Pseudorotations in Molecules: Electronic Orbital Triplets

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This work had its genesis in a collaboration with Roy R. Douglas on applications of algebraic topology to the Jahn-Teller effect and related phenomena in multi-body quantum mechanics. This paper is dedicated to his memory.

Abstract. Topological and geometrical methods are used to calculate the pseudorotational part of the vibronic spectrum for an electronic triplet of an octahedral, tetrahedral, or icosahedral molecule. The calculations take into account the nontrivial geometry inherent in the Jahn-Teller effect. It is shown that the Jahn-Teller effect gives rise to a geometry, which is related to the isoparametric geometry of E. Cartan. The pseudorotational spectra correspond to the spectra of connection Laplacians on nontrivial line bundles over base spaces with this geometry. Globally, the isoparametric submanifolds form a totally geodesic foliation of $S^4$ and the spectral flow of these connection Laplacians on this foliation is computed.

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1. Introduction

The Jahn-Teller effect for electronic orbital triplets can occur for molecules with tetrahedral, octahedral or icosahedral symmetry. The main consequence of the Jahn-Teller effect is that the minimal energy configuration for such a molecule in an orbital triplet state will not be when the nuclei are in the completely symmetric configuration. Instead, the minimal energy occurs on an extended compact manifold of asymmetric configurations. Pseudorotations are vibronic excitations arising from free distortions of the molecular geometry on this compact manifold. The most general pseudorotational modes of electronic triplets involve a 5-dimensional space of normal mode coordinates for the positions of the nuclei within the molecule. These pseudorotations appear in the $T \otimes (e \oplus t)$ Jahn-Teller effect of tetrahedral molecules, the $T \otimes (e_g \oplus t_{2g})$ of octahedral molecules and the $T \otimes h_g$ Jahn-Teller effect of icosahedral molecules.

An important example of the Jahn-Teller effect for tetrahedral symmetry occurs for the methane cation $\text{CH}_4^+$. The lowest electronic orbital state of $\text{CH}_4^+$ is known to be a triplet and the resulting $T \otimes (e \oplus t_2)$ Jahn-Teller effect leads to a distortion of the molecule away from tetrahedral symmetry [56, 40, 54, 72, 22, 59]. Octahedral symmetry is common in nature and the $T \otimes (e_g \oplus t_{2g})$ Jahn-Teller effect has been studied extensively [50, 27, 51, 52, 14, 15]. For example, it occurs in cubic crystals such as $\text{CaO:Fe}^{2+}$ [35, 37] and $\text{MgO:Fe}^{2+}$ [33]. Also, it pays an important role in transition metal perovskite crystals such as $\text{BaTiO}_3$ [8] and $\text{KFe}_2^+\text{F}_3$ [41, 57] and triangular lattice Heisenberg antiferromagnetic crystals such as $\text{LiVO}_2$ and $\text{NaTiO}_2$ [55]. The importance of the Jahn-Teller effect in perovskites suggests that it may be important for high $T_c$ superconductivity. Another example of the $T \otimes (e_g \oplus t_{2g})$ Jahn-Teller effect are transition metal hexafluorides such as $\text{ReF}_6$ and $\text{OsF}_6$ [32, 46]. To date, the most famous example of an icosahedral molecule is the buckminsterfullerene molecule $\text{C}_{60}$. The $T \otimes h_g$ Jahn-Teller effect for this molecule is discussed in [23, 1, 45]. This brief survey of triplet Jahn-Teller effects is by no means exhaustive and we refer to [30, 20, 6, 7, 38, 8, 39] for more complete reviews.

The role of topology in the Jahn-Teller effect was first demonstrated in calculations of the $E \otimes e$ Jahn-Teller pseudorotations in triangular molecules [43, 71, 69, 70, 28]. Moreover, these calculations have been experimentally confirmed in [18]. It was realized that $E \otimes e$ pseudorotational wave functions are sections in the Möbius band, the unique nontrivial real line bundle over the circle. The simplicity of the Möbius band allowed the calculation to be treated as a boundary value problem. In other words, it sufficed to solve for wave functions on the interval $[0, 2\pi]$ satisfying $\psi(0) = -\psi(2\pi)$, rather than the usual boundary condition $\psi(0) = \psi(2\pi)$ for wave functions on a circle. We will see that topology permeates the Jahn-Teller problem for orbital triplets to a much greater extent and boundary value methods no longer suffice.

