^Y \) and \( C_2^Z \) on \( D^J_{M,K} \) can be determined in a similar manner giving finally the following results:
Since the $M$ is no longer needed, it will be dropped form hereon.

One can now proceed to simplify the eigenfunctions somewhat. To do this one lets the four elements of the Four Group act on the $\psi^a_{J,J_\gamma}$ which leads to

$$I \psi^a_{J,J_\gamma} = \sum_{K=0}^{J} b_{J,J_\gamma,K,0} \phi^S_{J,K,0} + \sum_{K=1}^{J} b_{J,J_\gamma,K,1} \phi^S_{J,K,1}$$

$$c_2^x \psi^a_{J,J_\gamma} = (-1)^{J+1} \sum_{K=0}^{J} b_{J,J_\gamma,K,0} \phi^S_{J,K,0}$$

$$+ (-1)^{J+1} \sum_{K=1}^{J} b_{J,J_\gamma,K,1} \phi^S_{J,K,1}$$

$$c_2^y \psi^a_{J,J_\gamma} = (-1)^{J+K} \sum_{K=0}^{J} b_{J,J_\gamma,K,0} \phi^S_{J,K,0}$$

$$+ (-1)^{J+K+1} \sum_{K=1}^{J} b_{J,J_\gamma,K,1} \phi^S_{J,K,1}$$

$$c_2^z \psi^a_{J,J_\gamma} = (-1)^{K} \sum_{K=0}^{J} b_{J,J_\gamma,K,0} \phi^S_{J,K,0}$$

$$+ (-1)^{K} \sum_{K=1}^{J} b_{J,J_\gamma,K,1} \phi^S_{J,K,1}$$

Now each of the $2J+1$ eigenfunctions $\psi^a_{J,J_\gamma}$ associated with a given value of $J$ and $\gamma$ must transform as some one of the irreducible representations of the Four Group. This requires that
only some of the $2J+1 \, b_{J, \tau, K, \nu}$ that appear in the expansion can be unequal to zero. In order to see which coefficients drop out of the expansion one considers separately even and odd $J$ values.

For even $J$ values one sees that

$$1 \psi_{J, \tau}^a = \sum_{K=0}^{J} b_{J, \tau, K, 0} \varphi_{J, K, 0}^s + \sum_{K=1}^{J} b_{J, \tau, K, 1} \varphi_{J, K, 1}^s$$

$$c_{2}^x \psi_{J, \tau}^a = \sum_{K=0}^{J} b_{J, \tau, K, 0} \varphi_{J, K, 0}^s - \sum_{K=1}^{J} b_{J, \tau, K, 1} \varphi_{J, K, 1}^s$$

$$c_{2}^y \psi_{J, \tau}^a = \sum_{K=0}^{J} (-1)^K b_{J, \tau, K, 0} \varphi_{J, K, 0}^s - \sum_{K=1}^{J} (-1)^K b_{J, \tau, K, 1} \varphi_{J, K, 1}^s$$

$$c_{2}^z \psi_{J, \tau}^a = \sum_{K=0}^{J} (-1)^K b_{J, \tau, K, 0} \varphi_{J, K, 0}^s + \sum_{K=1}^{J} (-1)^K b_{J, \tau, K, 1} \varphi_{J, K, 1}^s$$

Note that if $b_{J, \tau, K, 1} = 0$ for even $\tau$ and all $K$ and also if $b_{J, \tau, K, 0} = 0$ for even $\tau$ and odd $K$ then

$$\psi_{J, \tau}^a = \sum_{K=0}^{J} b_{J, \tau, K, 0} \varphi_{J, K, 0}^s \quad (\tau = J, J-4, \ldots -J)$$

This now contains $\frac{J}{2} + 1$ terms and transforms as the representation $A$. If now $b_{J, \tau, K, 1} = 0$ for odd $\tau$ and all $K$ and if $b_{J, \tau, K, 0} = 0$ for odd $\tau$ and even $K$ then

$$\psi_{J, \tau}^a = \sum_{K=1}^{J-1} b_{J, \tau, K, 0} \varphi_{J, K, 0}^s \quad (\tau = J-1, J-5, \ldots -J+3)$$

This now contains $\frac{J}{2}$ terms and transforms as $B$. If $b_{J, \tau, K, 0} = 0$ for even $\tau$ and all $K$ and if $b_{J, \tau, K, 1} = 0$ for even $\tau$ and odd $K$ one has
\[ \psi_{J, \gamma}^a = \sum_{K=2}^{J} b_{J, \gamma, K, 1} \varphi_{J, K, 1}^S \left( \gamma = J-2, J-6, \ldots, -J+2 \right) \]

There are again \( \frac{J}{2} \) terms and the functions transform as \( B_z \). Finally, if \( b_{J, \gamma, K, 0} = 0 \) for odd \( \gamma \) and all \( K \) and if \( b_{J, \gamma, K, 1} = 0 \) for odd \( \gamma \) and even \( K \) one obtains

\[ \psi_{J, \gamma}^a = \sum_{J=1}^{J-1} b_{J, \gamma, K, 1} \varphi_{J, K, 1}^S \left( \gamma = J-3, J-7, \ldots, -J+1 \right) \]

There are \( \frac{J}{2} \) terms and the functions transform as \( B_y \).

Similar arguments are used to eliminate certain of the expansion coefficients for odd \( J \). The results are summarized in Tables 3 and 4.

This completes the reduction of the eigenfunctions as far as it can be carried on the basis of symmetry considerations.

From this point on the expansion for \( \psi_{J, \gamma}^a \) will be written as

\[ \psi_{J, \gamma}^a = \sum_{K=0}^{J} b_{J, \gamma, K, \gamma} \varphi_{J, K, \gamma}^S \]

and it will be understood that this reduction has been carried out in accordance with the results given above. This also completes the assignment of \( K \) values to be associated with the various \( \gamma \) values. Note that this assignment is done on the basis of symmetry considerations and not on the basis of energy considerations. There is, therefore, no reason to suppose that the highest \( \gamma \) values go with the highest energy values as is often the case in making these assignments.
<table>
<thead>
<tr>
<th>Even ( J )</th>
<th>Eigenfunctions</th>
<th>Number of Terms</th>
<th>Representation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \psi_{J,\gamma}^a = \sum_{K=0}^{J} b_{J,\gamma,K,0} \phi_{J,K,0}^s ) ( \gamma = J, J-4, \ldots, -J ) ( \frac{J}{2} + 1 ) ( A )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \psi_{J,\gamma}^a = \sum_{K=1}^{J-1} b_{J,\gamma,K,0} \phi_{J,K,0}^s ) ( \gamma = J-1, J-5, \ldots, -J+3 ) ( \frac{J}{2} ) ( B_x )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \psi_{J,\gamma}^a = \sum_{K=1}^{J-1} b_{J,\gamma,K,1} \phi_{J,K,1}^s ) ( \gamma = J-3, J-7, \ldots, -J+1 ) ( \frac{J}{2} ) ( B_y )</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \psi_{J,\gamma}^a = \sum_{K=2}^{J} b_{J,\gamma,K,1} \phi_{J,K,1}^s ) ( \gamma = J-2, J-6, \ldots, -J+2 ) ( \frac{J}{2} ) ( B_z )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**TABLE 3**

**THE ASYMMETRIC ROTATOR EIGENFUNCTIONS**

*(for Even \( J \))"
<table>
<thead>
<tr>
<th>Odd ( J )</th>
<th>Eigenfunctions</th>
<th>Number of Terms</th>
<th>Representation</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \psi_{J, \gamma}^a = \sum_{K=0}^{J-1} b_{J, \gamma, K, 0} \varphi_{J, K, 0}^s (\gamma = J-1, J-5 \ldots -J+1) )</td>
<td>( \frac{J+1}{2} )</td>
<td>( B_z )</td>
<td></td>
</tr>
<tr>
<td>( \psi_{J, \gamma}^a = \sum_{K=1}^{J} b_{J, \gamma, K, 1} \varphi_{J, K, 1}^s (\gamma = J, J-4 \ldots -J+2) )</td>
<td>( \frac{J+1}{2} )</td>
<td>( B_y )</td>
<td></td>
</tr>
<tr>
<td>( \psi_{J, \gamma}^a = \sum_{K=1}^{J} b_{J, \gamma, K, 1} \varphi_{J, K, 1}^s (\gamma = J-2, J-6 \ldots -J) )</td>
<td>( \frac{J+1}{2} )</td>
<td>( B_x )</td>
<td></td>
</tr>
<tr>
<td>( \psi_{J, \gamma}^a = \sum_{K=0}^{J-1} b_{J, \gamma, K, 0} \varphi_{J, K, 0}^s (\gamma = J-3, J-7 \ldots -J+3) )</td>
<td>( \frac{J-1}{2} )</td>
<td>( A )</td>
<td></td>
</tr>
</tbody>
</table>

**TABLE 4**

**THE ASYMMETRIC ROTATOR EIGENFUNCTIONS**
CHAPTER II

THE EIGENVALUE PROJECTION OPERATORS

The Operators and some of their Properties

At this point the form for the energies has been given as
\[ E_{J',\tau} (a,b,c) = acJ(J+1) + a \epsilon_{J',\tau} (b) \]
where the \( \epsilon_{J',\tau} (b) \) are the eigenvalues of the reduced Hamiltonian \( \hat{h} = \frac{1}{a} (\hat{H} - ac^2) \). The eigenfunctions have also been put into the simplest form allowed by symmetry considerations. There are further simplifications which are possible for the \( \epsilon_{J',\tau} (b) \). While it is possible to achieve this in a variety of ways, it will be done here by means of the eigenvalue projection operators introduced by Löwdin.*

Before introducing these operators it is desirable to invert the expanded form for the eigenfunctions. This has been given as
\[ \psi^{a}_{J',\tau} = \sum_{K=0}^{J} b_{J',\tau',K,Y} \phi^{s}_{J,K,Y} \]
where for a particular \( J \) and \( \tau \) it is known which of the \( b_{J',\tau',K,Y} \) are unequal to zero. This represents a unitary transformation from one set of eigenfunctions, the \( \phi^{s}_{J,K,Y} \), to another, the \( \psi^{a}_{J',\tau} \). Since the coefficients are real the transformation is actually orthogonal and can be inverted by noting that the inverse is simply its transpose. Thus one sees that
\[ \phi^{s}_{J,K,Y} = \sum_{J'=-J}^{+J} b_{J',\tau',K,Y} \psi^{a}_{J',\tau} \]  

(2.1)
where the \( T \) values included in the sum are those which transform together according to the particular irreducible representation of the Four Group which is involved. These values are indicated in Table 3.

It is necessary now to record the effect of the full Hamiltonian \( \hat{H} \) and the reduced Hamiltonian \( \hat{h} \) on the functions

\[
\varphi_{J,K}^S \quad \text{Since } \hat{H} = ac \hat{P}^2 + ah \text{ and } \hat{P}^2 \text{ is diagonal, one sees that}
\]

\[
\hat{H} \varphi_{J,K}^S = ac \hat{P}^2 \varphi_{J,K}^S + ah \varphi_{J,K}^S
\]

\[
= acJ(J+1) \varphi_{J,K}^S + ah \varphi_{J,K}^S
\]

Now we have seen that \( \hat{h} = \hat{P}_Z^2 + \frac{b}{2} (\hat{P}_x^2 + \hat{P}_y^2) \). \( \hat{P}_Z \) is a diagonal operator with respect to the \( \varphi_{J,K}^S \) which form the \( \varphi_{J,K}^S \) so that

\[
\hat{P}_Z \varphi_{J,K}^S = K \varphi_{J,K}^S, \quad \hat{P}_Z^2 \varphi_{J,K}^S = K^2 \varphi_{J,K}^S
\]

Also

\[
\hat{P}_{x+y} \varphi_{J,K}^S = \left[(J_x^2 - K_y^2)(J_y^2 - K_x^2)\right]^{\frac{1}{2}} \varphi_{J,K}^S
\]

\[
\hat{P}_Z^2 \varphi_{J,K}^S = \left[(J_x^2 - K_y^2)(J_y^2 - K_x^2)\right]^{\frac{1}{2}} \varphi_{J,K}^S
\]

One sees that now

\[
\hat{h} \varphi_{J,K}^S = K^2 \varphi_{J,K}^S + \frac{b}{2} \left\{ \left[\left(J^2 - (K+1)^2\right)(J+1)^2 - (K+1)^2\right]^{\frac{1}{2}} \varphi_{J,K}^S \right. \\
+ \left. \left[\left(J^2 - (K+1)^2\right)(J+1)^2 - (K-1)^2\right]^{\frac{1}{2}} \varphi_{J,K-2}^S \right\}
\]

and that

\[
\hat{h} \varphi_{J,-K}^S = K^2 \varphi_{J,-K}^S + \frac{b}{2} \left\{ \left[\left(J^2 - (-K+1)^2\right)(J+1)^2 - (-K+1)^2\right]^{\frac{1}{2}} \varphi_{J,-K}^S \right. \\
+ \left. \left[\left(J^2 - (-K+1)^2\right)(J+1)^2 - (-K-1)^2\right]^{\frac{1}{2}} \varphi_{J,-K-2}^S \right\}
\]
Therefore \( \hat{h} \Phi_{J,0,0}^s \):

\[
\hat{h} \Phi_{J,0,0}^s = b \left[ \frac{(J^2 - 1)(J^2 + 1)}{2} \right]^{1/2} \Phi_{J,2,0}^s
\]  \hspace{1cm} (2.1)

\[
\hat{h} \Phi_{J,1,\nu}^s = \left( 1 + \frac{(-1)^\nu b}{2} J(J + 1) \right) \Phi_{J,1,\nu}^s
\]  \hspace{1cm} (2.2a)

\[
\hat{h} \Phi_{J,2,\nu}^s = \left( 1 + (-1)^\nu \right) \frac{b}{2} \left[ (J^2 - 2^2) (J^2 + 1) \right]^{1/2} \Phi_{J,0,\nu}^s
\]  \hspace{1cm} (2.2b)

\[
\hat{h} \Phi_{J,3,\nu}^s = \frac{b}{2} \left[ (J^2 - 2^2) (J^2 - 2^2) \right]^{1/2} \Phi_{J,2,\nu}^s
\]  \hspace{1cm} (2.2c)

\[
\hat{h} \Phi_{J,4,\nu}^s = \frac{b}{2} \left[ (J^2 - 2^2) (J^2 - 2^2) \right]^{1/2} \Phi_{J,4,\nu}^s
\]  \hspace{1cm} (2.2d)

for \( K \geq 3 \). This may be summarized by

\[
\hat{h} \Phi_{J,K,\nu}^s = h_{K,K-2} \Phi_{J,K-2,\nu}^s + h_{K,K} \Phi_{J,K,\nu}^s + h_{K,K+2} \Phi_{J,K+2,\nu}^s
\]  \hspace{1cm} (2.2)

where \( h_{K,K} \) are the matrix elements of \( \hat{h} \) with respect to the \( \Phi_{J,K,\nu}^s \).

At this point the projection operators may be introduced. They are defined as

\[
\mathcal{O}_{J,\nu}^s (\hat{H}) = \tau_{\nu} \tau'_{\nu} \frac{\hat{H} - E_{J,\nu}}{(E_{J,\nu} - E_{J,\nu}')}
\]  \hspace{1cm} (2.3)

where the product contains all those \( \tau' \) values except \( \tau \) itself which transform according to the same irreducible representation. (Actually it can contain all \( \tau' \) associated with a given \( J \) except for \( \tau \) itself, since those transforming according to other representations
will not contribute in any way.) Since $\hat{H} = ac\hat{p}^2 + a\hat{n}$, if these operators act upon any member of a set of eigenfunctions for which $\hat{p}^2$ is a diagonal operator, one sees that

$$0_{J,\tau}^{\hbar} (\hat{H}) \psi_J = 0_{J,\tau}^{\hbar} \left( \frac{\hat{H} - E_J \tau'}{E_J \tau - E_J \tau'} \right) \psi_J$$

$$= 0_{J,\tau}^{\hbar} \left( \frac{\hbar - \epsilon_{J,\tau'}}{\epsilon_{J,\tau} - \epsilon_{J,\tau'}} \right) \psi_J = 0_{J,\tau}^{\hbar} (\hbar) \psi_J .$$

Since all functions used here will satisfy this property, it is evident that for the purpose of this work one may say that

$$0_{J,\tau}^{\hbar} (\hat{H}) = 0_{J,\tau}^{\hbar} (\hbar) . \quad (2.4)$$

One can now determine the effect of this operator on the inverted expansion of the eigenfunctions

$$\Phi_{J,K,Y} = \sum_{-J}^{+J} b_{J,\tau''}^{K,\tau',} \psi_{J,\tau''}^{a} .$$

It is clear that when the projection operator acts on a member of this sum, such that $\tau'' \neq \tau'$, there will be a $\tau'$ in the product which will equal $\tau''$ and will give no contribution. On the other hand, when it acts on a member of this sum such that $\tau'' = \tau'$, there will be no such cancellation, since in the product $\tau \neq \tau'$. Thus in the latter case each factor $\frac{\hbar - \epsilon_{J,\tau'}}{\epsilon_{J,\tau} - \epsilon_{J,\tau'}}$ will give unity. (The energy difference in the denominator is simply to normalize the contribution to 1.)

Since all the other terms give no contribution one sees that

$$0_{J,\tau}^{\hbar} (\hat{H}) \Phi_{J,K,Y} = \sum_{-J}^{+J} b_{J,\tau''}^{K,\tau',} \psi_{J,\tau''}^{a} .$$

$$= b_{J,\tau,K,Y} \psi_{J,\tau}^{a} . \quad (2.5)$$
The effect then of these operators is to project out of the sum the term associated with a given \( J \) and \( \gamma \). That these are in fact projection operators is readily seen by computing \( O^2_J, \gamma (h) \) and \( O_J, \gamma (h) \).

One easily sees that

\[
O^2_J, \gamma (h) \psi_{J,K,\gamma}^S = b_J, \gamma, K, \gamma O_J, \gamma (h) \psi_{J,\gamma}^a = b_J, \gamma, K, \gamma \psi_{J,\gamma}^a
\]

and that

\[
O_J, \gamma' (h) O_J, \gamma (h) \psi_{J,K,\gamma}^S = b_J, \gamma, K, \gamma O_J, \gamma' (h) \psi_{J,\gamma}^a = 0
\]

so that

\[
O_J, \gamma' (h) O_J, \gamma (h) = \delta_{\gamma, \gamma'} O_J, \gamma (h)
\]

which are the defining relations for projection operators.

From this one sees that if the eigenvalues \( \epsilon_J, \gamma (b) \) are known that one can easily determine the coefficients

\( b_J, \gamma, K, \gamma \)

from the use of these projection operators. At this point one can show that even without prior knowledge of the eigenvalues one can get some information that is useful.

**Use of the Projection Operators to Determine the Eigenvector Equations**

One use of these projection operators is in setting up the eigenvector equations for the coefficients \( b_J, \gamma, K, \gamma \).

As has been seen the number of terms in the expansion for \( \psi_{J,\gamma}^a \) is dependent upon whether \( J \) is even or odd and also the symmetry properties. To obtain these eigenvector equations allow \( O_J, \gamma (h) \) to act upon \( \varphi_{J,K,\gamma}^S \) to obtain

\[
O_J, \gamma (h) \varphi_{J,K,\gamma}^S = b_J, \gamma, K, \gamma \varphi_{J,\gamma}^a = b_J, \gamma, K, \gamma \sum_{K'=0}^{J} b_J, \gamma, K', \gamma \varphi_{J,K',\gamma}^S.
\]
Now allow the reduced Hamiltonian to act on this expansion
\[ \hat{h}_{J',r} \psi_{J',K',\gamma} = b_J,\gamma,K,\gamma \hat{\psi}_{J',\gamma} = b_J,\gamma,K,\gamma \psi_{J',K',\gamma} \]
\[ = \varepsilon_{J',\gamma} b_J,\gamma,K,\gamma \sum_{K'=0}^J b_J,\gamma,K',\gamma \varphi_{J',K',\gamma} \]
\[ = b_J,\gamma,K,\gamma \sum_{K'=0}^J b_J,\gamma,K',\gamma \varphi_{J',K',\gamma} \hat{\psi}_{J',K',\gamma} \]
\[ = b_J,\gamma,K,\gamma \sum_{K'=0}^J b_J,\gamma,K',\gamma \left\{ h_{K',K'-2} \varphi_{J'+K'-2,\gamma} \right\} \]
\[ + h_{K',K'} \varphi_{J',K',\gamma} + h_{K',K'+2} \varphi_{J',K'+2,\gamma} \}
\[ = b_J,\gamma,K,\gamma \sum_{K'=0}^J \left\{ b_J,\gamma,K'-2,\gamma \ h_{K'-2,K'} + b_J,\gamma,K',\gamma \ h_{K',K'} \right\} \varphi_{J',K',\gamma} \]
\[ + b_J,\gamma,K'+2,\gamma h_{K'+2,K'} \}
\[ \varphi_{J',K',\gamma} \]
This leads immediately to
\[ b_J,\gamma,K'-2,\gamma h_{K'-2,K'} + b_J,\gamma,K',\gamma (h_{K',K'} - \varepsilon_{J',\gamma}) \]
\[ + b_J,\gamma,K'+2,\gamma h_{K'+2,K'} = 0 \]
(2.6)
which are the eigenvector equations. From this set of equations one can extract the secular determinant which is simply the determinant of the matrix whose elements are the coefficients of
\[ b_J,\gamma,K,\gamma \]. This could then, of course, be expanded by minors to obtain the secular equation. The form of the equation is then that which is given by Herzberg, Nielsen, Randall, Dennison, Ginsburg and Weber and Ginsburg.

Use of the Projection Operators to determine the Invariants of the Secular Equation

The purpose of the present section is to evaluate the invariants of the secular equation with the projection operators
and to show how the eigenvalues $\varepsilon_{J,\gamma}$ (b) can be at least partially determined without solving the secular equation. These invariants are given from $J=0$ to $J=6$ in reference 8, to $J=10$ in reference 9, to $J=11$ in reference 10 with some errors of 9 corrected and extended to $J=15$ in reference 11. This is shown in detail only for the values that transform as A for even $J$. All other cases follow in like manner.

The eigenfunctions are

$$\psi_{J,\gamma}^a = \sum_{K=0}^{J} b_{J,\gamma,K,0} \Psi_{J,K,0} \quad (\gamma = J, J-4, \cdots, J)$$

and the inverted form is

$$\Psi_{J,K,0} = \sum_{\gamma=-J}^{J} b_{J,\gamma,K,0} \psi_{J,\gamma}^a$$

Now consider $K=0$ and allow $O_{J,\gamma}(h)$ to act on $\Psi_{J,0,0}^s$.

$$O_{J,\gamma}(h) \Psi_{J,0,0}^s = b_{J,\gamma,0,0} \psi_{J,\gamma}^a = \sum_{K=0}^{J} b_{J,\gamma,0,0} b_{J,\gamma,K,0} \Psi_{J,K,0}^s$$

Earlier the effect of the projection operator on the right side of the expansion was determined. Its effect on the left side is now found. In order to do this one notes that

$$\hat{h} = -\varepsilon_{J,\gamma} \quad \Psi_{J,0,0}^s = (h_{0,0} - \varepsilon_{J,\gamma}) \Psi_{J,0,0}^s + h_{02} \Psi_{J,2,0}^s$$

$$= c_{J,\gamma,0,0,0} \Psi_{J,0,0}^s + c_{J,\gamma,0,2,0} \Psi_{J,2,0}^s$$

$$\hat{h} = -\varepsilon_{J,\gamma} \quad \Psi_{J,2,0}^s = h_{20} \Psi_{J,0,0}^s + (h_{22} - \varepsilon_{J,\gamma}) \Psi_{J,2,0}^s + h_{24} \Psi_{J,4,0}^s$$

$$= c_{J,\gamma,2,0,0} \Psi_{J,0,0}^s + c_{J,\gamma,2,2,0} \Psi_{J,2,0}^s + c_{J,\gamma,4,0} \Psi_{J,4,0}^s$$

$$\hat{h} = -\varepsilon_{J,\gamma} \quad \Psi_{J,K,0}^s = h_{K,K-2} \Psi_{J,K-2,0}^s + (h_{K,K} - \varepsilon_{J,\gamma}) \Psi_{J,K,0}^s$$

$$+ h_{K,K+2} \Psi_{J,K+2,0}^s = c_{J,\gamma,K,K-2,0} \Psi_{J,K-2,0}^s + c_{J,\gamma,K,K+2,0} \Psi_{J,K+2,0}^s$$

where
\[ C_{J,\tau}^1, K, K, 0 = h_{K, K} - \epsilon_{J, \tau} \]
\[ C_{J,\tau}^1, K, K - 2, 0 = h_{K, K - 2} \]
\[ C_{J,\tau}^1, K, K + 2, 0 = h_{K, K + 2} \]

and \( h_{K, K} = K^2 \), \( h_{02} = h_{20} = \left( \frac{(J^2 - 1)^2}{2} \right) \), \( b \)

\[ h_{K, K - 2} = h_{K - 2, K} = \left[ \frac{(J^2 - (K - 1)^2)}{2} \right] \), \( b \)

\[ h_{K, K + 2} = h_{K + 2, K} = \left[ \frac{(J^2 - (K + 1)^2)}{2} \right] \), \( b \)

Now one sees that when \( O_{J, J}(h) \) acts upon \( \varphi^s_{J, 0, 0} \) the result is

\[ 0_{J, J}(h) \varphi^s_{J, 0, 0} = \frac{\mathcal{T}}{\epsilon_{J, J} - \epsilon_{J, \tau}} \varphi^s_{J, 0, 0} \]

\[ = D_{J, \tau} \frac{\mathcal{T}}{\epsilon_{J, J} - \epsilon_{J, \tau}} \varphi^s_{J, 0, 0} \]

where

\[ D_{J, \tau} = \frac{\mathcal{T}}{\epsilon_{J, J} - \epsilon_{J, \tau}} \]

This becomes

\[ D_{J, \tau} \varphi^s_{J, J - 4} \left( \hat{h} - \epsilon_{J, \tau} \right) \left\{ C_{J, J - 4, 0, 0, 0}^1 \varphi^s_{J, 0, 0} + C_{J, J - 4, 0, 2, 0}^1 \varphi^s_{J, 2, 0} \right\} \]

where \( C_{J, J - 4, 0, 0, 0}^1 \) are defined above. This has expanded the factor in which \( \tau = J - 4 \). Now let the next factor corresponding to \( \tau = J - 8 \) go through and the result is

\[ D_{J, \tau} \varphi^s_{J, J - 8} \left( \hat{h} - \epsilon_{J, \tau} \right) \left\{ C_{J, J - 8, 0, 0, 0}^2 \varphi^s_{J, 0, 0} + C_{J, J - 8, 0, 2, 0}^2 \varphi^s_{J, 2, 0} + C_{J, J - 8, 0, 0, 0}^1 \right\} \]

where \( C_{J, J - 8, 0, 0, 0}^1 = C_{J, J - 4, 0, 0, 0} \)

\[ + C_{J, J - 4, 0, 2, 0} \left( h_{02} \right) \left( \hat{h}_{02} \right) \left( h_{00} - \epsilon_{J, J - 4} \right) \left( h_{00} - \epsilon_{J, J - 8} \right) \]

\[ = \epsilon_{J, J - 4} \epsilon_{J, J - 8} h_{00} \left( \epsilon_{J, J - 4} \epsilon_{J, J - 8} + h_{00} + h_{02} h_{20} \right) \]
\[ C_{J-8,0,2,0}^2 = c_{J-4,0,0,0}^1 c_{J-8,0,2,0} \]
\[ + c_{J-8,0,2,0} c_{J-8,2,2,0} = (h_{00} - \epsilon_{J,J-4}) h_{02}^2 + h_{02} (h_{22} - \epsilon_{J,J-8}) \]
\[ = h_{02} (h_{00} + h_{22} - \epsilon_{J,J-4} - \epsilon_{J,J-8}) \]
\[ C_{J-8,0,4,0}^2 = c_{J-4,0,0,0}^1 c_{J-8,0,4,0} \]
\[ \text{Now let the factor for which } \tau = J-12 \text{ act on the sum of three terms to its right and one obtains} \]
\[ D_{J,\tau} \tau J-12 \left( h_{\tau} - \epsilon_{J,\tau} \right) \left\{ c_{J-12,0,0,0}^3 \phi_{J,0,0}^S \right. \]
\[ + c_{J-12,0,2,0} \phi_{J,2,0}^S + c_{J-12,0,4,0} \phi_{J,4,0}^S + c_{J-12,2,0} \phi_{J,6,0}^S \right\} \]

where
\[ c_{J-12,0,0,0}^3 = c_{J-8,0,0,0} c_{J-12,0,0,0} + c_{J-8,0,2,0} c_{J-12,2,0,0} \]
\[ = - \epsilon_{J,J-4} \epsilon_{J,J-8} \epsilon_{J,J-12} h_{00} \left\{ \epsilon_{J,J-4} \epsilon_{J,J-8} \epsilon_{J,J-12} \right\} \]
\[ + \epsilon_{J,J-8} \epsilon_{J,J-12} \left( h_{00}^2 + h_{02} h_{20} \right) \left( \epsilon_{J,J-4} \epsilon_{J,J-8} \epsilon_{J,J-12} \right) \]
\[ + e_{J,J-12,0,2,0} c_{J-12,0,0,0}^3 + c_{J-12,0,2,0} c_{J-12,2,0,0} \]
\[ + c_{J-8,0,4,0} c_{J-12,4,2,0} = h_{02} \left\{ \epsilon_{J,J-4} \epsilon_{J,J-8} \epsilon_{J,J-12} \right\} \]
\[ + \epsilon_{J,J-8} \epsilon_{J,J-12} \left( h_{00}^2 + h_{02} h_{20} \right) \left( \epsilon_{J,J-4} \epsilon_{J,J-8} \epsilon_{J,J-12} \right) + h_{00}^2 + h_{00} h_{22} + h_{22}^2 + h_{02} h_{20} + h_{24} h_{42} \]
\[ c_{J-12,0,4,0} = c_{J-8,0,2,0} c_{J-12,2,4,0} + c_{J-8,0,4,0} c_{J-12,4,4,0} \]
\[ = h_{02} h_{24} \left\{ \epsilon_{J,J-4} \epsilon_{J,J-8} \epsilon_{J,J-12} \right\} + h_{00} + h_{22} + h_{44} \]
\[ c_{J-12,0,6,0} = c_{J-8,0,4,0} c_{J-12,4,6,0} = h_{02} h_{42} h_{46} \]

This procedure may be continued until all factors are exhausted and gives
\[ O_{J,J}(\hat{h}) \mathcal{S}_{J,0,0} = D_{J,J} \mathcal{T}_{J,J-4n} \left( \mathcal{F}_{J,J-4n} \right) \sum_{K=0}^{2n} \frac{1}{\mathcal{F}_{J,J-4n}} \phi_{J,K,0} \]

\[ = \mathcal{T}_{J,J} \sum_{K=0}^{\frac{J}{2}} \frac{1}{\mathcal{F}_{J,J}} \phi_{J,0,K,0} \phi_{J,K,0} \quad (K \text{ even}) \quad (2.7) \]

where

\[ C_{J,J} = \begin{cases} \frac{J}{2} - 1 & \text{if } J = J-4,0,0 \text{ to } J-6,0,0 \\ \frac{J}{2} & \text{otherwise} \end{cases} \]

\[ C_{J,J} = \begin{cases} \frac{J}{2} - 1 & \text{if } J = J+4,0,0 \text{ to } J+6,0,0 \\ \frac{J}{2} & \text{otherwise} \end{cases} \]
From this one can readily see the effect of any \( O_{j, \gamma} (h) \) on any \( \Phi_{j, K, \gamma}^S \). The general result is

\[
O_{j, \gamma} (h) \Phi_{j, K, \gamma}^S = b_{j, \gamma, K, \gamma} \Phi_{j, \gamma, K, \gamma}^a
\]

\[
= \sum_{K'=0}^{J} b_{j, \gamma, K, \gamma} b_{j, \gamma, K', \gamma} \Phi_{j, K', \gamma}^S \Phi_{j, K, \gamma}^S
\]

\[
= \gamma^{J, \gamma} \sum_{K'=0}^{J} \sum_{K'=0}^{J} \sum_{K'=0}^{J} \sum_{K'=0}^{J} c_{j, K, K', \gamma} \Phi_{j, K, \gamma}^S \Phi_{j, K', \gamma}^S \cdot \tag{2.8}
\]

The superscript \( n \) refers to the number of factors in the projection operator. The first subscript of \( C \) refers to the \( J \) values; the second to the last factor of the expansion; the third to the particular \( K \) value in question; the fourth to the \( K' \) value in the sum, while the last is just 0 or 1. While evaluating the \( C \)'s, it is desirable to use the second subscript and the superscript to keep track of the various values in the product. Once this is completed it is desirable to change the second subscript to indicate the \( \gamma \) of \( O_{j, \gamma} (h) \) and to omit the superscript so that the above equation may be written as

\[
O_{j, \gamma} (h) \Phi_{j, K, \gamma}^S = \sum_{K'=0}^{J} b_{j, \gamma, K, \gamma} b_{j, \gamma, K', \gamma} \Phi_{j, K', \gamma}^S \Phi_{j, K, \gamma}^S
\]

\[
= \gamma^{J, \gamma} \sum_{K'=0}^{J} \sum_{K'=0}^{J} \sum_{K'=0}^{J} \sum_{K'=0}^{J} c_{j, \gamma, K, K', \gamma} \Phi_{j, K, \gamma}^S \Phi_{j, K', \gamma}^S \cdot \tag{2.9}
\]

Earlier the eigenvector equations for the \( b_{j, \gamma, K, \gamma} \) were explicitly given. Since the above equation gives

\[
b_{j, \gamma, K, \gamma} b_{j, \gamma, K', \gamma} = \gamma^{J, \gamma} \sum_{K'=0}^{J} \sum_{K'=0}^{J} \sum_{K'=0}^{J} \sum_{K'=0}^{J} c_{j, \gamma, K, K', \gamma} \Phi_{j, K, \gamma}^S \Phi_{j, K', \gamma}^S
\]

one sees that a similar set of equations holds for either the \( c_{j, \gamma, K, K', \gamma} \) or the \( d_{j, \gamma, K, K', \gamma} \) defined above. Both of these will be used in the pages that follow. Initially the equations for the \( c_{j, \gamma, K, K', \gamma} \)'s will be needed. These are simply
\[ C_{J',\gamma',K',-2} \psi_{K',-2} + C_{J',\gamma',K',2} + C_{J',\gamma',K',0} (h_{K',K'} - \epsilon_{J',\gamma'}) \]
\[ + C_{J',\gamma',K',+2} \psi_{K',+2} = 0 \]  

(2.10)

where the \( C \) 's can be determined in terms of the \( h_{K,K'} \) 's and the \( \epsilon_{J,J'} \) 's.

The secular equation may be written as

\[ \epsilon_{J,J'} + P_1 \epsilon_{J,J'} + P_2 \epsilon_{J,J'} + \ldots + P_{n-1} \epsilon_{J,J'} + P_n = 0 \]

where the \( P_i \) represent the invariants of the problem. Thus \( P_1 \)

is minus the sum of the \( \epsilon_{J,J'} \) that belong to the same representation, \( P_2 \) is the sum of these taken two at a time, etc. The expression for the \( C_{J,\gamma,K,K'} \) may now be used to evaluate these invariants. As mentioned earlier this will be shown in detail only for the states that transform as \( A \) for even \( J \).

The Invariant \( P_1 \)

Returning now to the states that transform as \( A \) for even \( J \) values and also choosing \( K = 0 \) the above equation for the

\[ C_{J,\gamma,K,K',0} \]

becomes

\[ C_{J,\gamma,0,K',-2} \psi_{K',-2} + C_{J,\gamma,0,K',0} (h_{K',K'} - \epsilon_{J,J'}) \]
\[ + C_{J,\gamma,0,K',+2} \psi_{K',+2} = 0 \]

The invariant \( P_1 \) results from setting \( K' = J \). If this is done one sees that

\[ C_{J,\gamma,0,J-2} \psi_{J-2} + C_{J,\gamma,0,J} + C_{J,\gamma,0,J} (h_{J,J} - \epsilon_{J,J'}) = 0 \]

The simplest procedure would be to evaluate this for several \( J \) values.

\[ J = 2, \gamma = \frac{1}{2}, \frac{3}{2} \]

\[ C_{2,\gamma,0,0,2} \psi_{0,2} + C_{2,\gamma,0,2,0} \psi_{2,0} (h_{2,2} - \epsilon_{2,2}) = h_{0,2} (h_{0,0} + h_{2,2} - \epsilon_{2,2} - \epsilon_{2,2}) \] or
\[ \sum \varepsilon_{2\gamma} = h_{00} + h_{22} \]
\[
J = 4, \gamma = 0, \pm 4 \\
C_{4\gamma} 020 h_{24} + C_{4\gamma} 040 (h_{44} - \varepsilon_{5\gamma}) = h_{02} h_{24} (h_{00} + h_{22} + h_{44} - \varepsilon_{4\gamma} - \varepsilon_{4\gamma} - \varepsilon_{4\gamma}) \\
= 0 \text{ or } \sum \varepsilon_{4\gamma} = h_{00} + h_{22} + h_{44} \\
J = 6, \gamma = \pm 2, \pm 6 \\
C_{6\gamma} 040 h_{46} + C_{6\gamma} 060 (h_{66} - \varepsilon_{6\gamma}) = h_{02} h_{46} (h_{00} + h_{22} + h_{44} + h_{66} - \varepsilon_{6\gamma}) \\
= 0 \text{ or } \sum \varepsilon_{6\gamma} = h_{00} + h_{22} + h_{44} + h_{66}
\]
If this is continued for higher J values, the result is
\[ \sum \varepsilon_{J, \gamma} = \sum_{K=0}^{J} h_{K,K} = \sum_{K=0}^{J} K^2 \quad (K \text{ even}) \]
This may be readily expressed as a function of J and gives
\[ \sum \varepsilon_{J, \gamma} = \frac{1}{6} J(J+1)(J+2) \quad (2.11) \]
If this procedure is followed for the other \( \gamma \)-values going with even J and also all \( \gamma \)-values going with odd J, similar results hold. These results are summarized in Table 5.

At this point a slight simplification and partial determination of the eigenvalues can be introduced. The secular equation for this case is
\[ \varepsilon_{\frac{J}{2} + 1} P_1 \leq \frac{J}{2},\gamma + \cdots + \frac{J}{2} P_{\frac{J}{2}} \leq \frac{J}{2},\gamma + \frac{J}{2} + 1 = 0 \quad (2.12) \]
The first invariant \( P_1 \) is just \( \sum \varepsilon_{J, \gamma} \). The normal form of the equation is found by letting
\[ \varepsilon_{\frac{J}{2} + 1} P_1 \leq \frac{J}{2},\gamma = \frac{1}{3} J(J+1) + \frac{2}{3} J,\gamma \]
and substituting into the regular form. This gives an equation
<table>
<thead>
<tr>
<th>Representation</th>
<th>Number of States</th>
<th>$\frac{1}{\sqrt{J}} \sum_{J}^{J} \epsilon_{J}\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Even J</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A$</td>
<td>$\frac{J}{2} + 1$</td>
<td>$\frac{1}{6} J(J+1)(J+2)$ ($\gamma = J, J-4, \ldots, -J$)</td>
</tr>
<tr>
<td>$B_z$</td>
<td>$\frac{J}{2}$</td>
<td>$\frac{1}{6} J(J+1)(J+2)$ ($\gamma = J-2, J-6, \ldots, -J+2$)</td>
</tr>
<tr>
<td>$B_x$</td>
<td>$\frac{J}{2}$</td>
<td>$\frac{1}{6}(J-1)J(J+1) + \frac{b}{2} J(J+1)$ ($\gamma = J-1, J-5, \ldots, -J+3$)</td>
</tr>
<tr>
<td>$B_y$</td>
<td>$\frac{J}{2}$</td>
<td>$\frac{1}{6}(J-1)J(J+1) - \frac{b}{2} J(J+1)$ ($\gamma = J-3, J-7, \ldots, -J+1$)</td>
</tr>
<tr>
<td><strong>Odd J</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$A$</td>
<td>$\frac{J-1}{2}$</td>
<td>$\frac{1}{6}(J-1)J(J+3)$ ($\gamma = J-3, J-7, \ldots, -J+3$)</td>
</tr>
<tr>
<td>$B_z$</td>
<td>$\frac{J+1}{2}$</td>
<td>$\frac{1}{6}(J-1)J(J+1)$ ($\gamma = J-1, J-5, \ldots, -J+1$)</td>
</tr>
<tr>
<td>$B_x$</td>
<td>$\frac{J+1}{2}$</td>
<td>$\frac{1}{6} J(J+1)(J+2) - \frac{b}{2} J(J+1)$ ($\gamma = J-2, J-6, \ldots, -J$)</td>
</tr>
<tr>
<td>$B_y$</td>
<td>$\frac{J+1}{2}$</td>
<td>$\frac{1}{6} J(J+1)(J+2) + \frac{b}{2} J(J+1)$ ($\gamma = J, J-4, \ldots, -J+2$)</td>
</tr>
</tbody>
</table>

**TABLE 5**

THE INVARIANT $P_1$
of degree $\frac{J}{2} + 1$ for the $f_{J, \gamma}$ so defined. The coefficient of $f_{J, \gamma}$ in this equation will be $-\sum f_{J, \gamma}$ and will vanish. Thus the normal form is

$$f_{J, \gamma}^2 + \frac{J}{2} f_{J, \gamma} + \frac{1}{2} f_{J, \gamma}^2 + \cdots + \frac{1}{2} f_{J, \gamma}^2 + \cdots + f_{J, \gamma}^2 f_{J, \gamma} + f_{J, \gamma}^2 = 0$$

where the $I_1$ that appear are the invariants of this equation and are simply the sum of the products of the $f_{J, \gamma}$ taken $i$ at a time with the correct algebraic sign.