In order to determine the topology of the space of nuclear pseudorotations for an orbital triplet state, we first study spaces of $3 \times 3$ real symmetric matrices which have eigenvalues of predetermined multiplicities. The space of pseudorotations is
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isometric to a manifold constructed from the electronic eigenstates. A detailed description of both the topology and the Riemannian geometry of this manifold is presented. As a consequence of the nontrivial topology of the manifold of pseudorotations, the usual Born-Oppenheimer approximation cannot be applied to this problem. However, using a generalisation of the Born-Oppenheimer approximation to nontrivial vector bundles, we are able to compute vibronic energy levels in the strong Jahn-Teller coupling limit. In Section V, we use our results to compute the pseudorotational spectrum of $\text{CH}_4^+$. Our calculations are compared to measurements of the vibronic lines in the photoelectron spectrum of methane reported in [56].

2. Born-Oppenheimer Approximation

Consider a molecule with $a$ nuclei of mass $M$ and $z$ electrons of mass $m$. Neglecting contributions from electron spin, the molecular Hamiltonian is

$$H_{\text{mol}} = -\frac{1}{2M} \sum_{j=1}^{a} \Delta a_j - \frac{1}{2m} \sum_{i=1}^{z} \Delta z_i + V(a, z) + V_{\text{nuc}}(a) , \quad (2.1)$$

where $a_j$ is the position vector for the $j^{th}$ nucleus, $z_i$ is the position vector for the $i^{th}$ electron, and $\Delta x$ denotes the Laplacian for a coordinate vector $x$. Collectively, the coordinate vectors $a_j$ define a total configuration vector $a \in \mathbb{R}^{3a}$ for the nuclei and the $z_i$ define a total configuration vector $z \in \mathbb{R}^{3z}$ for the electrons. The term $V(a, z)$ is the potential energy for all electron-electron and electron-nucleus interactions and $V_{\text{nuc}}(a)$ is the potential energy for all nucleus-nucleus interactions. These potentials $V$ and $V_{\text{nuc}}$ are the summations over the usual sets of two-body Coulomb potential functions. For simplicity we have assumed that all of the nuclei have the same mass; however, this assumption is not essential for the results which we obtain.

Although the nuclear mass is at least four orders of magnitude larger than the electron mass, it has long been known that generally molecular vibrations cannot be described in terms of classical nuclear motion. Instead an understanding of molecular energy levels must take into account the quantum mechanical coupling between the electrons and the nuclei. To this end, the Hamiltonian $H_{\text{mol}}$ is usually treated using the Born-Oppenheimer approximation [10, 17, 25, 26]. In this approximation, one considers multiplets of $a$-dependent eigenvalues of the electronic Hamiltonian

$$H_{\text{el}}(a) = -\frac{1}{2m} \sum_{i=1}^{z} \Delta z_i + V(a, z) . \quad (2.2)$$

Taking the direct sum of all eigenspaces associated with the eigenvalues in a multiplet defines for each multiplet a $a$-dependent vector subspace of $L^2(\mathbb{R}^{3z}; \mathbb{C})$, the Hilbert space of complex-valued square-integrable functions on $\mathbb{R}^{3z}$. For each multiplet, an operator called the Born-Oppenheimer Hamiltonian is obtained by expanding $H_{\text{mol}}$ with respect to a $a$-dependent orthonormal basis for this subspace. At sufficiently low energy, the point spectrum of $H_{\text{mol}}$ is approximated by the union

\footnote{The term vibronic (vibrational + electronic) is usually used to describe this coupling.}
of the point spectra of the Born-Oppenheimer Hamiltonians obtained by subdividing
the point spectrum of $H_{\text{el}}(a)$ into disjoint multiplets. A complete description of
how much of the point spectrum of $H_{\text{mol}}$ may be approximated in this manner is
too detailed for inclusion here and we refer the reader to [17, 25, 26].