This can be done for all other $\gamma$ and $J$ values and will in general give the result $\xi_{J, \gamma} = e_{J, \gamma} + f_{J, \gamma}$. This, at least, partially determines $\xi_{J, \gamma}$ and also gives one invariant in the problem which will vanish and hence should make any solution attempted somewhat easier. The $e_{J, \gamma}$ are thus determined by dividing the invariant $P_1$ by the number of states appearing in the expansion. These quantities are the same for all $\gamma$ values appearing in the expansion. While this has been done only for even $J$ states that transform as $A$, the same quantity may also be found for all other $\gamma$ values going with even $J$ and also for all $\gamma$ values going with odd $J$. These results are summarized for all $J$ and $\gamma$ in Table 6.

Since the $e_{J, \gamma}$ are all the same for all $\gamma$ values that transform according to a particular irreducible representation, one can alter the form of the reduced Hamiltonian and the projection operators since they also contain only $\gamma$ values that go with a particular irreducible representation. Thus one can say that $\hat{h} = \hat{e} + \hat{f}$ where $\hat{h}$ is the reduced Hamiltonian, $\hat{e}$ is a
number operator whose eigenvalues are given in Table 6, while \( \hat{f} \) is that part of the Hamiltonian whose eigenvalues are yet to be determined. This enables one to alter the form of the eigenvalue projection operators as follows

\[
C_{J, \gamma, 0, K', 0} C_{J, \gamma, 0, J-4, 0} \mathcal{H}_{J-4, J-2} C_{J, \gamma, 0, J-2, 0} = 0
\]

Furthermore, one may now express the eigenvalues of \( \hat{h} \) as \( \varepsilon_{J, \gamma}^{(b)} \) and the eigenvalues of \( \hat{H} \) as

\[
E_{J, \gamma}(a, b, c) = ac(J+1) + \varepsilon_{J, \gamma}^{(b)}
\]

(2.15)

The matrix elements of the operator \( \hat{f} \) are just those of \( \hat{h} \) with the numerical value of \( \varepsilon_{J, \gamma}^{(b)} \) subtracted from the diagonal terms only since \( \hat{e} \) is a diagonal number operator. This has the effect of simplifying the problem of determining the eigenvalues of the reduced Hamiltonian as well as simplifying the notation to be used in Chapter III.

The Invariant \( P_2 \)

The invariant \( P_2 \) in the secular equation or \( I_2 \) in the normal form of the secular equation can now be determined. This is accomplished by setting \( K' = J - 2 \) in the equation for the

\[
C_{J, \gamma, 0, K', 0} C_{J, \gamma, 0, J-4, 0} \mathcal{H}_{J-4, J-2} C_{J, \gamma, 0, J-2, 0} = 0
\]

As in the case of \( P_1 \) this is easily evaluated by considering several \( J \) values.
<table>
<thead>
<tr>
<th>Representation</th>
<th>Even J</th>
<th>Odd J</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>( \frac{J}{2} + 1 )</td>
<td>( \frac{J}{2} - 1 )</td>
</tr>
<tr>
<td>B_x</td>
<td>( \frac{J}{2} )</td>
<td>( \frac{J}{2} + 1 )</td>
</tr>
<tr>
<td>B_y</td>
<td>( \frac{J}{2} )</td>
<td>( \frac{J}{2} - 1 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Number of States</th>
<th>( e_{J, \gamma} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Even J</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>( \frac{1}{3} J(J+1) ) (( \gamma = J, J-4, \ldots, -J ))</td>
</tr>
<tr>
<td>B_x</td>
<td>( \frac{1}{3} (J+1)(J+2) ) (( \gamma = J-2, J-6, \ldots, -J+2 ))</td>
</tr>
<tr>
<td>B_y</td>
<td>( \frac{1}{3} (J-1)(J+1) + b(J+1) ) (( \gamma = J-1, J-5, \ldots, -J+3 ))</td>
</tr>
</tbody>
</table>

| Odd J            |                     |
| A                | \( \frac{1}{3} J(J+1) \) (\( \gamma = J-3, J-7, \ldots, -J+3 \)) |
| B_x              | \( \frac{1}{3} J(J-1) \) (\( \gamma = J-1, J-5, \ldots, -J+1 \)) |
| B_y              | \( \frac{1}{3} J(J+2) - bJ \) (\( \gamma = J-2, J-6, \ldots, -J \)) |

**TABLE 6**

THE QUANTITY \( e_{J, \gamma} \)
\[ J = 2, \gamma = \pm 2 \]
\[ C_{2 \gamma 000}(\varepsilon_{00} - \varepsilon_{2 \gamma}) + C_{2 \gamma 020}h_{20} = (\varepsilon_{00} - \varepsilon_{2 \gamma})(\varepsilon_{00} - \varepsilon_{2 \gamma}) \]
\[ + h_{02}h_{20} = 0 \quad \text{or} \]
\[ \gamma \neq \gamma \in 2 \gamma = h_{00} \sum_{\gamma} \varepsilon_{2 \gamma} - h_{00}^2 - h_{02}h_{20} = h_{00}h_{22} - h_{02}h_{20} = -12b^2. \]
\[ J = 4, \gamma = 0, \pm 4 \]
\[ C_{4 \gamma 000}h_{02} + C_{4 \gamma 020}(h_{22} - \varepsilon_{2 \gamma}) + C_{4 \gamma 040}h_{42} \]
\[ = h_{02}\left\{ \sum_{\gamma} \varepsilon_{4 \gamma} - h_{00}(\varepsilon_{4 \gamma} + \varepsilon_{3 \gamma}) + h_{00}^2 + h_{02}h_{20} \right\} \]
\[ + (h_{22} - \varepsilon_{4 \gamma})(h_{00} + h_{22} - \varepsilon_{4 \gamma} - \varepsilon_{3 \gamma}) + h_{24}h_{42}\} = 0 \]
\[ \text{or} \]
\[ \sum_{\gamma \neq \gamma} \varepsilon_{4 \gamma} - h_{00}h_{22}h_{44} - h_{22}h_{44} - h_{02}h_{20}h_{24}h_{42} = 64 - 208b^2. \]
\[ J = 6, \gamma = \pm 2, \pm 6 \]
\[ C_{6 \gamma 020}h_{24} + C_{6 \gamma 040}(h_{44} - \varepsilon_{6 \gamma}) + C_{6 \gamma 060}h_{64} \]
\[ = h_{02}\left( \sum_{\gamma \neq \gamma} \varepsilon_{6 \gamma} - (h_{00} + h_{22}) \sum_{\gamma \neq \gamma} \varepsilon_{6 \gamma} + h_{00}^2 + h_{02}h_{22}h_{24}h_{42} \right) \]
\[ + h_{02}h_{20} + h_{24}h_{42} + (h_{44} - \varepsilon_{6 \gamma}) \left\{ - \sum_{\gamma \neq \gamma} \varepsilon_{6 \gamma} + h_{00} + h_{22}h_{44} \right\} + h_{46}h_{64}\} = 0 \]
\[ \text{or} \]
\[ \sum_{\gamma \neq \gamma} \varepsilon_{6 \gamma} - h_{22}h_{44} - h_{64} - h_{02}h_{20}h_{24}h_{42} = 46h_{64} \]
\[ = h_{00}(h_{22} + h_{44} + h_{66}) + h_{22}(h_{44} + h_{66}) + h_{44}h_{66} - h_{02}h_{20} + h_{24}h_{42} = 46h_{64} \]
\[ = 784 - 1176b^2. \]

If this is continued for higher J values the result

\[ \sum_{\gamma \neq \gamma} \varepsilon_{j \gamma} \left( \sum_{k^*}^{J-2} h_k, k<k^* \right)_{k^*>k=0}^{J-2} = \sum_{k=0}^{h_k, k+2 h_k+2, K} \]
If this is evaluated in terms of \( J \) and \( b \) one obtains

\[
\sum_{\gamma} \xi_{J, \gamma} \xi_{J, \gamma'} = \frac{J(J+1)(J+2)}{360} \left\{ (J-2)(J-1)(5J+12)-6(J+14)(4J-3) b^2 \right\}.
\]

This may now be expressed in terms of the \( f_{J, \gamma} \) as follows

\[
\sum_{\gamma} \xi_{J, \gamma} \xi_{J, \gamma'} = \sum_{\gamma} \left( \frac{1}{3} J(J+1) f_{J, \gamma} \right) \left( \frac{1}{3} J(J+1) f_{J, \gamma'} \right)
\]

\[
= \sum_{\gamma} \left\{ \frac{1}{6} J^2(J+1)^2 \left\{ J(J+1) f_{J, \gamma} + f_{J, \gamma'} \right\} + f_{J, \gamma} f_{J, \gamma'} \right\}
\]

\[
= \frac{J^2(J+1)^2}{72} + \frac{1}{2} J^2(J+1) \sum_{\gamma} f_{J, \gamma} + \sum_{\gamma \neq \gamma'} f_{J, \gamma} f_{J, \gamma'}
\]

or

\[
\sum_{\gamma} f_{J, \gamma} f_{J, \gamma'} = \frac{-J(J+1)(J+2)(J+4)(4J-3)(1+3b^2)}{180} \quad (2.17)
\]

where \( \sum_{\gamma} \xi_{J, \gamma} \xi_{J, \gamma'} \) is the invariant \( P_2 \) of the secular equation and \( \sum_{\gamma} f_{J, \gamma} f_{J, \gamma'} \) is the invariant \( I_2 \) of the normal form of the secular equation. This has been shown explicitly only for the states that transform as \( \Delta \) for even \( J \). The invariant \( P_2 \) is given for the remaining \( \gamma \)-values for even \( J \) and all \( \gamma \)-values for odd \( J \) in Tables 7 and 8.

One may now determine part of \( f_{J, \gamma} \) through the use of the invariant \( I_2 \). The normal form of the secular equation is of degree \( \frac{J+1}{2} \) and has \( \frac{J}{2} \) non-zero invariants. The remaining invariant is zero as indicated earlier. Thus each of the roots may be expressed as suitable combinations of \( \frac{J}{2} \) independent quantities.

One may employ a polar coordinate representation for these \( \frac{J}{2} \) quantities as follows

\[
A_{J, \gamma, 1} = \alpha_{J, \gamma} a_{J, \gamma, 1}
\]

\[
A_{J, \gamma, 2} = \alpha_{J, \gamma} a_{J, \gamma, 2}
\]
TABLE 7

THE INVARIANT $P_2$ FOR EVEN $J$

<table>
<thead>
<tr>
<th>Representation</th>
<th>Number of States</th>
<th>$\sum_{\gamma \neq \gamma'} \in J, \gamma' \in J, \gamma'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>$\frac{J}{2} + 1$</td>
<td>$\frac{J(J+1)(J+2)}{360} \left( (J-2)(J-1)(5J+12) - 6(J+4)(4J-3)b^2 \right)$</td>
</tr>
<tr>
<td>$B_z$</td>
<td>$\frac{J}{2}$</td>
<td>$\frac{J(J+1)(J+2)(J-2)}{360} \left( (J-1)(5J+12) - 6(4J-9)b^2 \right)$</td>
</tr>
<tr>
<td>$B_x$</td>
<td>$\frac{J}{2}$</td>
<td>$\frac{(J-2)J(J+1)}{360} \left( (J-3)(J-1)(5J+7) + 30(J^2 + 2J + 3)b^2 - 3(8J^2 + 13J + 9)b^2 \right)$</td>
</tr>
<tr>
<td>$B_y$</td>
<td>$\frac{J}{2}$</td>
<td>$\frac{(J-2)J(J+1)}{360} \left( (J-3)(J-1)(5J+7) - 30(J^2 + 2J + 3)b^2 - 3(8J^2 + 13J + 9)b^2 \right)$</td>
</tr>
</tbody>
</table>

(\( \gamma' = J-4, \ldots, -J \))

(\( \gamma' = J+2, J-6, \ldots, -J+2 \))

(\( \gamma' = J-1, J-5, \ldots, -J+3 \))

(\( \gamma' = J-3, J-7, \ldots, -J+1 \))
<table>
<thead>
<tr>
<th>Representation</th>
<th>Number of States</th>
<th>( \sum_{\tau'-\tau} \epsilon_{\tau'} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>( \frac{J-1}{2} )</td>
<td>( \frac{(J-3)(J-1)J(J+1)}{360} ) (( J=J-3, J-1, \ldots, J+3 ))</td>
</tr>
<tr>
<td>( B_z )</td>
<td>( \frac{J+1}{2} )</td>
<td>( \frac{(J-1)J(J+1)}{360} ) (( J=J-1, J-5, \ldots, J+1 ))</td>
</tr>
<tr>
<td>( B_x )</td>
<td>( \frac{J+1}{2} )</td>
<td>( \frac{(J-1)J(J+1)}{360} ) (( J=J-2, J-6, \ldots, J ))</td>
</tr>
<tr>
<td>( B_y )</td>
<td>( \frac{J+1}{2} )</td>
<td>( \frac{(J-1)J(J+1)}{360} ) (( J=J, J-4, \ldots, J+2 ))</td>
</tr>
</tbody>
</table>

**TABLE 8**

THE INVARIANT \( P_2 \) FOR ODD \( J \)
\[ a_{j, \gamma, 1} = \cos \Theta_{j, \gamma} \]
\[ a_{j, \gamma, 2} = \sin \Theta_{j, \gamma} \cos \Theta_{j, \gamma} \]
\[ a_{j, \gamma, 3} = \sin \Theta_{j, \gamma} \sin \Theta_{j, \gamma} \cos \Theta_{j, \gamma} \]

This specifies a radial coordinate \( R_{j, \gamma} \) and \( \frac{J}{2} - 1 \) angular coordinates.

The roots \( f_{j, \gamma} \) of the secular equation are now chosen as linear combinations of the quantities \( A_{j, \gamma, i} \) such that
\[ \sum_{j, \gamma} f_{j, \gamma} = 0 \]
This enables one to separate the radial coordinate from the angular coordinates in each case and gives
\[ f_{j, \gamma} = \alpha_{j, \gamma} \epsilon_{j, \gamma} \]
where \( \epsilon_{j, \gamma} \) represent suitable linear combinations of the \( a_{j, \gamma, i} \) which in turn depend only on the \( \frac{J}{2} - 1 \) angular coordinates. Since \( \sum_{j, \gamma} f_{j, \gamma} = 0 \) one also sees that \( \sum_{j, \gamma} \epsilon_{j, \gamma} = 0 \)
and one can also show that
\[ \sum_{\tau \neq \tau'} \frac{\hat{f}_{J,\tau}}{\tau} \hat{e}_{J,\tau} = \sum_{\tau \neq \tau'} \frac{\alpha_{J,\tau}}{\tau} \hat{e}_{J,\tau} \hat{e}_{J,\tau'} = -\alpha_{J,\tau}^{2} \]
where
\[ \alpha_{J,\tau}^{2} = -I_{2} = \frac{J(J+1)(J+2)(+4)(4J-3)(1+3b^{2})}{180} \]  
Again this has been shown only for the states that transform as \( A \) for even \( J \). Similar results hold for all other \( \tau \) and \( J \) values and are summarized in Tables 9 and 10.

In terms of the quantities \( \hat{e}_{J,\tau} \) one now sees that
\[ \sum_{\tau} \hat{e}_{J,\tau} = 0 \quad \text{and} \quad \sum_{\tau \neq \tau'} \hat{e}_{J,\tau} \hat{e}_{J,\tau'} = -1. \]  
This holds for all \( J \) and \( \tau \). The remaining invariants of the problem can also be determined in this way and may also be expressed in terms of the \( \hat{e}_{J,\tau} \).

Earlier it was seen that the energies are given by
\[ E_{J,\tau}(a,b,c) = acJ(J+1)+aE_{J,\tau}(b) \]
where \( E_{J,\tau}(b) \) is specified for all \( J \) and \( \tau \). One may now express \( E_{J,\tau}(b) \) as \( \alpha_{J,\tau}(b) \hat{e}_{J,\tau}(b) \) for all \( J \) and \( \tau \). At this point the energies are completely given except for the \( \hat{e}_{J,\tau} \) which may not in general be determined exactly.

The partial determination of \( \hat{f}_{J,\tau} \) which has just been demonstrated will not be used in the approximations which follow. The reason is that, while the formal part of the calculations are somewhat simplified, the actual approximations used are made more difficult to handle with the separation of the radial coordinate \( \alpha_{J,\tau} \). It thus appears simpler to determine an approximation to \( \hat{f}_{J,\tau} \) directly rather than the \( \hat{e}_{J,\tau} \).
\begin{table}
\begin{tabular}{|c|c|}
\hline
Representation & Number of States \\
\hline
A & \( J/2 + 1 \) \\
B_z & \( J/2 \) \\
B_x & \( J/2 \) \\
B_y & \( J/2 \) \\
\hline
\end{tabular}

\[ \alpha_{J, \tau}^2 = -I_2 = -\sum_{\tau' \neq \tau} f_{J, \tau} f_{J, -\tau} \]

\[ J(J+1)(J+2)(J+4)(4J-3)(1+3b^2) \]
\[ 180 \]

\[ (\tau' = J, J-4, \ldots, -J) \]

\[ (J-2)J(J+1)(J+2)(4J+11+3(4J-9)b^2) \]
\[ 180 \]

\[ (\tau' = J-2, J-6, \ldots, -J+2) \]

\[ (J-2)J(J+1)(J+2) \left( 2(J-1) - 15b + 3(2J+3)b^2 \right) \]
\[ 90 \]

\[ (\tau' = J-1, J-5, \ldots, -J+3) \]

\[ (J-2)J(J+1)(J+2) \left( 2(J-1) + 15b + 3(2J+3)b^2 \right) \]
\[ 90 \]

\[ (\tau' = J-3, J-7, \ldots, -J+1) \]

\hline
\end{table}

\textbf{Table 9.}

\textbf{The Quantity } \( \alpha_{J, \tau}^2 \text{ For Even } J \).
<table>
<thead>
<tr>
<th>Representation</th>
<th>Number of States</th>
<th>( \alpha_j, \tau^2 = -I_2 = - \sum_{\tau \neq j, \tau'} f_{j, \tau} f_{j, \tau'} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A )</td>
<td>( \frac{J-1}{2} )</td>
<td>( \frac{(J-3)(J-1)J(J+4)(4J+7)(1+3b^2)}{180} ) ( \tau = J-3, J-7, \ldots, -J+3 )</td>
</tr>
<tr>
<td>( B_z )</td>
<td>( \frac{J+1}{2} )</td>
<td>( \frac{(J-1)J(J+1)(J+3)(4J-7+3(4J+3)b^2)}{180} ) ( \tau = J-1, J-5, \ldots, -J+1 )</td>
</tr>
<tr>
<td>( B_x )</td>
<td>( \frac{J+1}{2} )</td>
<td>( \frac{(J-1)J(J+1)(J+3)(2J+15b^2+3(2J-1)b^2)}{90} ) ( \tau = J-2, J-6, \ldots, -J )</td>
</tr>
<tr>
<td>( B_y )</td>
<td>( \frac{J+1}{2} )</td>
<td>( \frac{(J-1)J(J+1)(J+3)(2J+15b^2+3(2J-1)b^2)}{90} ) ( \tau = J, J-4, \ldots, -J+2 )</td>
</tr>
</tbody>
</table>

**TABLE 10**

*THE QUANTITY \( \alpha_j, \tau^2 \) FOR ODD J*
Remark on the Determination of the other Invariants

At this point the first two invariants $P_1$ and $P_2$ or alternatively $I_1$ and $I_2$ have been determined as functions of both $J$ and $b$ for all $J$ and $\gamma$. Clearly this process could be continued in the same manner in order to specify the remaining invariants. Since $P_1$ involves a polynomial to the third degree in $J$ and $P_2$ to the sixth degree in $J$, then evidently $P_3$ would involve a polynomial to the ninth degree in $J$, etc. The specific determination of the remaining invariants becomes extremely tedious and will not be pursued here.
AN APPROXIMATE METHOD FOR EVALUATING $f_{J^*}^{T'}$

Approximations to the Eigenvalue Projection Operators

Earlier it was seen that when $O_{J',T'}(f)$ acts on $\Phi^S_{J',K',Y}$ the result is

$$O_{J',T'}(f)\Phi^S_{J',K',Y} = \sum_{K'=0}^{J} D_{J',T',K,K'}^{J',T',J} \Phi^S_{J',K',Y}$$

where

$$D_{J',T',K,K'}^{J',T',J} = \frac{1}{\sqrt{\tau'/\tau}} \frac{\tau - \tau'}{2} C_{J',T',K,K'}^{J,T} b_{J',T',K,K'}^{J,T}$$

In order to make direct use of these projection operators, one needs to know the energy eigenvalues. In the absence of knowing these eigenvalues one may assume an approximate form for them. There are several ways that are available for determining approximations. The simplest is to consider the symmetric rotator limits for which $b = 0$ and $-1$ and make a linear approximation. While more sophisticated approximations can be made, the linear approximation has the advantage of keeping the subsequent approximations simpler in form and seems therefore to be preferable to a more accurate starting approximation.

Let this linear approximation, designated by $f_0^{T'}$, be used in the projection operators which are now specified as

$$O_{J',T'}^{0}(f) = \frac{\tau - f_0^{T'}}{\tau' + f_0^{T'}}(f_0^{T'} - f_0^{T'})$$

This now constitutes an approximation to the projection operator $O_{J',T'}(f)$. Note that it is now no longer a projection operator as such but only an approximation to a projection operator. If this approximation is now allowed to act on $\Phi^S_{J,K,Y}$ the result is

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Thus if a particular choice of \( f_{j,\gamma}^j \) is used in \( \hat{f}_{j,\gamma}^0 \) the result should be an approximation to \( b_{j,\gamma,K,v} \). The coefficients \( b_{j,\gamma,K,v} \) are then approximations to \( b_{j,\gamma,K,v} \), while the \( D_{j,\gamma,K,v}^0 \) approximate the \( D_{j,\gamma,K,v} \).

If the operator \( \hat{f} \) is allowed to act upon \( \hat{f}_{j,\gamma}^j \), the result is

\[
\hat{f}_{j,\gamma}^j(\hat{f}) \varphi_{j,K,v}^S = \sum_{K'=0}^J \sum_{K''=0}^J \sum_{K''''=0}^J D_{j,\gamma,K,v}^0 \varphi_{j,K,v}^S \]

Thus if a particular choice of \( f_{j,\gamma}^j \) is used in \( \hat{f}_{j,\gamma}^0 \) the result should be an approximation to \( b_{j,\gamma,K,v} \). The coefficients \( b_{j,\gamma,K,v} \) are then approximations to \( b_{j,\gamma,K,v} \), while the \( D_{j,\gamma,K,v}^0 \) approximate the \( D_{j,\gamma,K,v} \).

If the operator \( \hat{f} \) is allowed to act upon \( \hat{f}_{j,\gamma}^j \), the result is

\[
\hat{f}_{j,\gamma}^j(\hat{f}) \varphi_{j,K,v}^S = \sum_{K'=0}^J \sum_{K''=0}^J \sum_{K''''=0}^J D_{j,\gamma,K,v}^0 \varphi_{j,K,v}^S \]

Thus if a particular choice of \( f_{j,\gamma}^j \) is used in \( \hat{f}_{j,\gamma}^0 \) the result should be an approximation to \( b_{j,\gamma,K,v} \). The coefficients \( b_{j,\gamma,K,v} \) are then approximations to \( b_{j,\gamma,K,v} \), while the \( D_{j,\gamma,K,v}^0 \) approximate the \( D_{j,\gamma,K,v} \).

Each of the coefficients of \( D_{j,\gamma,K,v}^0 \varphi_{j,K,v}^S \) where \( f_{K,K,v} = h_{K,K,v} \) and \( f_{K,K,v} = h_{K,K,v} \) is seen to represent an approximation to the eigenvalues of the operator \( \hat{f} \).

The eigenvalues are given by \( f_{j,\gamma} \), the approximations used to compute \( \hat{f}_{j,\gamma}^j(\hat{f}) \) by \( f_{j,\gamma}^j \), and the coefficients of

\[
D_{j,\gamma,K,v}^0 \varphi_{j,K,v}^S \]

will be designated as \( f_{j,\gamma,K,v}^0 \).

Note that the number of terms in the sum is just the number of states whose eigenfunctions transform according to a particular irreducible representation as was discussed earlier. If this number is \( n \), then there are \( n^2 \) functions \( f_{j,\gamma,K,v}^0 \) since there
are also n functions \( \varphi^S_{J,K,Y} \) for which this sequence of operations may be carried out. Not all are independent, however, as

\[ f^0_{J,Y,K,K',Y} = f^0_{J,Y,K,K',Y} \]

so that \( \frac{n(n+1)}{2} \) of the \( f^0_{J,Y,K,K',Y} \) are independent and will in general be different from one another.

**Use of the Approximations to the Projection Operators**

Before discussing the use of the approximations to the projection operators there is a change of notation to be introduced. The projection operators have been designated as \( O_{J,Y} (\hat{f}) \).

From this point on this will be written as \( \hat{O}_{J,Y} \). The approximations to the projection operators will then be \( O_{J,Y}^0 \).

There are several methods that could be used in an effort to obtain improvements in the approximations to \( f_{J,Y} \).

One would be to compute the average of the \( f^0_{J,Y,K,K',Y} \) and equate this average \( f^1_{J,Y} \) which would presumably represent a better approximation to \( f_{J,Y} \) than does \( f^0_{J,Y} \). The functions \( f^1_{J,Y} \) could then be used to compute different approximations \( \hat{O}_{J,Y}^1 \) to the projection operators. The whole process of allowing these to act on the \( \varphi^S_{J,K,Y} \) and allowing the operator \( \hat{f} \) to act on the results is repeated. This would give a new set of \( f^1_{J,Y,K,K',Y} \) which could be averaged and the process continued. Assuming convergence, each successive average of the \( f^n_{J,Y,K,K',Y} \) should more closely approximate \( f_{J,Y} \) than the previous ones. There are several disadvantages to this procedure, so it will not be discussed further.
An alternative is to determine the average of the
\[ J_{ij}, r, K, K', \gamma \] and equate it to \( f^1_{ij}, r \) as before. However, one
can now return to the expression
\[
\Phi_{ij,k}^S = \sum_{K'=0}^J D_{ij, r, K', K', \gamma} \Phi_{ij,k, \gamma}^S
\]
and operate again with
\[
\Phi_{ij,k}^S \text{ to give } (\Phi_{ij,k}^S)^2 \Phi_{ij,k, \gamma}^S = \sum_{K'=0}^J D_{ij, r, K, K', \gamma} \Phi_{ij,k, \gamma}^S
\]
\[ = \sum_{K'=0}^J \sum_{K''=0}^J D_{ij, r, K, K', \gamma} D_{ij, r, K, K''} \Phi_{ij,k, \gamma}^S
\]
\[ = \sum_{K''=0}^J D_{ij, r, K, K''} \Phi_{ij,k, \gamma}^S
\]
where \( D_{ij, r, K, K', \gamma} = \sum_{K'=0}^J D_{ij, r, K, K', \gamma} \Phi_{ij,k, \gamma}^S \).

Since \( \Phi_{ij,k}^S \) is assumed to approximate \( b_{ij,r,K,\gamma} \) as \( b_{ij,r,K,\gamma} \) then one would expect that \((\Phi_{ij,k}^S)^2 \) would approximate \( b_{ij,r,k,\gamma} \) where \( D_{ij,r,k,k',\gamma} = b_{ij,r,k,\gamma} \) and \( D_{ij,r,k,k',\gamma} = b_{ij,r,k,\gamma} \).
The latter would represent a better approximation to the eigen-
functions if the process converges. Thus, if the operator \( \hat{f} \) is applied to \((\Phi_{ij,k}^S)^2 \) the result is
\[
\hat{f}(\Phi_{ij,k}^S)^2 \Phi_{ij,k, \gamma}^S \sum_{K'=0}^J D_{ij, r, K, K', \gamma} \hat{f}(\Phi_{ij,k, \gamma}^S)
\]
\[ = \sum_{K'=0}^J \left( \frac{D_{ij, r, K', K'-2, \gamma}}{D_{ij, r, K', K', \gamma}} \Phi_{k'-2, \gamma}^S \right)
\]
The coefficients of $D^j_{J, \gamma, K, K', \gamma}$ may be called $f^j_{J, \gamma, K, K', \gamma}$ and could be averaged to determine an $f^2_{J, \gamma}$.

This process could be continued and each successive $f^n_{J, \gamma}$ so computed should better represent $f^i_{J, \gamma}$ if it converges.

A variation of this latter procedure would seem to represent the best course to follow. Returning to $\hat{0}^0_{J, \gamma} \Phi^S_{J, K, \gamma}$ we saw that $\hat{0}^0_{J, \gamma} \Phi^S_{J, K, \gamma} = \sum_{K' = 0}^J D^0_{J, \gamma, K, K', \gamma} \Phi^S_{J, K', \gamma}$

and also

$$\hat{0}^0_{J, \gamma} \Phi^S_{J, K, \gamma} = \sum_{K' = 0}^J f^0_{J, \gamma, K, K', \gamma} \Phi^S_{J, K, \gamma}$$

(3.4)

where

$$f^0_{J, \gamma, K, K', \gamma} = \frac{D^0_{J, \gamma, K, K', \gamma}}{D^0_{J, \gamma, K, K', \gamma}} f_{K', -2, K'}$$

$$+ f_{K', K'} + \frac{D^0_{J, \gamma, K, K', \gamma}}{D^0_{J, \gamma, K, K', \gamma}} f_{K', K'}$$

If $\hat{0}^0_{J, \gamma}$ is allowed to act, say $n+1$ times, on $\Phi^S_{J, K, \gamma}$ the result is

$$(\hat{0}^0_{J, \gamma})^{n+1} \Phi^S_{J, K, \gamma} = \sum_{K' = 0}^J D^n_{J, \gamma, K, K', \gamma} \Phi^S_{J, K', \gamma}$$

(3.5)

and
\[ f^{(0)}_{J', \gamma} (m+1) = \sum_{J'=0}^{\infty} \Phi_{J', K', \gamma}^S = \sum_{K'=0}^{\infty} \Phi_{J', K', \gamma}^S D_{J', \gamma, K', \gamma}^n \] (3.6)

where

\[ D_{J', \gamma, K', \gamma}^n = \sum_{K''=0}^{\infty} D_{J', \gamma, K'', \gamma}^{n-1} \] (3.7)

and

\[ f_{J', \gamma, K', \gamma}^n = \frac{D_{J', \gamma, K', \gamma}^{n-2, \gamma}}{D_{J', \gamma, K', \gamma}^n} f_{K'-2, \gamma}^{n-2, \gamma} + f_{K', \gamma}^{n-2, \gamma} + \frac{D_{J', \gamma, K', \gamma}^{n+2, \gamma}}{D_{J', \gamma, K', \gamma}^n} f_{K'+2, \gamma}^{n+2, \gamma} \] (3.8)

In this form these equations are not particularly useful. It is possible to express the equations for the

\[ D_{J', \gamma, K', \gamma}^n \] in a simpler form but this is very difficult to do in general. The final form of the equation is a recursion relation involving

\[ D_{J', \gamma, K', \gamma}^m \] (m < n)

and which contains many terms. This causes the equations for

\[ f_{J', \gamma, K', \gamma}^n \] to assume a relatively simple form. This simpler form shows that in general each of the \( f_{J', \gamma, K', \gamma}^n \) for a particular \( J \) and will approach the same limit as \( n \) increases without regard to the particular \( K \) and \( K' \) involved. Since this is the case, it would appear simpler to
make a particular choice of $K$ and $K'$ and concentrate on it rather than attempt to compute averages over all $K$ and $K'$. However, because it is very difficult to show these results for an arbitrary $J$ and $\gamma$, no effort is made here to do so. Rather than this, several special cases will be considered in detail in this chapter. These will serve to illustrate the kind of results which are possible.

Before going on to discuss the special cases a word is in order on the means of determining the accuracy of the approximations. In the cases which can be solved exactly one could simply define the error in the approximation as $\delta f^\mathcal{n}_{J,\gamma} = f^\mathcal{n}_{J,\gamma} - f^\mathcal{n}_{J,\gamma}$ and compute it for each $n$. In general, however, one cannot find $f^\mathcal{n}_{J,\gamma}$ and an alternative means of determining $\delta f^\mathcal{n}_{J,\gamma}$ is needed. It is possible to compute approximate values of the invariants from $f^\mathcal{n}_{J,\gamma}$ and then compare the results of the actual invariants. Thus from a given set of $f^\mathcal{n}_{J,\gamma}$ one can compute $I^\mathcal{n}_i$ where the index $i$ identifies the invariant in question. The error in the invariant is then given as $\delta I^\mathcal{n}_i = I^\mathcal{n}_i - I^\mathcal{n}_i$. The error in the invariant can be used to compute an estimate to $\delta f^\mathcal{n}_{J,\gamma}$.

This can be seen by considering the normal form of the secular equation. This may be written as

$$f^\gamma_1 + f^\gamma_2 I_2 + \ldots + f^\gamma_{q-1} I_{q-1} + f^\gamma_q I_q = 0$$

where $q$ is the degree of the equation and the subscript $J$ has been dropped from $f$ for now. If the error in $f^\mathcal{n}_\gamma$ is defined as $\delta f^\mathcal{n}_\gamma = f^\mathcal{n}_\gamma - f^\mathcal{n}_\gamma$ one sees that $f^\mathcal{n}_\gamma = f^\mathcal{n}_\gamma + \delta f^\mathcal{n}_\gamma$. By computing
powers of \( f_\gamma \) in terms of \( f_{\gamma}^n \) and \( \delta f_{\gamma}^n \) and substituting into the normal form of the secular equation one can obtain a polynomial in \( \delta f_{\gamma}^n \). If this is done the result is

\[
F_{q+1} (\delta f_{\gamma}^n)^q + P_q (\delta f_{\gamma}^n)^q - 1 + \ldots + P_{q+1} (\delta f_{\gamma}^n)^{-1} + \ldots + P_2 \delta f_{\gamma}^n + P_1 = 0
\]

where

\[
F_1 = (f_{\gamma}^n)^q + I_1 (f_{\gamma}^n)^q - 2 + \ldots + I_i (f_{\gamma}^n)^q - 1 + \ldots + I_q - \delta f_{\gamma}^n + I_q
\]

and

\[
F_2 = \frac{dF_1}{df_{\gamma}^n}, F_3 = \frac{1}{2} \frac{dF_2}{df_{\gamma}^n}, \ldots, F_{i+1} = \frac{1}{i} \frac{dF_i}{df_{\gamma}^n}, \ldots, F_{q+1} = \frac{1}{q} \frac{dF_q}{df_{\gamma}^n}
\]

or

\[
F_{i+1} = \frac{1}{i!} \frac{d^i F_1}{d(f_{\gamma}^n)^i}
\]

This may not in general be solved exactly since its solution would give the exact solutions of the problem. One notes, however, that if \( f_{\gamma}^n \) is reasonably accurate, then \( \delta f_{\gamma}^n \) will be small enough to neglect the terms in powers of \( \delta f_{\gamma}^n \) greater than one. This leads to a linear approximation

\[
\delta f_{\gamma}^n \approx \frac{-F_1}{F_2}
\]

where

\[
F_2 = \frac{dF_1}{df_{\gamma}^n}
\]

This would seem to be a simple and reasonably accurate method of estimating \( \delta f_{\gamma}^n \).

That this approximation for \( \delta f_{\gamma}^n \) does indeed go to zero as \( n \) increases is very difficult to show in general. Rather than attempt to show this the results will simply be stated and then will later be illustrated for several particular \( J \) values.

The numerator \( F_1 \) in the approximation for \( \delta f_{\gamma}^n \) can be expressed in terms of powers of \( f_{\gamma}^n \) and the errors in the invariants rather
than the invariants themselves. The result of this is

\[ F_1 = \delta I_1^n (f^n_{\gamma})^{q-1} + \delta I_2^n (f^n_{\gamma})^{q-2} + \ldots + \delta I_1^n (f^n_{\gamma})^{q-1} + \ldots \]

\[ + \delta I_{q-1} f^n_{\gamma} + \delta I_q^n \]

where \( \delta I_1^n = I_1^n - I_1^n \). The denominator of the same expression may be expressed as

\[ F_2 = D_1^n + (q-1) \delta I_1^n (f^n_{\gamma})^{q-2} + \ldots + (q-1) \delta I_1^n (f^n_{\gamma})^{q-1} \]

\[ + \ldots + 2 \delta I_{q-2} f^n_{\gamma} + \delta I_q^n \]

where \( D_1^n = \gamma f_{\gamma} - f^n_{\gamma} \)

\[ = q(f^n_{\gamma})^{q-1} + (q-1) I_1^n (f^n_{\gamma})^{q-2} + \ldots + (q-1) I_1^n (f^n_{\gamma})^{q-1} \]

\[ + \ldots + 2 I_{q-2} f^n_{\gamma} + I_q^n \].

The term \( D^n_{\gamma} \) appearing in the denominator will not go to zero for any values of the asymmetry parameter \( b \) while the errors in the invariants which appear in both \( F_1 \) and \( F_2 \) will go to zero for all values of \( b \) when \( n \) becomes large. This then causes the estimate \( \delta f^n_{\gamma} \approx \frac{-1}{F_2} \) to vanish as \( n \) increases without limit.

As stated above all of this is difficult to prove, so specific results will be shown following the determination of \( f^n_{J, \gamma} \) for several different \( J \) values. Attention will be confined to states that transform as \( A \) for even \( J \) values. All others can be seen to follow in the same manner.

Approximations to the \( f^n_{J, \gamma} \) for \( J=2 \)

In this case the secular equation is just a quadratic and the exact solutions are readily found. The \( K \) values that appear in the expanded form for the eigenfunctions are just \( K=0 \) and \( 2 \). The eigenfunctions are given by

\[ \psi_{\pm 2} = b_{\pm 20} \phi_{0}^{\pm} + b_{\pm 22} \phi_{2}^{\pm} \]
where the subscripts for J=2 and \( \Upsilon = 0 \) have been omitted for now.

The inverted form of this expansion is then

\[
\varphi^s_K = b_{2,K} \psi^a_2 + b_{-2,K} \psi^a_{-2} \quad (K=0,2)
\]

The projection operators become

\[
\hat{\Omega}^{+2} = \frac{\hat{\Omega} - \hat{\Omega}_{+2}}{\hat{\Omega}_{+2} - \hat{\Omega} - 2}
\]

where again the J index has been dropped for now.

Remembering that \( \mathcal{T} = \pm \frac{\pi}{2} \) one may now apply \( \hat{\Omega} \) to \( \varphi^s_0 \)

with the result that

\[
\hat{\Omega} \varphi^s_0 = \frac{(\hat{\Omega} - \hat{\Omega}')}{(\hat{\Omega}' - \hat{\Omega})} \varphi^s_0
\]

\[
= \frac{1}{\hat{\Omega}' - \hat{\Omega}} \left( (\hat{\Omega}'_0 - \hat{\Omega}') \varphi^s_0 + \hat{\Omega}'_0 \varphi^s_2 \right)
\]

\[
= \frac{1}{\hat{\Omega}' - \hat{\Omega}} \left( -(2 + \hat{\Omega}') \varphi^s_0 + 2\sqrt{3} \ b \ \varphi^s_2 \right)
\]

\[
= D_{\mathcal{T}00} \varphi^s_0 + D_{\mathcal{T}02} \varphi^s_2
\]

Also

\[
\hat{\Omega} \varphi^s_0 = \hat{\Omega}(D_{\mathcal{T}00} \varphi^s_0 + D_{\mathcal{T}02} \varphi^s_2)
\]

\[
= D_{\mathcal{T}00} \left( \hat{\Omega}'_0 \varphi^s_0 + \hat{\Omega}'_2 \varphi^s_2 \right) + D_{\mathcal{T}02} \left( \hat{\Omega}'_0 \varphi^s_0 + \hat{\Omega}'_2 \varphi^s_2 \right)
\]

\[
= (\hat{\Omega}'_0 + \hat{\Omega}'_2 \frac{D_{\mathcal{T}02}}{D_{\mathcal{T}00}}) D_{\mathcal{T}00} \varphi^s_0 + (\hat{\Omega}'_0 + \hat{\Omega}'_2 \frac{D_{\mathcal{T}00}}{D_{\mathcal{T}02}}) D_{\mathcal{T}02} \varphi^s_2
\]

\[
= \hat{\Omega} \varphi^a_{\mathcal{T}K} = \hat{\Omega} (D_{\mathcal{T}00} \varphi^s_0 + D_{\mathcal{T}02} \varphi^s_2)
\]

or \( \hat{\Omega} = \hat{\Omega} \varphi^s_0 + \hat{\Omega} \varphi^s_2 \), \( \hat{\Omega} = \hat{\Omega} \varphi^s_0 + \hat{\Omega} \varphi^s_2 \)

The second of these gives

\[
\hat{\Omega} = \hat{\Omega} - 2 + 2 = -\hat{\Omega} \quad \text{or} \quad \hat{\Omega} + \hat{\Omega} = 0
\]

while the first gives
\[ f_{\gamma} = -2 - \frac{12b^2}{f_{\gamma} + 2} \]

or

\[ f_{\gamma} + 2 = -\frac{12b^2}{f_{\gamma} + 2} \]

which becomes \( f_\gamma f_{\gamma'} + 2(f_\gamma + f_{\gamma'}) + 4(1 + 3b^2) = 0 \).

These are just the invariants of the secular equation and can be written as

\[ I_1 = -\sum f_\gamma = 0, \quad I_2 = f_{\gamma} f_{\gamma'} = -4(1 + 3b^2). \]

Thus \( f_{-2} = -f_2 \) and \( f_2^2 = 4(1 + 3b^2) \) so that \( f_{\pm2} = \pm 2(1 + 3b^2)^{1/2} \).