It follows from established results [75] that the eigenspaces of the electronic
Hamiltonian are classified by irreducible representations of the molecular symmetry
group. In this paper, we are considering 3-dimensional eigenspaces of $H_{\text{el}}$, which
are possible for molecules having tetrahedral, octahedral or icosahedral symme-
try. Denoting the fully symmetric nuclear configuration vector by $a_0 \in \mathbb{R}^{3a}$, the
eigenspaces of $H_{\text{el}}(a_0)$ are representation spaces of the molecular symmetry group.
This group is either the tetrahedral group $T_d$, the extended octahedral group $O_h$, or
the extended icosahedral group $Y_h$.

The 24-element group $T_d$ is the complete symmetry group of a regular tetrahe-
dron. In a common nomenclature, the irreducible representations of $T_d$ are $A_1$ and
$A_2$ of dimension one, $E$ of dimension two, and $T_1$ and $T_2$ of dimension three. Refer-
ence [44] may be consulted for a review of the representation theory of molecular
symmetry groups.

The complete symmetry group of a regular octahedron is $O_h$, which is isomor-
phic to the direct product of the octahedral group $O$ with the 2-element group $Z_2$.
The octahedral group $O$ consists of the 24 rotations about the symmetry axes of a
regular octahedron, whereas the extended octahedral group also includes reflections
in the plane perpendicular to each symmetry axis. The irreducible representations
of $O$ are $A_1$ and $A_2$ of dimension one, $E$ of dimension two, and $T_1$ and $T_2$ of dimension three. Each irreducible representation of $O$ determines two irreducible
representations of $O_h$. One of these, denoted by the subscript $u$, is odd under in-
verson about the origin and the other, denoted by the subscript $g$, is even under
inversion.

The complete symmetry group of a regular icosahedron is the extended icosa-
hedral group $Y_h$. This is a 120-element group, which is isomorphic to the direct
product of $Z_2$ with the icosahedral group $Y$. The irreducible representations of $Y$
are $A$ of dimension one, $T_1$ and $T_2$ of dimension three, $G$ of dimension four, and
$H$ of dimension five. As with $O_h$ above, each irreducible representation of $Y$ deter-
mines two irreducible representations of $Y_h$, one of which is even under inversion
and the other of which is odd under inversion.

We are considering a triplet eigenvalue of $\lambda$ of $H_{\text{el}}(a_0)$. The associated eigen-
value is classified by a 3-dimensional irreducible representation $T$ of the molecular
symmetry group. This representation must be one of the $T_1$ or $T_2$ representations
of $T_d$, the $T_{1u}$, $T_{1g}$, $T_{2u}$, or $T_{2g}$ representations of $O_h$, or the $T_{1u}$, $T_{1g}$, $T_{2u}$ or $T_{2g}$
representations of $Y_h$. Of course, nuclear motion will not preserve the molecular
symmetry and the degenerate eigenvalue $\lambda$ will be split into an almost degenerate
triplet $\{\lambda_1(a), \lambda_2(a), \lambda_3(a)\}$.

A convenient coordinate system for describing displacements of the nuclei
about the symmetric configuration $a_0$ are normal mode coordinates [42]. The nu-
clear configuration is specified by a normal mode coordinate vector $q \in \mathbb{R}^{3a-6}$,
where we have followed the usual procedure of eliminating the the coordinates for
rigid rotations and translations of the molecule. In this coordinate system, the symmetric configuration of the nuclei corresponds to $q = 0$. The advantage of normal mode coordinates is that they are also classified by the irreducible representations of the molecular symmetry group \([74, 42]\). Reducing the total vibrational representation of the molecular symmetry group into $l$ irreducible representations of dimensions $d_k$, for $k = 1, 2, \ldots, l$, induces a decomposition of the vector $q$ as

$$q = (q^1_1, q^1_2, \ldots, q^1_{d_1}, q^2_1, q^2_2, \ldots, q^2_{d_2}, \ldots, q_l^1, q_l^2, \ldots, q_l^{d_l}) . \tag{2.3}$$

Each subvector $q^k \in \mathbb{R}^{d_k}$ transforms according to one of the irreducible representations in the total vibrational representation.