The total energies of these states are then given as

\[ E_{\pm2}(a, b, c) = 6ac + 2a \pm 2a(1 + 3b^2)^{1/2} \]

In the limits as \( b \) goes to 0 and -1 the energies become

\[ E_{\pm2}(a, 0, c) = 6ac + ak^2 \begin{cases} \gamma = 2, \quad K = 2 \\ \gamma = -2, \quad K = 0 \end{cases} \]

and

\[ E_{\pm2}(a, -1, c) = 6ac - 2ak^2 \begin{cases} \gamma = 2, \quad K = 0 \\ \gamma = -2, \quad K = 2 \end{cases} \]

or \( f_{\pm2}(0) = \pm 2, \quad f_{\pm2}(-1) = \pm 4 \). An obvious choice for approximation to \( f_{\gamma} \) is \( f_0^{\pm2} = \pm 2(1 - b) \) or \( f_0^{\pm2} = \pm 2(1 + b^2) \). Eventually the former one of these will be used even though the latter is a more accurate choice. These have been chosen so that \( I_1^0 = f_{\pm2}^0 + f_{\pm2}^0 = 0 \) and \( I_2^0 = f_{+2}^0 f_{+2}^0 = -4(1 - b)^2 \) for the former choice of \( f_{\gamma}^0 \). The error between the actual function of \( f_{\gamma} \) and the approximate functions \( f_{\gamma}^0 \) will be designated as

\[ \delta f_{\gamma}^0 = f_{\gamma} - f_{\gamma}^0 \]

while the error between the actual invariants and those computed from \( f_{\gamma}^0 \) will be

\[ \delta I_1^0 = I_1 - I_1^0 = 0, \quad \delta I_2^0 = I_2 - I_2^0 = -8b(1 + b). \]
To see how the approximations work here one can now consider the approximations to the projection operators which are
\[ \hat{O}_r^0 = \frac{f - f^0_r}{f - f^0_r} = \frac{f^0 - f^0_r}{D^0_r} \text{ where } r \neq r' \text{ and } D^0_r = f^0_r - f^0_r = 2f^0_r. \]

It is necessary to calculate \((\hat{O}_r^0)^{n+1} (f) \varphi^s_0\) and \((\hat{O}_r^0)^{n+1} (f) \varphi^s_2\).

To begin with one gets

\[ \hat{O}_r^0 \varphi^s_0 = D^0_r \varphi^s_0 + D^0_r \varphi^s_2 \]
\[ \hat{O}_r^0 \varphi^s_2 = D^0_r \varphi^s_0 + D^0_r \varphi^s_2 \]

where

\[ D^0_{r00} = \frac{-f^0_r + 2}{D^0_r} = \frac{f^0 - 2}{D^0_r} \]
\[ D^0_{r22} = \frac{-f^0_r + 2}{D^0_r} = \frac{f^0 + 2}{D^0_r} \]
\[ D^0_{r02} = D^0_{r20} = \frac{2\sqrt{3} b}{D^0_r} \]

Repeating this gives

\[ (\hat{O}_r^0)^2 \varphi^s_0 = D^1_{r00} \varphi^s_0 + D^1_{r02} \varphi^s_2 \]
\[ (\hat{O}_r^0)^2 \varphi^s_2 = D^1_{r20} \varphi^s_0 + D^1_{r22} \varphi^s_2 \]

where

\[ D^1_{r00} = (D^0_{r00})^2 + D^0_{r02} D^0_{r20} = D^0_{r00} \left( D^0_{r00} + \frac{(D^0_{r02})^2}{D^0_{r00}} \right) \]
\[ = \frac{D^0_{r00}}{D^0_r} \left( f^0_r - 2 + \frac{12b^2}{f^0_r - 2} \right) \]
\[
\begin{align*}
\frac{d^0_{\gamma 00}}{d^0_\gamma} & = \frac{d^0_{\gamma 00}}{d^0_\gamma} \left( 2d^0_\gamma - \left(d^0_\gamma + 2\right) + \frac{12b^2}{d^0_\gamma - 2} \right) \\
& = \frac{d^0_{\gamma 00}}{d^0_\gamma} \left( d^0_\gamma - \frac{1}{d^0_\gamma - 2} \left( (d^0_\gamma + 2) (d^0_\gamma - 2) - 12b^2 \right) \right) \\
& = \frac{d^0_{\gamma 00}}{d^0_\gamma} \left( d^0_\gamma - \frac{1}{d^0_\gamma - 2} \left( (d^0_\gamma)^2 - 4 (1 + 3b^2) \right) \right) \\
& = \frac{d^0_{\gamma 00}}{d^0_\gamma} \left( d^0_\gamma - \frac{1}{d^0_\gamma - 2} (I_2 - I_2^0) \right) = d^0_{\gamma 00} \left( 1 - \frac{S_{12}^0}{d^0_\gamma d^0_{\gamma 00}} \right) \\
D^1_{\gamma 22} &= \left( d^0_{\gamma 02} \right)^2 \left( d^0_{\gamma 22} \right)^2 = \left( d^0_{\gamma 22} + \frac{\left( d^0_{\gamma 22} \right)^2}{d^0_{\gamma 02}} \right) d^1_{\gamma 22} \\
& = d^0_{\gamma 22} \left( 1 - \frac{S_{12}^0}{d^0_{\gamma 02}} \right) \\
D^1_{\gamma 02} &= D^1_{\gamma 20} = d^0_{\gamma 00} d^0_{\gamma 02} + d^0_{\gamma 02} d^0_{\gamma 22} = d^0_{\gamma 02} \left( d^0_{\gamma 00} + d^0_{\gamma 22} \right) \\
& = d^0_{\gamma 02}
\end{align*}
\]

Continuing this

\[
(0^0_\gamma)^3 \varphi_0^s = d^2_{\gamma 00} \varphi_0^s + d^2_{\gamma 02} \varphi_2^s
\]

\[
(0^0_\gamma)^3 \varphi_2^s = d^2_{\gamma 20} \varphi_0^s + d^2_{\gamma 22} \varphi_2^s
\]

where

\[
D^2_{\gamma 00} = D^1_{\gamma 00} d^0_{\gamma 02} + d^1_{\gamma 20} d^0_{\gamma 02} = d^0_{\gamma 00} \left( d^1_{\gamma 00} + \frac{d^1_{\gamma 02} d^0_{\gamma 02}}{d^0_{\gamma 00}} \right) \\
& = d^0_{\gamma 00} \left( d^0_{\gamma 00} \left( 1 - \frac{S_{12}^0}{d^0_{\gamma 02}} \right) + \frac{\left( d^0_{\gamma 02} \right)^3}{d^0_{\gamma 00}} \right) \\
& = d^0_{\gamma 00} \left( d^0_{\gamma 00} + \frac{(d^0_{\gamma 02})^2}{d^0_{\gamma 00}} - \frac{S_{12}^0}{\left( d^0_{\gamma 02} \right)^3} \right) = d^1_{\gamma 00} - \frac{S_{12}^0}{\left( d^0_{\gamma 02} \right)^3} d^0_{\gamma 00}
\]
\[
\begin{align*}
\mathcal{D}^2_{\gamma 22} &= \mathcal{D}^1_{\gamma 20} \mathcal{D}^0_{\gamma 02} + \mathcal{D}^1_{\gamma 22} \mathcal{D}^0_{\gamma 22} = \mathcal{D}^0_{\gamma 22} \left( \frac{\mathcal{D}^1_{\gamma 22} + \mathcal{D}^1_{\gamma 02} \mathcal{D}^0_{\gamma 02}}{\mathcal{D}^0_{\gamma 22}} \right) \\
&= \mathcal{D}^0_{\gamma 22} \left( \mathcal{D}^0_{\gamma 22} \left( 1 - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \right) + \left( \frac{\mathcal{D}^0_{\gamma 02}}{\mathcal{D}^0_{\gamma 22}} \right)^2 \right) \\
&= \mathcal{D}^0_{\gamma 22} \left( \mathcal{D}^0_{\gamma 22} + \frac{(\mathcal{D}^0_{\gamma 02})^2}{(\mathcal{D}^0_{\gamma 22})^2} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \right) = \mathcal{D}^1_{\gamma 22} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \mathcal{D}^0_{\gamma 22} \\
\mathcal{D}^2_{\gamma 02} &= \mathcal{D}^2_{\gamma 20} = \mathcal{D}^1_{\gamma 00} \mathcal{D}^0_{\gamma 02} + \mathcal{D}^1_{\gamma 02} \mathcal{D}^0_{\gamma 22} = \mathcal{D}^0_{\gamma 02} \left( \mathcal{D}^1_{\gamma 00} + \mathcal{D}^1_{\gamma 22} \right) \\
&= \mathcal{D}^0_{\gamma 02} \left( \mathcal{D}^0_{\gamma 02} + \mathcal{D}^0_{\gamma 22} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \right) = \mathcal{D}^0_{\gamma 02} \left( 1 - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \right) \\
&= \mathcal{D}^0_{\gamma 02} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \mathcal{D}^0_{\gamma 02}.
\end{align*}
\]

If this process is continued one finds that

\[
\begin{align*}
(0_{\gamma})^{n+1} \phi^s_0 &= \mathcal{D}^n_{\gamma 00} \phi^s_0 + \mathcal{D}^n_{\gamma 02} \phi^s_2 \\
(0_{\gamma})^{n+1} \phi^s_2 &= \mathcal{D}^n_{\gamma 20} \phi^s_0 + \mathcal{D}^n_{\gamma 22} \phi^s_2
\end{align*}
\]

where

\[
\begin{align*}
\mathcal{D}^n_{\gamma 02} &= \mathcal{D}^n_{\gamma 20} = \mathcal{D}^{n-1}_{\gamma 00} \mathcal{D}^0_{\gamma 02} + \mathcal{D}^{n-1}_{\gamma 02} \mathcal{D}^0_{\gamma 22} = \mathcal{D}^{n-1}_{\gamma 02} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \mathcal{D}^{n-2}_{\gamma 02} \quad (3.13a) \\
\mathcal{D}^n_{\gamma 00} &= \mathcal{D}^{n-1}_{\gamma 00} \mathcal{D}^0_{\gamma 02} + \mathcal{D}^{n-1}_{\gamma 20} \mathcal{D}^0_{\gamma 22} = \mathcal{D}^{n-1}_{\gamma 00} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \mathcal{D}^{n-2}_{\gamma 00} \quad (3.13b) \\
\mathcal{D}^n_{\gamma 22} &= \mathcal{D}^{n-1}_{\gamma 20} \mathcal{D}^0_{\gamma 02} + \mathcal{D}^{n-1}_{\gamma 22} \mathcal{D}^0_{\gamma 22} = \mathcal{D}^{n-1}_{\gamma 22} - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \mathcal{D}^{n-2}_{\gamma 22} \quad (3.13c)
\end{align*}
\]

The last two of these may also be written as

\[
\begin{align*}
\mathcal{D}^n_{\gamma 00} &= \frac{\mathcal{D}^0_{\gamma 00}}{\mathcal{D}^0_{\gamma 02}} \mathcal{D}^n_{\gamma 02} \left( 1 - \frac{\delta^1_{\gamma 2}}{(\mathcal{D}^0_{\gamma 22})^2} \frac{\mathcal{D}^{n-1}_{\gamma 02}}{\mathcal{D}^0_{\gamma 02}} \right)
\end{align*}
\]
\[ D_{\gamma 22}^n = \frac{D_{\gamma 22}^0}{D_{\gamma 02}^0} \left( 1 - \frac{I_2^0}{D_{\gamma 02}^0} \right) \left( \frac{D_{\gamma 02}^{n-1}}{D_{\gamma 02}^0} \right) \]

It is now necessary to compute the \( \gamma, \gamma', K, K' \) whose form can be given as

\[ \gamma, K, K' = \frac{D_{\gamma, K, K'}^n}{D_{\gamma, K, K'}^0} \]

For \( n = 0 \) these become

\[ f_{\gamma 00} = f_{\gamma 00} + \frac{D_{\gamma 02}^0}{D_{\gamma 00}^0} f_{20} = -2 + 2\sqrt{3} b \]
\[ f_{\gamma 02} = f_{\gamma 02} + \frac{D_{\gamma 00}^0}{D_{\gamma 02}^0} f_{02} + f_{22} = 2 + 2\sqrt{3} b \]
\[ f_{\gamma 22} = f_{\gamma 22} + \frac{D_{\gamma 22}^0}{D_{\gamma 22}^0} f_{02} + f_{22} = 2 + 2\sqrt{3} b \]

For \( n = 1 \)

\[ D_{\gamma 22}^1 = \frac{D_{\gamma 22}^0}{D_{\gamma 02}^0} \left( 1 - \frac{I_2^0}{D_{\gamma 02}^0} \right) \left( \frac{D_{\gamma 02}^{1-1}}{D_{\gamma 02}^0} \right) \]

\[ \gamma, K, K' = \frac{D_{\gamma, K, K'}^1}{D_{\gamma, K, K'}^0} \]

For \( n = 0 \) these become

\[ f_{\gamma 00} = f_{\gamma 00} + \frac{D_{\gamma 02}^0}{D_{\gamma 00}^0} f_{20} = \frac{-2(f_{\gamma}^0 - 2) + 12b^2}{f_{\gamma}^0 - 2} \]
\[ f_{\gamma 02} = f_{\gamma 02} + \frac{D_{\gamma 00}^0}{D_{\gamma 02}^0} f_{02} + f_{22} = \frac{-2f_{\gamma}^0 + 4(1+3b^2)}{f_{\gamma}^0 - 2} \]
\[ f_{\gamma 22} = f_{\gamma 22} + \frac{D_{\gamma 22}^0}{D_{\gamma 22}^0} f_{02} + f_{22} = \frac{2f_{\gamma}^0 + 4(1+3b^2)}{f_{\gamma}^0 + 2} \]

For \( n = 1 \)
\[
\begin{align*}
\frac{\mathcal{I}_0}{\mathcal{I}_{700}} &= \frac{\mathcal{I}_0 + \frac{\mathcal{I}_{702}}{\mathcal{I}_{700}}}{\mathcal{I}_{700}} = -2 + 2\sqrt{3}b \frac{\mathcal{I}_{702}}{\mathcal{I}_{700}}, \\
-2\mathcal{I}^0_{700} \left(1 - \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2}\right) + 2\sqrt{3}b\mathcal{I}^0_{702} &= -2\mathcal{I}^0_{700} + 2\sqrt{3}b\mathcal{I}^0_{702} + \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2}, \\
\frac{\mathcal{I}^0_{700} \mathcal{I}^0_{702} + 2\mathcal{I}^0_{12}}{(D^0_{700})^2} &= \mathcal{I}^0_{700} \left(1 - \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2}\right), \\
\mathcal{I}^0_{700} - \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2} &= 0, \\
\mathcal{I}^0_{700} - \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2} &= 0, \\
\mathcal{I}^0_{700} - \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2} &= 0, \\
\mathcal{I}^0_{700} - \frac{\mathcal{I}^0_{12}}{(D^0_{700})^2} &= 0.
\end{align*}
\]
while

\[
\frac{r_1}{r_{02}} = \frac{r_1}{r_{20}} = D_{r_{02}}^1 \quad r_0 + r_2 = 2 + 2\sqrt{3} \frac{D_{r_{00}}^1}{D_{r_{02}}^1} = 2n_{r_{02}} + 2\sqrt{3}bD_{r_{00}}^1
\]

\[
= 2D_{r_{02}}^0 + 2\sqrt{3} \frac{D_{r_{00}}^0}{D_{r_{02}}^0} - 2\sqrt{3}b \frac{\delta_{r_{22}}^0}{(D_{r_{22}}^0)^2} = 2 + \frac{r_0}{r_2} - 2 - \frac{\delta_{r_{22}}^0}{D_{r_{22}}^0}
\]

\[
d_{r_{02}}^0
\]

\[
= r_2 \left( 1 - \frac{\delta_{r_{22}}^0}{r_0 D_{r_{22}}^0} \right)
\]

\[
\frac{r_1}{r_{22}} = \frac{r_1}{r_{20}} \quad r_0 + r_2 = r_2 \left( 1 - \frac{\delta_{r_{22}}^0}{r_0 D_{r_{22}}^0} \right)
\]

For \( n \geq 2 \) one sees that

\[
\frac{r_n}{r_{02}} = \frac{r_n}{r_{20}} = D_{r_{02}}^n \quad r_0 + r_2 = 2 + 2\sqrt{3} \frac{D_{r_{00}}^n}{D_{r_{02}}^n} = 2n_{r_{02}} + 2\sqrt{3}bD_{r_{00}}^n
\]

\[
= 2 \left( D_{r_{02}}^{n-1} - \frac{\delta_{r_{22}}^0}{(D_{r_{22}}^0)^2} D_{r_{02}}^{n-2} \right) + 2\sqrt{3}b \left( D_{r_{00}}^{n-1} - \frac{\delta_{r_{22}}^0}{(D_{r_{22}}^0)^2} D_{r_{00}}^{n-2} \right)
\]

\[
d_{r_{02}}^n
\]

\[
= 2n_{r_{02}} + 2\sqrt{3} \frac{D_{r_{00}}^{n-1}}{D_{r_{02}}^{n-1}} - \frac{\delta_{r_{22}}^0}{(D_{r_{22}}^0)^2} \left( 2n_{r_{02}}^{n-2} + 2\sqrt{3}b D_{r_{00}}^{n-2} \right)
\]

\[
d_{r_{02}}^n
\]

\[
= \frac{r_n}{r_{02}} \frac{D_{r_{02}}^{n-1}}{D_{r_{02}}^{n-1}} - \frac{\delta_{r_{22}}^0}{(D_{r_{22}}^0)^2} \frac{r_n^{n-2} D_{r_{02}}^{n-2}}{D_{r_{02}}^{n-2}}
\]
This may also be expressed as

\[
\frac{f_n}{\eta_0} = \frac{2D_{\eta_0}^0 + 2\sqrt{3}bD_{\eta_0}^0}{D_{\eta_0}^0} = \frac{2D_{\eta_0}^0 + 2\sqrt{3}bD_{\eta_0}^0}{(D_{\eta}^0)^2} \left( 1 - \frac{\delta I_2^0}{f_{\eta_0}^0} \right) \frac{D_{\eta_0}^0}{\eta_0}
\]

The other \( f_{\eta, K, K'} \) may be given as

\[
f_{\eta_0} = f_{\eta_0}^0 \left( 1 - \frac{\delta I_2^0}{f_{\eta_0}^0} \right) \frac{D_{\eta_0}^0}{\eta_0}
\]

\[
f_{\eta_22} = f_{\eta_22}^0 \left( 1 - \frac{\delta I_2^0}{f_{\eta_22}^0} \right) \frac{D_{\eta_22}^0}{\eta_22}
\]

This has shown that a simple recursion relation results for the \( D_{\eta, K, K'}^n \) and also for the \( f_{\eta, K, K'}^n \). These may be summarized
as \( D^n_{\gamma, K, K'} = D^{n-1}_{\gamma, K, K'} - \frac{\delta I^0_2}{(D^0_{\gamma})^2} D^{n-2}_{\gamma, K, K'} \)

\[ = D^0_{\gamma, K, K'} \frac{D^n_{\gamma, K, K'}}{D^0_{\gamma, K, K'}} \left( 1 - \frac{\delta I^0_2}{(D^0_{\gamma})^2 D^0_{\gamma, K, K'}} \right) \frac{D^{n-1}_{\gamma, K, K'}}{D^0_{\gamma, K, K'}} \)

and \( r^n_{\gamma, K, K'} \)

\[ = \left( 1 - \frac{\delta I^0_2}{(D_{\gamma})^2} \frac{D^{n-1}_{\gamma, K, K'}}{D^n_{\gamma, K, K'}} \right). \]

It is easily seen from this that all \( r^n_{\gamma, K, K'} \) approach the same limit as \( n \) gets very large. This is apparent from expressing the recursion relation for \( D^n_{\gamma, K, K'} \) as

\[ D^n_{\gamma, K, K'} = 1 + \frac{\delta I^0_2}{(D_{\gamma})^2} D^{n-1}_{\gamma, K, K'} - \frac{\delta I^0_2}{2(D_{\gamma})^2} D^{n-2}_{\gamma, K, K'} \]

Now define \( R_{n, 1} = D^n_{\gamma, K, K'} \), \( R_{n, m} = D^n_{\gamma, K, K'} \) and one obtains

\[ R_{n, 1} = 1 + \frac{\delta I^0_2}{2(D_{\gamma})^2} R_{n-1, 1} R_{n, 1}. \]

As \( n \) increases without limit, one sees that \( R_{n-1, 1} \rightarrow R_{n, 1} \) so that the recursion relation becomes

\[ R = 1 + \frac{\delta I^0_2}{2(D_{\gamma})^2} R^2. \]

If we now define \( \alpha = \frac{\delta I^0_2}{2(D_{\gamma})^2} \), this may be written as \( R^2 - R + 1 = 0 \).

The solutions to this equation are \( R = \frac{1}{2\alpha} \pm \frac{1}{2\alpha} \sqrt{1 - 4\alpha} \).
These may be substituted into the expression for \( f_{J,\gamma}^n, K, K' \) which

as \( n \to \infty \) becomes

\[
\begin{align*}
f_{J,\gamma}^0 (1 - 2 \alpha K) &= f_{J,\gamma}^0 (1 - 1 + \frac{1}{1 - 4\alpha}) \\
&= \pm f_{J,\gamma}^0 \sqrt{1 - 4\alpha} = \pm f_{J,\gamma}^0 \sqrt{1 - \frac{1}{1 - 4\alpha}} = \pm f_{J,\gamma}^0 \sqrt{1 - \frac{5I_2^0}{1 - \frac{1}{2}}} = \pm \sqrt{\left(\frac{f_{J,\gamma}^0}{f_{J,\gamma}^0}\right)^2 - \frac{5I_2^0}{2}} \\
&= \pm \sqrt{-I_2} = \pm 2 (1+3b^2)^{\frac{1}{2}}
\end{align*}
\]

which are just the exact solutions mentioned earlier where the

plus sign goes with \( \gamma = 2 \) and the minus sign with \( \gamma = -2 \). Note

that this form of the solution is independent of the \( K \) and \( K' \)

used for the \( f_{J,\gamma}^n, K, K' \).