It was shown by Jahn and Teller \([36]\) that the symmetric configuration is not a simultaneous minimum of the eigenvalues $\lambda_1(q)$, $\lambda_2(q)$ and $\lambda_3(q)$. They showed that for all molecules except linear molecules\(^2\)

$$\frac{\partial \lambda_1}{\partial q^k_j}(0) = \frac{\partial \lambda_2}{\partial q^k_j}(0) = \frac{\partial \lambda_3}{\partial q^k_j}(0) = 0, \quad \text{for all } j \text{ and } k, \tag{2.4}$$

if and only if the product representation $V[T^2]$ does not contain the identity representation. Here $[T^2]$ denotes the symmetric square of the electronic representation $T$ and $V$ denotes the vibrational representation. The complete list of these product representations for all molecular symmetry groups was decomposed in \([36]\) and it was found that with the exception of the axial symmetry groups, $V[T^2]$ always contains the identity representation\(^3\).

For the remainder of this paper we will use the labelling convention that

$$\lambda_1(q) \leq \lambda_2(q) \leq \lambda_3(q) . \tag{2.5}$$

Note that the imposition of this convention will mean that the $\lambda_i$ will not in general be differentiable at 0, because the eigenvalues will be re-ordered as $q$ passes through the point of degeneracy at 0.

For the symmetry group $T_d$, Jahn and Teller concluded that if the electronic irreducible representation $T$ is either of the representations $T_1$ or $T_2$, then the molecular symmetry will not be stable with respect to molecular distortions in normal modes classified by either of the $E$ and $T_2$ irreducible representations. In other words, equation (2.4) will not hold for $q^k$ corresponding to either of these representations. This Jahn-Teller effect is called the $T \otimes (e_g \oplus t_{2g})$ Jahn-Teller effect, where we are following the convention in the literature of using lower case to denote irreducible representations when they classify normal modes and upper case to denote irreducible representations when they classify eigenspaces of $H_{el}(a_0)$. The $e$ and $t_2$ normal modes are said to be Jahn-Teller coupled to the $T$ electronic state. Similarly, if $T$ is one of the 3-dimensional irreducible representations $T_{1g}$, $T_{1u}$, $T_{2g}$ or $T_{2u}$ of the group extended octahedral group $O_h$, then normal mode distortions classified by both the $E_g$ and $T_{2g}$ representations were found to be Jahn-Teller coupled to $T$. This is the $T \otimes (e_g \oplus t_{2g})$ Jahn-Teller effect of the molecular symmetry group $O_h$.

\(^2\)These are molecules having the axial symmetry groups $C_{\infty v}$ and $D_{\infty h}$.

\(^3\)It is now known how to prove the Jahn-Teller theorem without resorting to an itemisation of all irreducible representations of all molecular symmetry groups \([61, 9]\). These more sophisticated proofs shed light on the mathematical content of the Jahn-Teller theorem.
For the extended icosahedral group \( \mathcal{Y}_h \), if \( T \) is one of the 3-dimensional irreducible representations \( T_{1g}, T_{1u}, T_{2g} \) or \( T_{2u} \), then normal modes classified by the \( H_g \) representation are Jahn-Teller coupled to \( T \). This is the \( T \otimes h_g \) Jahn-Teller effect. Our results in this paper apply to all three of these Jahn-Teller effects.

In studying low energy excitations of the molecule, we will restrict the nuclear configuration space \( \mathbb{R}^{3a-6} \) to the 5-dimensional subspace \( N \subset \mathbb{R}^{3a-6} \) in which only the Jahn-Teller coupled normal modes are nonzero. Furthermore, we shall restrict \( q \) to a suitably bounded neighbourhood \( N' \) of \( 0 \) in the vector space \( N \). Specifically, \( N' \) should be starlike \(^4 \) from \( q = 0 \), which implies that \( N' \) is contractible. An appropriate bound on the diameter of \( N' \) ensures that the triplet \( \{ \lambda_1(q), \lambda_2(q), \lambda_3(q) \} \) will be bounded away from the remainder of the spectrum of \( H_{el}(q) \), for all \( q \in N' \). This amounts to assuming that we are studying distortions in which the molecule remains reasonably close to its symmetric configuration. In other words, we are considering molecular distortions, rather than some more general many-body problem.

Define \( Z(q) \) to be the 3-dimensional direct sum of the eigenspaces for the triplet \( \{ \lambda_1(q), \lambda_2(q), \lambda_3(q) \} \). Note that for some nonzero values of \( q \in N' \), the eigenvalues \( \lambda_i(q) \) will have twofold degeneracies. Contractibility of \( N' \) implies that there exists a globally defined smooth basis \( \{ e_1(q), e_2(q), e_3(q) \} \) for \( Z(q) \) over all \( q \in N' \). However, we shall see that it is not possible to choose this basis such that even one of the basis vectors \( e_i(q) \) is an eigenvector of \( H_{el}(q) \) for all \( q \in N' \).