It would be well to summarize what has been done for

this case. The approximations to the projection operators can

be made by defining a set of functions \( f_{J,\gamma}^0 \) which are readily

found from the limits \( b = 0 \) and \( -1 \). This led to

\[
(\hat{0}_{J,\gamma}) = \frac{\hat{f} - f_{J,\gamma}^0}{f_{J,\gamma}^0}.
\]

Then the effect of \( (\hat{0}_{J,\gamma})^{n+1} \) on \( \phi_{J,\gamma}^s, K, 0 \)

was determined and gave

\[
(\hat{0}_{J,\gamma})^{n+1} \phi_{J,\gamma}^s, K, 0 = \sum_{K',0} D_{J,\gamma}^{n-1} \phi_{J,\gamma}^s, K', 0 \phi_{J,\gamma}^s, K', 0
\]

where \( D_{J,\gamma}^{n-1} \phi_{J,\gamma}^s, K', 0 = \frac{\delta I_2^0}{(D_{J,\gamma}^0)^2} D_{J,\gamma}^{n-2} \phi_{J,\gamma}^s, K, K', 0 \).

Then operation with \( \hat{f} \) on both sides of the expression for

\( (\hat{0}_{J,\gamma})^{n+1} \phi_{J,\gamma}^s, K, 0 \) gave expression for the \( f_{J,\gamma}^n, K, K', 0 \) as coefficients

of the \( D_{J,\gamma}^{n-1} \phi_{J,\gamma}^s, K', 0 \). These expressions reduced to

\[
f_{J,\gamma}^n, K, K', 0 = f_{J,\gamma}^0 \left( 1 - \frac{\delta I_2^0}{f_{J,\gamma}^0} \frac{D_{J,\gamma}^{n-1}}{D_{J,\gamma}^0} \right) \right) \frac{\phi_{J,\gamma}^s, K', 0}{\phi_{J,\gamma}^s, K, 0}
\]

which in the limit

as \( n \) gets large go over to the exact solutions \( f_{J,\gamma}^* \).
This shows that since all $f^\infty_{J,\gamma, K, K', 0}$ approach the same limit it would be as well to choose an arbitrary pair of values $K$ and $K'$ and compute its $f^\infty_{J,\gamma, K, K', 0}$ calling it $f^\infty_{J,\gamma}$ rather than computing the average over all $K$ and $K'$ as mentioned earlier. There are two choices of $K$ and $K'$ which in all cases are easier to work with than are the other choices and which are then more desirable to use than the others. These choices are $K = 0, K' = J$ and $K = J, K' = 0$. Both of these give the same results and from hereon only the choice $K = 0, K' = J$ will be used.

Looking ahead for a moment to higher $J$ values and to states that transform according to other irreducible representations, there are several comments that would seem to be in order. The results are of a similar form, though of course, more complicated. The recursion relation for the $D^n_{J,\gamma, K, K', Y}$ will always involve at least one more term than the degree of the secular equation for that set of states, since the solution of the recursion relation as $n$ gets large becomes the exact solution to the problem. The approximations $f^\infty_{J,\gamma, K, K', Y}$ will also be somewhat more complicated. Also, there is always a choice of $K$ and $K'$ which is easier to work with than all other choices, though it is not always $K = 0, K' = J$, but rather $K = \text{minimum } K$ value appearing in the expansion while $K' = \text{maximum } K$ value appearing in the expansion.

At this point it would seem appropriate to return to the $J = 2, \gamma = \pm 2$ approximations and examine them more closely.
The n-th approximation is now given by

$$x^n_T = x^0_T + \frac{n-1}{2(x_T^0)^2} \frac{D_{\gamma 02}}{D_{\gamma 02}} = x^0_T \left( 1 - \frac{\delta I_2^n}{x_T^0} \frac{D_{\gamma 02}}{D_{\gamma 02}} \right)$$

$$= x^0_T \left( 1 - \frac{\delta I_2^0}{2(x_T^0)^2} \frac{D_{\gamma 02}}{D_{\gamma 02}} \right) = x^0_T \left( 1 + \frac{\delta I_2^0}{2x_T^0} \frac{D_{\gamma 02}}{D_{\gamma 02}} \right)$$

where $$I_2^0 = x_T^0 x_T^0 = -(x_T^0)^2$$.

In order to compare the approximations with the exact solutions, there are several quantities that need to be considered. In this simple case, since the exact solutions are easily determined, one can define the error in $$x^n_T$$ as $$\delta x^n_T = x_T - x^n_T$$ which is readily computed once $$x_T^0$$ is chosen.

One sees that the approximate equation for the error in $$x^n_T$$ reduces to

$$\delta x^n_T = \frac{(x_T^n)^2 + I_2^n}{2x_T^n} = \frac{-\delta I_2^n}{2x_T^n}.$$

To evaluate the approximations one then needs to choose $$x_T^0$$, compute

$$D_{\gamma 02}^n = D_{\gamma 02}^{n-1} - \delta I_2^0 \frac{D_{\gamma 02}^{n-2}}{(D_{\gamma 02}^0)^2},$$

find $$x_T^n = x_T^0 \left( 1 - \frac{\delta I_2^0}{x_T^0} \frac{D_{\gamma 02}^{n-1}}{D_{\gamma 02}^{n-1}} \right)$$

and then compute the invariants $$I^n_1$$ and $$I^n_2$$. Note that $$I^n_1 = I_1$$ or $$\delta I^n_1 = 0$$. The invariant $$I^n_2 \neq I_2$$ and is given as

$$I^n_2 = x_T^n x_T^n = x_T^0 x_T^0 \left( 1 + \frac{\delta I_2^0}{2x_T^0} \frac{D_{\gamma 02}^n}{D_{\gamma 02}^n} \right)^2.$$
\[ I_2 \left( \frac{\delta I_2^0}{I_2} \right) \frac{D^{n-1}}{\gamma_{02}} + \left( \frac{\delta I_2^0}{4I_2} \right)^2 \left( \frac{D^{n-1}}{\gamma_{02}} \right)^2 \]

and \( \delta I_2^n = I_2 - I_2^n = \delta I_2^0 - \delta I_2 \frac{D^{n-1}}{\gamma_{02}} - \left( \frac{\delta I_2^0}{4I_2} \right)^2 \left( \frac{D^{n-1}}{\gamma_{02}} \right)^2 \)

\[ = \frac{\delta I_2^0}{(D_{\gamma_{02}}^{n})^2} \left( \frac{D^{n-1}}{\gamma_{02}} \left( \frac{D^{n-1}}{\gamma_{02}} - \frac{D^{n-1}}{\gamma_{02}} \right) - \delta I_2^0 \left( \frac{D^{n-1}}{\gamma_{02}} \right)^2 \right) \]

\[ = \frac{(\delta I_2^0)^2}{4I_2^0 (D_{\gamma_{02}}^{n})^2} \left( \frac{D^{n-1}}{\gamma_{02}} \left( \frac{D^{n-1}}{\gamma_{02}} - \frac{D^{n-1}}{\gamma_{02}} \right) + \frac{\delta I_2^0}{4I_2} (D_{\gamma_{02}}^{n-2}) \right) \]

\[ = \frac{(-\delta I_2^0)^3}{(4I_2^0 (D_{\gamma_{02}}^{n})^2} \left( \frac{D^{n-1}}{\gamma_{02}} \left( \frac{D^{n-1}}{\gamma_{02}} - \frac{D^{n-1}}{\gamma_{02}} \right) \right) \]

\[ \times (-1)^{p+1} (\delta I_2^0)^{p+1} \frac{D^{n-p+1}}{4I_2^0 (D_{\gamma_{02}}^{n})^2} \left( \frac{D^{n-p-1}}{\gamma_{02}} - \frac{D^{n-p-1}}{\gamma_{02}} \right) \]
\[
\begin{align*}
&= \frac{(-1)^n (\delta I_2^n)}{D_{\gamma 02}^{n-1}} \left[ D_{\gamma 02}^2 n_\gamma^0 - (D_{\gamma 02}^1)^2 \right] \\
&= \frac{(-1)^n (\delta I_2^0)^n}{(4I_2^0)^{n-1}} \left( \left( \frac{D_{\gamma 02}^1 + \delta I_2^0}{4I_2^0} \right) D_{\gamma 02}^0 - (D_{\gamma 02}^1)^2 \right) \\
&= \frac{(-1)^n (\delta I_2^0)^{n+1}}{(4I_2^0)^n} \left( \frac{(D_{\gamma 02}^0)^2}{(4I_2^0)^2} \right) \delta I_2^0 \left( -\frac{I_2^0}{4I_2^0} \right) n \left( \frac{(D_{\gamma 02}^n)^2}{(4I_2^0)^2} \right) \quad (3.5)
\end{align*}
\]

From this one can then compute \( \delta \xi_\gamma^2 = -\frac{\delta I_2^n}{2I_\gamma^2} \).

In order to see how these approximations actually work, it is now necessary to use a specific form for \( I_\gamma^0 \) in these expressions and evaluate them as functions of the asymmetry parameter \( b \). To do this the linear approximation \( I_\gamma^0 = I_\gamma^0 = \delta I_\gamma^2 (1-b) \)
is used. Since the error in \( I_\gamma^2 \) is just minus the error in \( I_\gamma^0 \), this is done only for \( f_\gamma^2 \). First note that \( I_2^0 = I_2^0 f_\gamma^2 \\
= -(f_\gamma^2)^2 = -4(1-b)^2 \) and \( \delta I_2^0 = I_2^0 - I_2^0 = -4(1+3b^2) \cdot 4(1-b)^2 = -8b(1+b) \).
One may then determine the \( D_\gamma^n \) as follows

\[
\begin{align*}
D_\gamma^n &= D_\gamma^{n-1} + \frac{\delta I_2^0}{4I_2^0} D_\gamma^{n-2} \\
&= \frac{D_\gamma^{n-2}}{4I_2^0} + \frac{\delta I_2^0}{4I_2^0} \left[ D_\gamma^{n-3} + \frac{\delta I_2^0}{4I_2^0} \left( \frac{D_\gamma^{n-4}}{4I_2^0} + \frac{\delta I_2^0}{4I_2^0} \right) \right] \\
&= \frac{D_\gamma^{n-2}}{4I_2^0} + 2 \frac{\delta I_2^0}{4I_2^0} \frac{D_\gamma^{n-3}}{4I_2^0} + \frac{(\delta I_2^0)^2}{(4I_2^0)^2} \frac{D_\gamma^{n-4}}{4I_2^0} 
\end{align*}
\]
\[ D_0^{(0)} = \sum_{p=0}^{n-1} \frac{(n-p)!}{(n-2p)!} \frac{(\delta I_2^0)^p}{(4I_2^0)^p} \]
\[ D^0_{\gamma 2} = \frac{2\sqrt{3}b}{4(1-b)} \]
\[ D^1_{\gamma 02} = D^0_{\gamma 02} \]
\[ D^2_{\gamma 02} = D^0_{\gamma 02} \left( 1 + \frac{\delta_{\gamma 2}^0}{4I_2^0} \right) \]
\[ D^3_{\gamma 02} = D^0_{\gamma 02} \left( 1 + \frac{2\delta_{\gamma 2}^0}{4I_2^0} \right) \]
\[ D^4_{\gamma 02} = D^0_{\gamma 02} \left( 1 + \frac{3\delta_{\gamma 2}^0}{4I_2^0} + \frac{(\delta_{\gamma 2}^0)^2}{(4I_2^0)^2} \right) \]
\[ D^5_{\gamma 02} = D^0_{\gamma 02} \left( 1 + \frac{4\delta_{\gamma 2}^0}{4I_2^0} + \frac{3(\delta_{\gamma 2}^0)^2}{(4I_2^0)^2} \right) \]

etc. where \[ \delta_{\gamma 2}^0 = \frac{b(1+b)}{2(1-b)^2} \]

These may now be substituted into the expressions for \( f_{\gamma}^n \), \( \delta_{\gamma 2}^n \) and \( \delta_{\gamma 2}^n \) which can then be directly evaluated as functions of the asymmetry parameter \( b \). These results are shown below for several values of \( n \) and for \( \gamma = 2 \).

\[ D^0_{202} = \frac{2\sqrt{3}b}{4(1-b)} \]
\[ D^1_{202} = D^0_{202} \]
\[ D^2_{202} = D^0_{202} \left( 1 + \frac{b(1+b)}{2(1-b)^2} \right) \]
\[ D^3_{202} = D^0_{202} \left( 1 + \frac{b(1+b)}{(1-b)^2} \right) \]
\[ D_{202}^4 = D_{202}^0 \left( 1 + \frac{3b(1+b)}{2(1-b)^2} + \frac{b^2(1+b)^2}{4(1-b)^4} \right) \]
\[ D_{202}^5 = D_{202}^0 \left( 1 + \frac{2b(1+b)}{(1-b)^2} + \frac{3b^2(1+b)^2}{4(1-b)^4} \right) \]
\[ r_2^0 = 2(1-b) \]
\[ r_2^1 = r_2^0 \left( 1 + \frac{\delta_{12}^0}{D_{202}^0} \frac{D_{202}^0}{D_{202}^1} \right) = r_2^0 \left( 1 + \frac{b(1+b)}{(1-b)^2} \right) \]
\[ r_2^2 = r_2^0 \left( 1 + \frac{\delta_{12}^0}{2I_2^0} \frac{D_{202}^1}{D_{202}^2} \right) = r_2^0 \left( 1 + \frac{b(1+b)}{(1-b)^2} \cdot \frac{1}{\frac{1 + b(1+b)}{2(1-b)^2}} \right) \]
\[ r_2^3 = r_2^0 \left( 1 + \frac{\delta_{12}^0}{2I_2^0} \frac{D_{202}^2}{D_{202}^3} \right) = r_2^0 \left( 1 + \frac{\delta_{12}^0}{2I_2^0} \cdot \frac{1}{\frac{1 + \delta_{12}^0}{4I_2^0} \frac{D_{202}^1}{D_{202}^2}} \right) \]
\[ = r_2^0 \left( 1 + \frac{b(1+b)}{(1-b)^2} \cdot \frac{\frac{1 + b(1+b)}{2(1-b)^2}}{1 + \frac{b(1+b)}{(1-b)^2}} \right) \]
\[ r_2^4 = r_2^0 \left( 1 + \frac{\delta_{12}^0}{2I_2^0} \frac{D_{202}^3}{D_{202}^4} \right) = r_2^0 \left( 1 + \frac{b(1+b)}{(1-b)^2} \cdot \frac{\frac{1 + b(1+b)}{1 + 3b(1+b) + \frac{b^2(1+b)^2}{2(1-b)^2}}}{\frac{1 + 3b(1+b) + \frac{b^2(1+b)^2}{2(1-b)^2}}{4(1-b)^4}} \right) \]
\[ r_2^5 = r_2^0 \left( 1 + \frac{\delta_{12}^0}{2I_2^0} \frac{D_{202}^4}{D_{202}^5} \right) = r_2^0 \left( 1 + \frac{b(1+b)}{(1-b)^2} \cdot \frac{\frac{1 + 3b(1+b) + \frac{b^2(1+b)^2}{2(1-b)^2}}{1 + 3b(1+b) + \frac{b^2(1+b)^2}{2(1-b)^2}}}{\frac{1 + 3b(1+b) + \frac{b^2(1+b)^2}{2(1-b)^2}}{4(1-b)^4}} \right) \]
\[ \text{etc. and} \]
\[ \delta_{12}^n = \delta_{12}^0 \cdot \frac{(-\delta_{12}^0)^n}{(4I_2^0)^n} \cdot \frac{(r_{202}^0)^2}{(b_{202}^n)^2} \]
\[-8b(1+b) \left( \frac{-b(1+b)^{n}}{2(1-b)^{2}} \right) \left( \frac{D_{202}^{0}}{(D_{202}^{0})^{2}} \right) \]

\[= \frac{(-b(1+b))^{n+1}}{2^{n-2}(1-b)^{2n}} \frac{(D_{202}^{0})^{2}}{(D_{202}^{n})^{2}} \]

while \[\delta f_{2}^{n} = - \frac{\delta I_{2}^{n}}{2f_{2}^{n}}\]

The results of this are summarized in both tabular and graphical form. In Tables 11-16 the functions of \(f_{2}^{n}\), \(-\delta f_{2}^{n}\), \(\delta I_{2}^{n}\), and \(-\delta I_{2}^{n} = - \frac{\delta I_{2}^{n}}{2f_{2}^{n}}\) are given for values of the asymmetry parameter \(b\) ranging from \(b=0\) to \(b=-1\) in units of one tenth and for values of \(n\) ranging from \(n=0\) to \(n=5\). Each value of \(n\) is shown on a separate table. The first column lists the values of \(b\) used. The second column gives the exact solution for \(f_{2}\) as computed from \(f_{2} = 2(1+3b^{2})^{\frac{1}{2}}\). These were determined to one more significant figure than is shown and then rounded off. The third column gives the function \(f_{2}^{n}\) as computed by the method described above. The fourth column is the error in \(f_{2}^{n}\) as computed by subtracting column 3 from column 2. Note that when this quantity becomes smaller than \(10^{-3}\) it can no longer be given to three significant figures. For \(n=5\) as shown in Table 16 all values of \(-\delta f_{2}^{n}\) are simply listed as \(<10^{-5}\).

The fifth column gives \(\delta I_{2}^{n}\) the error in the invariant \(I_{2}\). This in conjunction with \(f_{2}^{n}\) is used to compute the estimate of the error \(\delta f_{2}^{n} = \frac{\delta I_{2}^{n}}{2f_{2}^{n}}\) which is shown in the last column of
<table>
<thead>
<tr>
<th>-b</th>
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<th>$-\delta x_2^0$</th>
<th>$\delta n_2$</th>
<th>$-\delta f_2^0 \approx \frac{\delta n_2}{2f_2^0}$</th>
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**TABLE II**

A SUMMARY OF THE NUMERICAL RESULTS FOR J=2, T=2 AND n=0
### TABLE 12

A SUMMARY OF THE NUMERICAL RESULTS FOR $J=2$, $\gamma=2$ AND $\nu=1$

<table>
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<tr>
<th>$-b$</th>
<th>$f_2$</th>
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<th>$\delta I_2^1$</th>
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**TABLE 13**

A SUMMARY OF THE NUMERICAL RESULTS FOR J=2, \( \gamma =2 \) AND n=2
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</table>

**TABLE 14**

A SUMMARY OF THE NUMERICAL RESULTS FOR $J=2, \gamma=2$ AND $n=3$
A summary of the numerical results for $J=2, T=2$ and $n=4$.
<table>
<thead>
<tr>
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<th>$f_2$</th>
<th>$f_2^5$</th>
<th>$-\delta f_2^5$</th>
<th>$\delta f_2$</th>
<th>$-\delta f_2^5 \approx \frac{\delta f_2}{2f_2^5}$</th>
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**TABLE 16**

A SUMMARY OF THE NUMERICAL RESULTS FOR $J=2, \tau =2$ AND $n=5$
the tables. Note that the estimate of the error as shown in
the last column is smaller than the error as listed in Column
4. The magnitude of the discrepancy tends to diminish as \( n \)
increases. For \( n=2 \) and above this is not apparent however,
since the error given in column 4 has become too small to
determine to three significant figures.

The entry in the last column of the tables represents
the quantity of interest since it gives a reliable estimate
of the error in \( \frac{r^n}{2} \). This shows that for a given \( n \) the max-
imum error occurs in the vicinity of the most asymmetric
case of \( b = -\frac{1}{3} \). This maximum error does shift from about \( b = -0.4 \)
for \( n=0 \) to about \( b = -0.3 \) for \( n=5 \). The error for all values of
\( b \) is seen to decrease at least an order of magnitude for each
increase in \( n \) so that the values of \( \frac{r^n}{2} \) for \( n=5 \) are actually
\(<10^{-6} \) for all values of \( b \). This estimate of the error is
shown in graphical form in Figure 2 which is a semi-logarithmic
plot. The various curves shown there are for values of \( n \)
ranging from \( n=0 \) to \( n=5 \). They readily show how the order of
magnitude of the error diminishes with increasing \( n \).

At this point it is perhaps superfluous to state
that this has been a very tedious means of approximating the
roots of a quadratic equation which is easily solvable. The
results for this case have been presented in rather complete
detail since they are somewhat simpler than those for the
higher \( J \) values where the degree of the polynomial whose
solutions are sought is higher than 2. These results also give
The six curves shown are the estimates of the errors in the approximations as given by $\delta_{2}^{\infty} = \frac{\delta_{2}^{n}}{2^{n_{2}}}$ for values of $n$ from 0 to 5. The abscissae represent values of the asymmetry parameter $b$. The values of $b$ shown range from $b = -1$ to $-9$. The ordinate is the quantity $\frac{\delta_{2}^{n}}{2^{n_{2}}}$ and is dimensionless. The values for the ordinate range from $10^{-7}$ to 1 on a logarithmic scale.
some insight into the form that the solutions for the higher J values assume. For the other examples to be discussed there will be fewer details shown in the derivation of the results. Rather the tendency will be to simply present the results of the calculations, discuss them and estimate the error involved with the approximations.