The basis \( \{ e_1(q), e_2(q), e_3(q) \} \) defines a continuous map \( H_Z \) from \( N' \) to \( \text{Herm}(3, \mathbb{C}) \), the 9-dimensional real vector space of \( 3 \times 3 \) hermitian matrices with complex entries. The \( (i, j) \) entry of the matrix \( H_Z(q) \) is defined by the inner product

\[
H_Z(q)_{ij} = (e_i(q), H_{el}(q) e_j(q)),
\]

where \( (\cdot, \cdot) \) is the Hilbert space inner product on \( L^2(\mathbb{R}^{3z}; \mathbb{C}) \). If the Hamiltonian \( H_{el}(q) \) is time-reversal invariant, then there exists a real structure \(^5 \) on \( H_Z(N') \subset \text{Herm}(3, \mathbb{C}) \). Therefore, without loss of generality, we may assume that \( H_Z(N') \) is a subset of \( \text{Herm}(3, \mathbb{R}) \), the 6-dimensional vector subspace of all \( 3 \times 3 \) symmetric matrices with real entries. As we have omitted spin from the molecular Hamiltonian \( H_{mol} \), the electronic Hamiltonian \( H_{el}(q) \) is time-reversal invariant, provided that there is no external magnetic field.

The Jahn-Teller Hamiltonian \( H_{JT} \) is defined as the traceless part of \( H_Z(q) \) by

\[
H_Z(q) = s_0(q) I + H_{JT}(q),
\]

where \( s_0(q) = \frac{1}{3} \text{trace} (H_Z(q)) \) and \( I \) is the \( 3 \times 3 \) identity matrix. The functions \( s_0(q) \) and \( H_{JT}(q) \) are usually approximated by writing them as polynomials in the components of \( q \).

For the \( T \otimes (e \oplus t_2) \) and \( T \otimes (e_g \oplus t_{2g}) \) Jahn-Teller effects, we shall consider the coordinate vector \( (q_1, q_2) \) to transform according to the \( e \) or \( e_g \) representation and the \( (q_3, q_5, q_5) \) to transform according to the \( t_2 \) or \( t_{2g} \) representation. In the

\footnote{A subset \( X \subset \mathbb{R}^n \) is called starlike from the point \( x \in X \) if for every \( y \in X \) the line segment from \( x \) to \( y \) lies entirely in \( X \).}

\footnote{A subset \( K \) of \( \text{Herm}(3, \mathbb{C}) \) is said to be a real subset if there exists a fixed \( 3 \times 3 \) unitary matrix \( U \) such that \( U^* K U \subset \text{Herm}(3, \mathbb{R}) \).}
linear approximation to the Jahn-Teller effect, the Hamiltonian is taken as

\[
H_{JT}(\mathbf{q}) = \begin{pmatrix}
\frac{1}{\sqrt{6}} \kappa_1 q_1 - \frac{1}{\sqrt{2}} \kappa_1 q_2 & -\frac{1}{\sqrt{2}} \kappa_2 q_5 & -\frac{1}{\sqrt{2}} \kappa_2 q_4 \\
-\frac{1}{\sqrt{2}} \kappa_2 q_5 & \frac{1}{\sqrt{6}} \kappa_1 q_1 + \frac{1}{\sqrt{2}} \kappa_1 q_2 & -\frac{1}{\sqrt{2}} \kappa_2 q_3 \\
-\frac{1}{\sqrt{2}} \kappa_2 q_4 & -\frac{1}{\sqrt{2}} \kappa_2 q_3 & -\sqrt{\frac{2}{3}} \kappa_1 q_1
\end{pmatrix}
\] (2.8)

where \(\kappa_1\) is the Jahn-Teller coupling constant for the \(e\) or \(e_g\) normal mode and \(\kappa_2\) is the Jahn-Teller coupling constant to the \(t_2\) or \(t_{2g}\) normal mode. The quadratic restoring term is

\[
s_0(\mathbf{q}) = \frac{1}{2} \beta_1 (q_1^2 + q_2^2) + \frac{1}{2} \beta_2 \left(q_3^2 + q_4^2 + q_5^2\right),
\] (2.9)

where \(\beta_1\) is the quadratic coupling constant for the \(e\) or \(e_g\) normal mode and \(\beta_2\) is the quadratic coupling constant for the \(t_2\) or \(t_{2g}\) normal mode.