In dealing with spectroscopy it is more customary to deal with frequencies than energies. Thus it might be appropriate to translate the results of the energy determination given above into the frequency notation commonly used. The Hamiltonian was given earlier as

\[ H = \frac{\hbar^2}{2I_x} \hat{p}_x^2 + \frac{\hbar^2}{2I_y} \hat{p}_y^2 + \frac{\hbar^2}{2I_z} \hat{p}_z^2 = \alpha \hat{p}_x^2 + \alpha \hat{p}_y^2 + a(b \hat{p}_x^2 - \hat{p}_y^2) \]

where

\[ \alpha = \frac{\hbar^2}{4} \left( \frac{1}{I_x} + \frac{1}{I_y} \right), \quad a = \frac{\hbar^2}{4} \left( \frac{1}{I_z} - \frac{1}{I_x} - \frac{1}{I_y} \right), \quad \alpha c = \frac{\hbar^2}{4} \left( \frac{1}{I_x} - \frac{1}{I_y} \right) \]

The energy eigenvalues have been given as

\[ E_{J,\gamma}(a,b,c) = \alpha c (J+1) + a E_{J,\gamma}(b) \]

where the \( E_{J,\gamma}(b) \) are given in Table 6.

The spectral frequencies are related to the energy eigenvalues by dividing the latter by the product of Planck's constant and the velocity of light. Since the symbol \( c \) has already been used to designate one of the rotational constants,
and since it is also customary to use it for the velocity of light, some change of notation is required. For now this will be achieved by the simple expedient of designating the velocity of light as $c_0$ rather than $c$.

One can then write an operator expression for the frequencies which is given by

$$\hat{P} = \frac{\hbar}{\hbar c_0} = \frac{ac}{\hbar c_0} + \frac{c}{\hbar c_0} \frac{x^2}{2\hbar c_0} + \frac{c}{\hbar c_0} (\frac{x^2}{2\hbar c_0} + \frac{x^2}{2\hbar c_0})$$

The frequencies themselves would be given as

$$P(J\gamma) = \frac{E_J}{\hbar c_0} = \frac{ac}{\hbar c_0} J(J+1) + \frac{c}{\hbar c_0} (e_J,\gamma + f_J,\gamma)$$

where the quantity $E_J = e_J,\gamma + f_J,\gamma$ is usually referred to as $\gamma$ in the literature. In terms of the usual spectroscopic notation the rotational constants would be

$$\frac{ac}{\hbar c_0} = \frac{1}{2} (A+B), \frac{c}{\hbar c_0} = \frac{1}{2} (2C-A-B), \frac{c}{\hbar c_0} = \frac{1}{2} (A-B),$$

and

$$A = \frac{\hbar}{8\pi^2 c_0 I_x}, \quad B = \frac{\hbar}{8\pi^2 c_0 I_y}, \quad C = \frac{\hbar}{8\pi^2 c_0 I_z}$$

and the frequencies could be given as

$$P(J\gamma) = \frac{1}{2} (A+B)J(J+1) + \frac{1}{2} (2C-A-B)(e_J,\gamma + f_J,\gamma).$$

At this point one can easily write out all of the frequencies associated with $J=0,1,2$. Using Tables 6 and 9 one sees that

$$P(0) = 0 \quad P(1) = A+B$$
\[ F(1_{\pm 1}) = A + B + \frac{1}{2} (2C - A - B)(1_{\pm b}) \]
\[ F(2_0) = 3(A + B) + 2(2C - A - B) \]
\[ F(2_{\pm 1}) = 3(A + B) + \frac{1}{2} (2C - A - B)(1_{\pm 3}) \]
\[ F(2_{\pm 2}) = 3(A + B) + \frac{1}{2} (2C - A - B)(2_{\pm 2}) \]

where \( f_2 = 2(1 + 3b^2)^{\frac{1}{4}} \) or may be taken from the approximations given above.

For the sake of numerical illustration one may assign values to the constants \( A, B \) and \( C \) in accord with the assignment given for \( I_x, I_y, \) and \( I_z \) in Chapter I. To do this let \( C = 1, \)
\[ \frac{1}{2}(A + B) = 2 \] and \( \frac{1}{2} (2C - A - B) = -1. \) For \( b = 0 \) this gives \( A = B = 2 \) while for \( b = -1 \) one sees that \( B = 1 \) and \( A = 3. \) With these restrictions one can study the frequencies as functions of the asymmetry parameter. Figure 3 shows the variation of these as the asymmetry parameter varies from \( b = 0 \) to \( b = -1 \) in steps of one-tenth for \( J = 0, 1, 2. \) Note that as was mentioned earlier the assignment of values for a given \( J \) is on the basis of symmetry considerations and hence the values do not increase with increasing frequency.

Approximations to the \( f_{J, \gamma} \) for \( J = 4 \)

The states for \( J = 4 \) which transform as \( A \) have been assigned values of \( \gamma = 4, 0 \) and \( -4. \) The eigenfunctions are given by
\[ \psi_\gamma = b_0,0 \varphi_0^S + b_{20} \varphi_{2}^S + b_{40} \varphi_{4}^S \quad (\gamma = 4, 0, -4) \]
and the inverted expansion by
\[ \varphi_K^S = b_{4K0} \psi_4^a + b_{0,K,0} \psi_0^a + b_{-4,K,0} \psi_{-4}^a \quad (K = 0, 2, 4) \]
FIGURE 3

THE FREQUENCIES $P(J_\nu)$ FOR $J=0, 1$ AND $2$
where the indices \( J \) and \( \gamma \) have been omitted from \( \Phi_{j,k,\gamma}^s \) and
\( \psi_{j,\gamma}^a \). The secular equation for this case is just
\[
\varepsilon_\gamma^2 - 20 \varepsilon_\gamma + (64 - 208b^2) \varepsilon_\gamma + 2880b^2 = 0.
\]
The normal form of the secular equation is found by setting
\[
\varepsilon_\gamma = \frac{20}{3} + \varepsilon_\gamma \quad \text{and substituting with the result}
\]
\[
f_\gamma^3 + I_2 f_\gamma + I_3 = 0
\]
where
\[
I_1 = -\sum f_\gamma = 0, \quad I_2 = \sum_{\gamma \neq \gamma'} f_\gamma f_\gamma' = \frac{-208}{3} \left(1+3b^2\right) \quad \text{and}
\]
\[
I_3 = -\sum_{\gamma \neq \gamma' \neq \gamma''} f_\gamma f_\gamma f_\gamma'' = \frac{-8 \cdot 20 \cdot 28}{3^3} \left(1-9b^2\right).
\]
The equation can be solved exactly and has as its solutions
\[
f_4 = -\frac{\omega}{2} \left(\cos \theta - 3 \sin \theta\right)
\]
\[
f_0 = \alpha \cos \theta
\]
\[
f_{-4} = -\frac{\omega}{2} \left(\cos \theta + 3 \sin \theta\right)
\]
where \( \alpha = \frac{8}{3} \left(1+3b^2\right)^\frac{1}{2}, \cos 3\theta = \frac{35(1-9b^2)}{\left(13(1+3b^2)^2\right)^{\frac{3}{2}}} \).

From these either the energy eigenvalues or the characteristic frequencies may be found. The solutions are somewhat difficult to work with and will not be discussed further.

For the purpose of determining approximations to these
one can make the following linear starting approximations.
\[
\begin{align*}
f_4^0 &= \frac{28}{3} (1-\frac{3}{7}b), \quad f_0^0 = \frac{8}{3} (1+3b), \quad f_{-4}^0 = \frac{-20}{3} (1-\frac{3}{5}b). \quad (3.17)
\end{align*}
\]
These are readily found from the two symmetric rotator limits of
\( b=0 \) and \( b=-1 \). They are chosen so that the approximate invariant
\( I_1^0 = 0 \) while
The errors in these invariants are then given by

\[ \delta I_1^0 = 0, \quad \delta I_2^0 = -3 \cdot 2^5 b (1+b), \quad \delta I_3^0 = 2^7 b (1+b) (1+3b). \]

The approximations to the projection operators are given by

\[ \hat{\varphi}^0_{\gamma'} = \frac{(\hat{f}^0_{\gamma'} - \hat{f}^0_{\gamma})(\hat{f}^0_{\gamma'} - \hat{f}^0_{\gamma})}{(\hat{f}^0_{\gamma} - \hat{f}^0_{\gamma})(\hat{f}^0_{\gamma} - \hat{f}^0_{\gamma})} \quad (\gamma \neq \gamma' \neq \gamma''). \]

If these are allowed to act upon the symmetrized symmetric rotator eigenfunctions the results are

\[ D^0_{\gamma \gamma} \varphi^s_K = D^0_{\gamma \gamma, 0} \varphi^s_0 + D^0_{\gamma \gamma, 2} \varphi^s_2 + D^0_{\gamma \gamma, 4} \varphi^s_4 \quad (K=0, 2, 4) \]

where

\[ D^0_{\gamma \gamma'} = 1 \quad (\hat{f}^0_{\gamma'} + \frac{20}{3} (\hat{f}^0_{\gamma'} - \hat{f}^0_{\gamma'}) + \frac{460}{9} + 180b^2) \]

\[ = \frac{1}{D^0_{\gamma'}} \left( \left( \hat{f}^0_{\gamma} - \frac{28}{3} \right) (\hat{f}^0_{\gamma} + \frac{8}{3}) - 28b^2 - \delta I_2^0 \right) \quad (3.18) \]

\[ D^0_{\gamma 22} = \frac{1}{D^0_{\gamma'}} \left( \hat{f}^0_{\gamma'} \hat{f}^0_{22} + \frac{8}{3} (\hat{f}^0_{\gamma'} + \hat{f}^0_{\gamma}) + \frac{64}{9} + 208b^2 \right) \]

\[ = \frac{1}{D^0_{\gamma'}} \left( \left( \hat{f}^0_{\gamma} - \frac{28}{3} \right) (\hat{f}^0_{\gamma} + \frac{20}{3}) - 5 \delta I_2^0 \right) \]

\[ D^0_{\gamma 44} = \frac{1}{D^0_{\gamma'}} \left( \hat{f}^0_{\gamma'} \hat{f}^0_{44} - \frac{28}{3} (\hat{f}^0_{\gamma'} + \hat{f}^0_{\gamma}) + \frac{764}{9} + 26b^2 \right) \]

\[ = \frac{1}{D^0_{\gamma'}} \left( \left( \hat{f}^0_{\gamma} + \frac{8}{3} \right) (\hat{f}^0_{\gamma} + \frac{20}{3}) - 180b^2 - 5 \delta I_2^0 \right) \]

\[ D^0_{\gamma 02} = D^0_{\gamma 20} = \frac{-6 \sqrt{5} b}{D^0_{\gamma'}} (\hat{f}^0_{\gamma} + \hat{f}^0_{\gamma} + \frac{28}{3}) \]

\[ = \frac{6 \sqrt{5} b}{D^0_{\gamma'}} (\hat{f}^0_{\gamma} - \frac{28}{3}) \]

\[ D^0_{\gamma 24} = D^0_{\gamma 42} = -2 \frac{\sqrt{7} b}{D^0_{\gamma'}} (\hat{f}^0_{\gamma} + \hat{f}^0_{\gamma} - \frac{20}{3}) \]

\[ = 2 \frac{\sqrt{7} b}{D^0_{\gamma'}} (\hat{f}^0_{\gamma} + \frac{20}{3}) \]
\[ D_0^\gamma_{04} = D_0^\gamma_{40} = \frac{12 \sqrt{35} \ell^2}{D_0^\gamma} \]

with
\[ D_0^\gamma = (f_0^\gamma - f_0^\gamma)(f_0^\gamma - f_0^\gamma) = 3(f_0^\gamma)^2 + f_0^2 \]

and
\[ D_0^\gamma_{00} + D_0^\gamma_{22} + D_0^\gamma_{44} = 1 - \frac{2 f_0^2}{D_0^\gamma} \]

If the operator \( \hat{f} \) is allowed to act on \( \phi_s^0 \), the result is
\[ \hat{f}_0^\gamma \phi_s^0 = f_0^\gamma_{00} D_0^\gamma_{00} \phi_s^0 + f_0^\gamma_{02} D_0^\gamma_{02} \phi_s^2 + f_0^\gamma_{04} D_0^\gamma_{04} \phi_s^4 \]

where
\[ f_0^\gamma_{04} = \frac{28}{3} + \frac{2\sqrt{7} b}{D_0^\gamma_{02}} = f_0^\gamma. \]

The remaining \( f_0^\gamma, K, K' \) could be listed, but since they are not to be used in any way they will not be shown here.

If one acts on \( \phi_s^0 \) with \( (\phi_s^0)^n+1 \) one obtains
\[ (\phi_s^0)^n+1 \phi_s^0 = D_0^\gamma_{00} \phi_s^0 + D_0^\gamma_{02} \phi_s^2 + D_0^\gamma_{04} \phi_s^4 \]

where
\[ D_0^\gamma_{00} = D_0^{n-1} \gamma_{00} D_0^\gamma_{00} + D_0^{n-1} \gamma_{02} D_0^\gamma_{02} + D_0^{n-1} \gamma_{04} D_0^\gamma_{04} \]
\[ D_0^\gamma_{02} = D_0^{n-1} \gamma_{02} D_0^\gamma_{02} + D_0^{n-1} \gamma_{04} D_0^\gamma_{04} \]
\[ D_0^\gamma_{04} = D_0^{n-1} \gamma_{04} D_0^\gamma_{04} \]

Also
\[ (\phi_s^0)^n+1 \phi_s^0 = f_0^\gamma_{00} D_0^\gamma_{00} \phi_s^0 + f_0^\gamma_{02} D_0^\gamma_{02} \phi_s^2 + f_0^\gamma_{04} D_0^\gamma_{04} \phi_s^4 \]

where
This could also be performed by repeating these operations on $\varphi_2^s$ and $\varphi_4^s$, but since in the limit of large $n$ all $f_n^\gamma_{,K,K'}$ approach the same functions, this will not be given here. Rather attention will be confined to $K=0$, $K'=4$ while $f_n^\gamma_{04}$ will be designated as $f_n^\gamma$ and will represent the $n$th approximation to $f_\gamma$. Note that while all nine $D_n^{\gamma_{,K,K'}}$ are needed, only three $D_n^{\gamma_{,0,0}}$ are necessary for computing $f_n^\gamma_{04}$. These are just the $D_n^{\gamma_{00}}$, $D_n^{\gamma_{02}}$ and $D_n^{\gamma_{04}}$ indicated above.

The following is a listing of all of the $D_n^{\gamma_{04}}$, $D_n^{\gamma_{02}}$, $D_n^{\gamma_{00}}$ and $f_n^{\gamma_{04}} = f_n^{\gamma}$ for values of $n$ ranging from $n=0$ to $n=5$. It is desirable to list the $D_n^{\gamma_{0,0,K}}$ since they are equal to $b_n^{\gamma_{0,0}} b_n^{\gamma_K}$ and can be used to evaluate approximations to the coefficients $b_n^{\gamma_K}$ that appear in the expansion for the eigenfunctions.

Also note that $\delta_2^0 = -96b(1+b)$, $\delta_3^0 = 128b(1+b)(1+3b)$ and $D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

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$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

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$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$

$D_4^0 = 3(f_0^0)^2 + f_2^0 = 64(3-2b-b^2) = 64(3+b)(1-b)$
\( n=0 \)

\[
D_{\gamma 04}^0 = \frac{12\sqrt{15} b^2}{D_{\gamma}^0} \tag{3.18}
\]

\[
D_{\gamma 02}^0 = \frac{6\sqrt{5} b}{D_{\gamma}^0} (x_{\gamma}^0 - \frac{28}{3})
\]

\[
D_{\gamma 00}^0 = \frac{1}{D_{\gamma}^0} \left( (x_{\gamma}^0 - \frac{28}{3})(x_{\gamma}^0 + \frac{8}{3}) - 28b^2 - 5I_2^0 \right)
\]

and the \( f_{\gamma}^0 \) are just those given in equation 3.17.

\( n=1 \)

\[
D_{\gamma 04}^1 = \left(1 - \frac{5I_2^0}{D_{\gamma}^0} \right) D_{\gamma 04}^0 \tag{3.19}
\]

\[
D_{\gamma 02}^1 = \left(1 - \frac{5I_2^0}{D_{\gamma}^0} \right) D_{\gamma 02}^0 - \frac{\sqrt{15} b}{D_{\gamma}^0} \left( \frac{5I_3^0 + 5I_2^0 x_{\gamma}^0}{(D_{\gamma}^0)^2} \right)
\]

\[
= \frac{D_{\gamma 02}^0}{D_{\gamma 04}^0} \left( \frac{1}{D_{\gamma 04}^0} - \frac{\sqrt{15} b}{D_{\gamma}^0} \left( \frac{5I_3^0 + 5I_2^0 x_{\gamma}^0}{(D_{\gamma}^0)^2} \frac{D_{\gamma 02}^0}{D_{\gamma 04}^0} \right) \right)
\]

\[
D_{\gamma 00}^1 = \left(1 - \frac{5I_2^0}{D_{\gamma}^0} \right) D_{\gamma 00}^0 - \frac{1}{(D_{\gamma}^0)^2} \left( (5I_3^0 + 5I_2^0 x_{\gamma}^0)(2x_{\gamma}^0 - \frac{20}{3}) - 5D_{\gamma}^0 \delta I_2^0 \right)
\]

\[
= \frac{D_{\gamma 00}^0}{D_{\gamma 04}^0} \left( \frac{D_{\gamma 04}^0}{D_{\gamma 04}^0} - \left( \frac{5I_3^0 + 5I_2^0 x_{\gamma}^0}{(D_{\gamma}^0)^2} \frac{D_{\gamma 02}^0}{D_{\gamma 04}^0} \right) \right)
\]

\[
x_{\gamma}^1 = x_{\gamma}^1_{04} = \frac{2\sqrt{15} b D_{\gamma 02}^1 + \frac{28}{3} D_{\gamma 04}^1}{D_{\gamma 04}^1}
\]

\[
x_{\gamma}^0 \left( 1 - \frac{5I_2^0 x_{\gamma}^0}{D_{\gamma}^0} \right) \frac{D_{\gamma 04}^0}{D_{\gamma 04}^1}
\]
\[ n = 2 \]

\[ \begin{align*}
D_r^2 &= (1 - \frac{S_{12}^0}{D_r^0}) n_r^1 - \frac{(3 S_{13}^0 (S_{13}^0 + S_{23}^0) - D_r^0 S_{12}^0)}{(D_r^0)^2} D_r^0 n_r^4 (3.20) \\
 n_r^2 &= (1 - \frac{S_{12}^0}{D_r^0}) n_r^1 - \frac{(3 S_{13}^0 (S_{13}^0 + S_{23}^0) - D_r^0 S_{12}^0)}{(D_r^0)^2} D_r^0 n_r^2
+ \frac{6 \sqrt{5} b S_{12}^0 (S_{13}^0 + S_{23}^0)}{(D_r^0)^3} \\
&= \frac{D_r^0 n_r^2}{D_r n_r^4} \left( D_r^2 - \frac{6 \sqrt{5} b (S_{13}^0 + S_{23}^0)}{(D_r^0)^2} \left( \frac{1}{D_r n_r^4} - \frac{S_{12}^0}{D_r^0} \right) \right)
\end{align*} \]

\[ \begin{align*}
D_r^2 &= (1 - \frac{S_{12}^0}{D_r^0}) n_r^1 - \frac{(3 S_{13}^0 (S_{13}^0 + S_{23}^0) - D_r^0 S_{12}^0)}{(D_r^0)^2} D_r^0 n_r^0
+ \frac{(S_{13}^0 + S_{23}^0) (S_{12}^0 - \frac{20}{3} S_{12}^0)}{(D_r^0)^3}
\end{align*} \]

\[ \begin{align*}
&= \frac{D_r^0 n_r^0}{D_r n_r^4} \left( D_r^2 - \frac{(S_{13}^0 + S_{23}^0) (2 S_{14}^0 - \frac{20}{3}) - D_r^0 S_{12}^0}{(D_r^0)^2} \right) n_r^1
+ \frac{(S_{13}^0 + S_{23}^0) (S_{12}^0 - \frac{20}{3} S_{12}^0)}{(D_r^0)^3} D_r^0 n_r^0
\end{align*} \]

\[ \begin{align*}
r_r^2 &= r_r^2 D_r^4 = \frac{2 \sqrt{7} b D_r^2}{D_r^4} + \frac{28}{3} D_r^2
\end{align*} \]