For the icosahedral \(T \otimes h_g\) Jahn-Teller effect, the entire 5-dimensional normal mode vector transforms according to the \(h_g\) representation. In this case there is one Jahn-Teller coupling constant \(\kappa\) and only one quadratic coupling constant \(\beta\). The linear Jahn-Teller Hamiltonian is

\[
H_{JT}(\mathbf{q}) = \kappa \begin{pmatrix}
\frac{1}{\sqrt{6}} q_1 - \frac{1}{\sqrt{2}} q_2 & -\frac{1}{\sqrt{2}} q_5 & -\frac{1}{\sqrt{2}} q_4 \\
-\frac{1}{\sqrt{2}} q_5 & \frac{1}{\sqrt{6}} q_1 + \frac{1}{\sqrt{2}} q_2 & -\frac{1}{\sqrt{2}} q_3 \\
-\frac{1}{\sqrt{2}} q_4 & -\frac{1}{\sqrt{2}} q_3 & -\sqrt{\frac{2}{3}} q_1
\end{pmatrix}
\] (2.10)

and the quadratic restoring term in the Hamiltonian is

\[
s_0(\mathbf{q}) = \frac{1}{2} \beta \left(q_1^2 + q_2^2 + q_3^2 + q_4^2 + q_5^2\right).
\] (2.11)

We will view \(H_{JT}\) as a continuous map from \(N'\) to \(\operatorname{Herm}_0(3, \mathbb{R})\), the 5-dimensional subspace of traceless matrices in \(\operatorname{Herm}(3, \mathbb{R})\). In this context, it is straightforward to verify that both (2.8) and (2.10) are vector space isomorphisms. If we define \(\operatorname{Herm}_0(3, \mathbb{R})\) as a metric space by endowing it with the metric product

\[
\langle A, B \rangle = \kappa^{-2} \operatorname{trace}(AB),
\] (2.12)

then the map \(H_{JT}\) defined in (2.10) is an isometry. Therefore, it is reasonable for us to simply identify \(N'\) with the corresponding open neighbourhood of the zero matrix in \(\operatorname{Herm}_0(3, \mathbb{R})\). Note that the inner product in (2.12) is proportional to the usual Hilbert-Schmidt metric on \(\operatorname{Herm}_0(3, \mathbb{R})\).

By making a judicious choice of another metric on \(\operatorname{Herm}_0(3, \mathbb{R})\), it is also possible to arrange for (2.8) to be an isometry. However, if we consider the equal coupling cases of the \(T \otimes (e \oplus t_2)\) and \(T \otimes (e_g \oplus t_{2g})\) Jahn-Teller effects, then the Hamiltonian (2.8) simplifies to (2.10) with \(\kappa_1 = \kappa_2 = \kappa\) and \(H_{JT}\) is an isometry with the metric defined in product (2.12). We shall assume for the remainder of this paper that the linear Jahn-Teller Hamiltonian is given by (2.10), because the simplicity of the inner product in (2.12) allows for a cleaner explanation of our methods. Nevertheless, our methods can be applied to more general inner product structures on \(\operatorname{Herm}_0(3, \mathbb{R})\), which allows the Jahn-Teller effect for the Hamiltonian (2.8) to be considered.
Let \( \mu_1, \mu_2 \) and \( \mu_3 \) denote the eigenvalues of \( H_J T \in \text{Herm}_0(3, \mathbb{R}) \). Note that \( \mu_i = \lambda_i - \frac{1}{3} \sum_{i=1}^3 \lambda_i \), for \( i = 1, 2, 3 \). We define within \( \text{Herm}_0(3, \mathbb{R}) \) the three maximal regions \( W_i \) for which the eigenvalue \( \mu_i \) is nondegenerate. We call these regions similar degeneracy regions. For example, \( W_1 \subset \text{Herm}_0(3, \mathbb{R}) \) consists of all matrices for which the bottom eigenvalue \( \mu_1 \) is nondegenerate. There are no constraints on \( \mu_2 \) and \( \mu_3 \), other than the imposed ordering
\[
\mu_1(q) < \mu_2(q) \leq \mu_3(q) \quad \tag{2.13}
\]
of the eigenvalues and the condition that the \( \sum_{i=1}^3 \mu_i \) vanish. From their definition, it is clear that each \( W_i \) is a smooth open submanifold of \( \text{Herm}_0(3, \mathbb{R}) \). In the following proposition, we determine the homotopy types of these similar degeneracy regions by constructing deformation retractions.