\[ \begin{align*}
f_r^0 &= \left( 1 - \frac{(S_{13}^0 + S_{23}^0)}{D_r^0} \right) \left( \frac{D_r^1}{D_r^4} - \frac{S_{12}^0}{D_r^0} \right) \left( \frac{D_r^0}{D_r^4} \right) \right) \\
&= \left( 1 - \frac{(S_{13}^0 + S_{23}^0)}{D_r^0} \right) \left( \frac{D_r^1}{D_r^4} - \frac{S_{12}^0}{D_r^0} \right) \left( \frac{D_r^0}{D_r^4} \right) \right) \\
&= \left( 1 - \frac{(S_{13}^0 + S_{23}^0)}{D_r^0} \right) \left( \frac{D_r^1}{D_r^4} - \frac{S_{12}^0}{D_r^0} \right) \left( \frac{D_r^0}{D_r^4} \right) \right) \\
&= \left( 1 - \frac{(S_{13}^0 + S_{23}^0)}{D_r^0} \right) \left( \frac{D_r^1}{D_r^4} - \frac{S_{12}^0}{D_r^0} \right) \left( \frac{D_r^0}{D_r^4} \right) \right) \\
&= \left( 1 - \frac{(S_{13}^0 + S_{23}^0)}{D_r^0} \right) \left( \frac{D_r^1}{D_r^4} - \frac{S_{12}^0}{D_r^0} \right) \left( \frac{D_r^0}{D_r^4} \right) \right)
\( n = 3 \)

\[
\begin{align*}
D^3_{704} &= (1 - \frac{\mathcal{I}^{0}_{3}}{D^0_{7}}) D^2_{704} - \frac{(3 \mathcal{I}^0_{2} (\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22}) - D^0_{7} \mathcal{I}^{0}_{2})}{(D^0_{7})^2} D^1_{704} \\
+ &\frac{(\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22})^2}{(D^0_{7})^3} D^0_{704} \tag{3.21}
\end{align*}
\]

\[
\begin{align*}
D^3_{702} &= (1 - \frac{\mathcal{I}^{0}_{3}}{D^0_{7}}) D^2_{702} - \frac{(3 \mathcal{I}^0_{2} (\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{2}) - D^0_{7} \mathcal{I}^{0}_{2})}{(D^0_{7})^2} D^1_{702} \\
+ &\frac{(\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22})^2}{(D^0_{7})^3} D^0_{702} - \frac{6\sqrt{3} \mathcal{I}^2_{2} (\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22})}{(D^0_{7})^4} D^0_{702}
\end{align*}
\]

\[
\begin{align*}
D^3_{700} &= (1 - \frac{\mathcal{I}^{0}_{3}}{D^0_{7}}) D^2_{700} - \frac{(3 \mathcal{I}^0_{2} (\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22}) - D^0_{7} \mathcal{I}^{0}_{2})}{(D^0_{7})^2} D^1_{700} \\
+ &\frac{(\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22})^2}{(D^0_{7})^3} D^0_{700} - \frac{\mathcal{I}^2_{2} (\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22}) (\mathcal{I}^{0}_{3} - \frac{20}{3} \mathcal{I}^{0}_{2})}{(D^0_{7})^4}
\end{align*}
\]

\[
\begin{align*}
\frac{n^0_{700}}{D^0_{704}} &= \frac{n^3_{704}}{D^3_{704}} - \frac{(\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22})(2 \mathcal{I}^{0}_{2} - \frac{20}{3} D^0_{7} \mathcal{I}^{0}_{2})}{(D^0_{7})^2} D^2_{704} \\
+ &\frac{(\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22})(\mathcal{I}^{0}_{3} - \frac{20}{3} \mathcal{I}^{0}_{2})}{(D^0_{7})^3} D^0_{700} \\
+ &\frac{2\sqrt{3} \mathcal{I}^0_{3} (\mathcal{I}^{0}_{3} - \frac{20}{3} \mathcal{I}^{0}_{2})}{D^0_{7}} \\
\end{align*}
\]

\[
\begin{align*}
x^3_{704} &= x^3_{704} + \frac{2\sqrt{3} n^3_{704}}{D^3_{704}} \\
\mathcal{R}_{704} &= \left(1 - \frac{\mathcal{I}^{0}_{3} + \mathcal{I}^{0}_{22}}{x^0_{704}} \right) \left( D^2_{704} - \frac{\mathcal{I}^{0}_{2}}{x^0_{704}} \right) \left( D^1_{704} + \frac{\mathcal{I}^{0}_{2}}{D^0_{704}} \right) \left( D^0_{704} \right) \frac{D^3_{704}}{D^3_{704}}
\end{align*}
\]
\[ n=4 \]

\[ D_{704}^4 = (1 - \frac{S_{I2}^0}{D_{7}^0}) D_{704}^3 - \left( \frac{3f_{7}^0 (S_{I3}^0 + S_{I2}^{o,0}) - D_{7}^0 S_{I2}^0}{(D_{7}^0)^2} \right) D_{704}^2 \]

\[ + \left( \frac{S_{I3}^0 + S_{I2}^{o,0}}{(D_{7}^0)^3} \right) \left( D_{704}^1 - \frac{S_{I2}^0}{D_{7}^0} D_{704}^0 \right) \]  

(3.22)

\[ D_{702}^4 = (1 - \frac{S_{I2}^0}{D_{7}^0}) D_{702}^3 - \left( \frac{3f_{7}^0 (S_{I3}^0 + S_{I2}^{o,0}) - D_{7}^0 S_{I2}^0}{(D_{7}^0)^2} \right) D_{702}^3 \]

\[ + \left( \frac{S_{I3}^0 + S_{I2}^{o,0}}{(D_{7}^0)^3} \right) \left( D_{702}^1 - \frac{S_{I2}^0}{D_{7}^0} D_{702}^0 \right) \]

\[ + \frac{6\sqrt{5} b S_{I2}^0 (S_{I3}^0 + S_{I2}^{o,0})}{(D_{7}^0)^5} \]

\[ D_{700}^4 = (1 - \frac{S_{I2}^0}{D_{7}^0}) D_{700}^3 - \left( \frac{3f_{7}^0 (S_{I3}^0 + S_{I2}^{o,0}) - D_{7}^0 S_{I2}^0}{(D_{7}^0)^2} \right) D_{700}^2 \]

\[ + \left( \frac{S_{I3}^0 + S_{I2}^{o,0}}{(D_{7}^0)^3} \right) \left( D_{700}^1 - \frac{S_{I2}^0}{D_{7}^0} D_{700}^0 \right) \]

\[ + \frac{S_{I2}^0 (S_{I3}^0 + S_{I2}^{o,0}) (S_{I3}^0 - \frac{20}{3} S_{I2}^0)}{(D_{7}^0)^5} \]

\[ = \frac{n_{700}^0}{D_{704}^0} \left( D_{704}^4 - \left( \frac{S_{I3}^0 + S_{I2}^{o,0}}{(D_{7}^0)^2} \right) \left( D_{704}^3 - \frac{S_{I2}^0}{D_{7}^0} D_{704}^2 \right) \right) \]

\[ + \left( \frac{S_{I3}^0 + S_{I2}^{o,0}}{(D_{7}^0)^3} \right) \left( D_{700}^1 - \frac{S_{I2}^0}{D_{7}^0} D_{700}^0 \right) \]

\[ + \frac{(S_{I3}^0 + S_{I2}^{o,0}) (S_{I3}^0 - \frac{20}{3} S_{I2}^0)}{(D_{7}^0)^3} \left( D_{700}^2 - \frac{S_{I2}^0}{D_{7}^0} D_{700}^1 + \frac{S_{I2}^0}{D_{7}^0} \right) D_{700} \]

\[ \tau_{7}^4 = \tau_{704}^4 - 2\sqrt{5} b D_{702}^4 + \frac{28}{3} D_{704}^4 \]

\[ D_{704}^4 \]
\[
\begin{align*}
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( \frac{D_7^{04} - S_2^0 D_7^{04} + \left( \frac{S_2^0}{D_7^0} \right)^2 D_7^{04} - \left( \frac{S_2^0}{D_7^0} \right)^3 D_7^{04}}{D_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right) \\
&= r_7^0 \left( 1 - \frac{S_2^0 + S_2^0 S_7^0}{r_7^0} \right) \left( d_7^{04} - \frac{S_2^0 d_7^{04} + \left( \frac{S_2^0}{d_7^0} \right)^2 d_7^{04} - \left( \frac{S_2^0}{d_7^0} \right)^3 d_7^{04}}{d_7^{04}} \right)
\end{align*}
\]
\[- \frac{n^0}{D^0_{704}} \left( D^5_{704} - \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} - \frac{20}{3} \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \right) \frac{D^4_{704}}{D_{704}^0} \]

\[+ \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \]

\[+ \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \]

\[\times \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \right) \]

\[\frac{D^5_{704}}{D_{704}^0} \]

For arbitrary values of \( n \) one evidently obtains

\[D^0_{704} = (1 - \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} - \frac{20}{3} \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \frac{D^4_{704}}{D_{704}^0} \]

\[+ \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \]

\[\times \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \left( \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \right) \right) \]

\[\frac{D^5_{704}}{D_{704}^0} \]

\[\left( 3 \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} - \frac{20}{3} \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) D_{704}^0 \left( \sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n} \right) \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]

\[\sum_{m=0}^{n-3} \left( \frac{\sum_{i=3}^{n} \sum_{j=2}^{n} \sum_{k=3}^{n}}{D_{704}^0} \right)^m \]
\[- \frac{6 \sqrt{3} b \left( \sum \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right)}{\left( D_{\gamma}^{0} \right)^{2}} \left( - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right)^{n-1} \]

\[- \frac{D_{\gamma}^{0}}{D_{\gamma}^{0}} \leq \left( 6 \sqrt{3} b \left( \sum \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right) \right) \leq \sum_{m=0}^{n-1} \left( - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right)^{m} D_{\gamma}^{0-n-m} \]

\[n_{\gamma}^{n-0} = \left( 1 - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right) n_{\gamma}^{1-n-1} \leq \left( \frac{3 \delta I_{3}^{0} \left( \sum \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right) - D_{\gamma}^{0} \delta I_{2}^{0}}{\left( D_{\gamma}^{0} \right)^{2}} \right) D_{\gamma}^{0-n-2} \]

\[+ \left( \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right)^{2} \sum_{m=0}^{n-3} \left( - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right)^{m} D_{\gamma}^{0-n-3-m} \]

\[+ \left( \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right) \left( \frac{\delta I_{3}^{0} - \frac{20}{3} \delta I_{2}^{0}}{D_{\gamma}^{0}} \right) \left( - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right)^{n-2} \]

\[- \frac{D_{\gamma}^{0}}{D_{\gamma}^{0}} \leq \left( 2V_{g} b \left( \sum \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right) \right) \leq \sum_{m=0}^{n-2} \left( - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right)^{m} D_{\gamma}^{0-n-2-m} \]

\[x_{\gamma}^{n} = x_{\gamma}^{0} = \frac{2V_{g} b}{D_{\gamma}^{0}} + \frac{28}{3} \frac{n^{n}}{D_{\gamma}^{0-n}} \]

\[x_{\gamma}^{0} = x_{\gamma}^{0} \left( 1 - \left( \frac{\delta I_{3}^{0} + \delta I_{2,2}^{0}}{D_{\gamma}^{0}} \right) \sum_{m=0}^{n-1} \left( - \frac{\delta I_{2}^{0}}{D_{\gamma}^{0}} \right)^{m} D_{\gamma}^{0-n-1-m} \right) \]

With these written in terms of the various \( D_{\gamma}^{n}, \ delta I_{2}^{0}, \)

\( delta I_{2,3}, D_{\gamma}^{0} \) and \( f_{\gamma}^{0} \) it is now a question of substituting the functions given earlier for the latter in order to obtain \( D_{\gamma}^{n} \)

and \( f_{\gamma}^{n} \) explicitly in terms of the asymmetry parameter \( b \). One
can also obtain an estimate of the error in $f^n_\gamma$ as a function of the asymmetry parameter. These will not be written here. Rather attention is called to Table 17 which shows the results of calculating $f^n_4$ from $n=0$ to $n=4$. The first column is just the asymmetry parameter $b$ in units of one tenth from $b=0$ to $b=1$. The second column is the exact solution as computed from the solution to the secular equation. The remaining columns give the approximations from $n=0$ to $n=4$.

It is seen that the improvement in the accuracy for the function is about an order of magnitude for each successive approximation. Actually near $b=0$, $b=\sqrt{33}$ and $b=\sqrt{10}$ it converges somewhat more rapidly than this. The maximum error is in the vicinity of $b=-.6$. For $f^n_0$ the convergence is not quite as rapid while for $f^n_{-4}$ it is a little more rapid. In each of these other cases, however, the rate of convergence does not greatly differ from that shown here for $f^n_4$.

At this point perhaps mention should be made of the remaining $\gamma$ values associated with $J=4$ as well as those connected with $J=3$. In the latter case the secular determinant is $7\times7$ and from symmetry breaks into a $1\times1$ and three $2\times2$ sub-determinants. The $1\times1$ gives rise to a constant solution while the three $2\times2$ sub-determinants give quadratic equations. The energies or frequencies may then be found by solving the quadratic equation or by approximating the roots as described in the previous section dealing with $J=2$. These approximations which are not given here
<table>
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<th>$f_4^0$</th>
<th>$f_4^1$</th>
<th>$f_4^2$</th>
<th>$f_4^3$</th>
<th>$f_4^4$</th>
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<td>10.4092</td>
<td>10.4372</td>
<td>10.4186</td>
<td>10.4180</td>
</tr>
<tr>
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<td>10.9417</td>
<td>10.9343</td>
<td>10.9315</td>
<td>10.9313</td>
</tr>
<tr>
<td>-0.8</td>
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<td>12.5333</td>
<td>11.6043</td>
<td>11.5905</td>
<td>11.5888</td>
<td>11.5888</td>
</tr>
<tr>
<td>-0.9</td>
<td>12.3936</td>
<td>12.9333</td>
<td>12.4010</td>
<td>12.3941</td>
<td>12.3937</td>
<td>12.3936</td>
</tr>
</tbody>
</table>

**TABLE 17**

The approximate function $f^n_{j,r}$ for $J=4$, $r=4$ and $n=0$ to $n=4$
tend to converge to the actual solutions at essentially the same rate as for J=2. For J=4 the secular determinant splits into a 3x3 and three 2x2 sub-determinants. The roots of the 3x3 have just been approximated above. The roots of the three 2x2 sub-determinants may then be found exactly or again approximately as were those for J=2.

The equations for the spectral frequencies for all \( \gamma \) values associated with both J=3 and J=4 are now listed.

\[
\begin{align*}
P(3_0) &= 6(A+B) + 2(2C-A-B) \\
P(3_{\pm 1}) &= 6(A+B) + \frac{1}{2}(2C-A-B) \left( 5 + 3b \pm 4 \left( 1 \pm \frac{3}{2}b + \frac{3}{2}b^2 \right)^{\frac{1}{2}} \right) \\
P(3_{\pm 2}) &= 6(A+B) + (2C-A-B) \left( 1 \pm \left( 1 + 15b^2 \right)^{\frac{1}{2}} \right) \\
P(3_{\pm 3}) &= 6(A+B) + \frac{1}{2}(2C-A-B) \left( 5 + 3b \pm 4 \left( 1 \pm \frac{3}{2}b + \frac{3}{2}b^2 \right)^{\frac{1}{2}} \right) \\
P(3_{\pm 4}) &= 6(A+B) + \frac{1}{2}(2C-A-B) \left( 5 + 3b \pm 4 \left( 1 \pm \frac{3}{2}b + \frac{3}{2}b^2 \right)^{\frac{1}{2}} \right)
\end{align*}
\]

The functions \( f_0 \) and \( f_{\pm 4} \) are the solutions to the cubic secular equation which have been approximated above. Note that the \( \pm \gamma \) values as they have been written do not in general have the same transformation properties.

For the purpose of numerical illustration reference is made to page 85 where specific values are assigned to the constants.
\frac{1}{2} (A+B) and \frac{1}{2}(2C-A-B). These values have been again used in Figures 4 and 5 for the purpose of illustrating the variation of the energies or frequencies as the asymmetry parameter varies. Note that the frequency scale has been changed by a factor of 2 in these figures from that which was used in Figure 3. Again the \gamma values have been assigned according the symmetry considerations rather than energy considerations. Also for this choice of the rotational constants there is now some overlapping between the J=2 and J=3 frequencies and also between the J=3 and J=4 frequencies.
Figure 4

The frequencies $P(J^\gamma)$ for $J = 3$
FIGURE 5

THE FREQUENCIES $F(J_{\pi})$ FOR $J=4$
CHAPTER IV

CONCLUSIONS

At this point the approximate method described early in Chapter III has been illustrated for two cases. The first of these cases was $J=2, \gamma = 2$. For the other $\gamma$ value associated with $\gamma = 2$ namely $\gamma = -2$ the results are of the same magnitude but opposite sign. The second illustration was $J=4, \gamma = 4$. The results for the other $\gamma$ values in the $J=4$ case, that is $\gamma = 0$ and $\gamma = -4$, are quite similar in nature. In each case the rate of convergence of the approximate solutions to the correct solutions was seen to be about an order of magnitude for each successive approximation.

Some calculations for the states that transform as $A$ for higher even $J$ values have been attempted. For $J=6$ it was felt for a time that the rate of convergence might be substantially reduced. This, however, does not now appear to be the case. It now appears that the approximations will converge at about the same rate as for the two cases illustrated. The calculations made for $J=8$ are not sufficient at this time to be at all conclusive.

This latter case of $J=8$ is, however, a very important one. The approximations for $J=2$ are to the roots of a quadratic equation. Those for $J=4$ are for a cubic equation and for $J=6$ to a quartic equation. $J=8$ represents the first instance of a quintic equation to arise. For all of the $J$ values below this the solutions can at least in principle be obtained in closed form by algebraic means. The solution for the cubic and quartic cases are not of
a convenient form but are nevertheless in closed form. The approximations for these two cases are more tedious to obtain but are perhaps in a more convenient form for subsequent use in analyzing spectra.

Perhaps the most crucial test of the method proposed here lies in the case for \( J=8 \). The quintic equation that arises cannot be solved in closed form by algebraic means. If the method proposed could yield approximations that converge at substantially the same rate as for lower \( J \) values, it would then appear to offer promise to continue to higher \( J \) values where the degree of the secular equation continues to increase.

The results as obtained are in the form of rational functions of the rotational constants. If one is willing to introduce irrational factors into the solutions it appears that one might get a slightly higher rate of convergence of the solutions. This, however, is felt to be more than offset by the fact that the solutions tend to be more difficult to handle. The irrational parts change with \( J \) and indeed for the various \( \gamma \) associated with a given \( J \) and would appear to make the solutions more difficult to use in analyzing spectra.

It would seem expedient then to keep the restriction that the approximations be in the form of rational functions. Assuming that the rate of convergence for the states that transform as \( A \) for \( J=8 \) is not substantially less than for the other cases, it would then appear that the method would give expressions for the eigenvalues of any accuracy desired. The limiting factor would
seem to lie with the patience of the person determining the approximations rather than with the method.

It also appears that the method can be extended to include some non-rigid distortion effects without too much difficulty. The centrifugal distortion terms giving rise to \((K|K^2)\) and \((K|K^4)\) terms in the energy matrix do not alter the symmetry of the problem. They could then be included in the determination of the invariants of the problem and carried over to the approximations without an undue change in the formalism. It is anticipated that this can be done in the not too distant future.

At least a word is in order about the eigenfunctions. The quantities \(D^n_{\gamma,k,k'}\), discussed in Chapter III are equal to 
\(b^n_{\gamma,k} b^n_{\gamma,k'}\), where the \(b^n_{\gamma,k}\) are approximations to the coefficients in the expansion of the asymmetric rotator wavefunctions in terms of the symmetric rotator wavefunctions. From the \(D^n_{\gamma,0,k}\) one could then determine \(b^n_{\gamma,0}\) when \(K=0\) and the remaining \(b^n_{\gamma,k}\) in a very straightforward manner. The coefficients so obtained then represent approximations to the actual coefficients with their accuracy increasing with increasing \(n\).

A distinct disadvantage to this, however, is that while for a given \(n\) one might be satisfied with the determination of the eigenvalues one might not be satisfied with the eigenfunctions. The reason is that there is no guarantee that the eigenfunctions so obtained will be orthogonal. While it is true that as \(n\) increases the degree of non-orthogonality decreases, this does not tell the whole story. As in most approximate quantum mechanical calculations
one can obtain eigenvalues that might be satisfactory while the
eigenfunctions that result leave something to be desired. If one
were to attempt to calculate expectation values of operators other
than the constants of the motion, say for the dipole moment operator,
with an eye on intensity calculations the lack of a guarantee of
complete orthogonality would no doubt make such calculations
suspect.

Recently it has come to light that there may be a way
out of this. It now appears that the $D_{\gamma_0, K}^R$ can be chosen in such
a way that the eigenfunctions will be orthogonal and that this will
still permit the eigenvalues to be expressed in the form of rational
functions whose rate of convergence is at least no worse than that
given above. If this turns out to be the case then at least a
necessary condition will be incorporated into the eigenfunctions.
Whether or not this is sufficient to yield eigenfunctions that will
be suitable for other than eigenvalue calculations remains to be
seen.

In summarizing one is then led to conclude that the method
used appears to give a means of determining eigenvalues in terms
of arbitrary values of the asymmetry parameter that can be expressed
in the form of rational functions and which can be made as accurate
as one wishes. Also it would appear that at least some non-rigid
terms can be included without undue complication and perhaps that
the eigenfunctions can be made orthogonal without unduly complicating
the form of the solutions.
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I have accepted a position as Assistant Professor of Physics at Clarkson College of Technology in Potsdam, New York.