**Proposition 2.1.** There exist strong deformation retractions
\[
r_1 : W_1 \longrightarrow R_1 , \quad \tag{2.14a}
\]
\[
r_2 : W_2 \longrightarrow R_2 , \quad \tag{2.14b}
\]
\[
r_3 : W_3 \longrightarrow R_3 . \quad \tag{2.14c}
\]
The subspaces \( R_1 \) and \( R_3 \) have the homotopy type of \( \mathbb{RP}(2) \), the 2-dimensional real projective space of 1-dimensional vector subspaces in \( \mathbb{R}^3 \). The subspace \( R_2 \) has the homotopy type of 3-dimensional flag manifold \( \mathbb{RF}(1, 1, 1) \), consisting of ordered triples of mutually orthogonal 1-dimensional vector subspaces in \( \mathbb{R}^3 \).

**Proof.** We first construct these deformation retractions on the subspace of diagonal matrices \( W^D_i \) in \( W_i \). To this end, introduce the coordinates
\[
b = \frac{\mu_2 - \mu_1}{\mu_3 - \mu_1} \quad \text{and} \quad r = \sqrt{\mu_1^2 + \mu_2^2 + \mu_3^2} \quad \tag{2.15}
\]
and define
\[
D(b, r) = \frac{r}{\sqrt{6(1 - b + b^2)}} \begin{bmatrix}
- (1 + b) & 0 & 0 \\
0 & 2b - 1 & 0 \\
0 & 0 & 2 - b
\end{bmatrix} \quad \tag{2.16}
\]
Note that this is a well defined coordinate system for the diagonal matrices in the similar degeneracy regions, because \( \mu_3 > \mu_1 \) in each of the regions. For each \( W_i \), we now define homotopies \( \phi_i : W^D_i \times [0, 1] \longrightarrow W^D_i \) as follows:
\[
\phi_1(D(b, r), t) = D(b - t(b - 1) , r - t(r - 1)) \quad \tag{2.17a}
\]
\[
\phi_2(D(b, r), t) = D(b - t(b - \frac{1}{2}) , r - t(r - 1)) \quad \tag{2.17b}
\]
\[
\phi_3(D(b, r), t) = D(b - tb , r - t(r - 1)) \quad \tag{2.17c}
\]
These homotopies are deformations of $W_i^D$ onto

$$
\phi_1(D, 1) = \begin{bmatrix}
-\sqrt{\frac{2}{3}} & 0 & 0 \\
0 & \frac{1}{\sqrt{6}} & 0 \\
0 & 0 & \frac{1}{\sqrt{6}}
\end{bmatrix}, \quad \phi_2(D, 1) = \begin{bmatrix}
-\frac{1}{\sqrt{2}} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \frac{1}{\sqrt{2}}
\end{bmatrix}, \quad (2.18)
$$

and

$$
\phi_3(D, 1) = \begin{bmatrix}
\frac{1}{\sqrt{6}} & 0 & 0 \\
0 & -\frac{1}{\sqrt{2}} & 0 \\
0 & 0 & \frac{1}{\sqrt{6}}
\end{bmatrix}
$$

The finite-dimensional spectral theorem or principal axis theorem implies that all matrices $A \in W_i$ may be written as $A = O D O^t$, where $O$ is an element of $O(3)$, the group of orthogonal $3 \times 3$ matrices. This allows us to extend the deformations $\phi_i$ to deformations $\phi_i$ of $W_i$. Specifically, for $A = O D O^t$, we define

$$
\phi_i(A, t) = O \phi_i(D, t) O^t \quad (2.19)
$$

Note that $O$ is not uniquely determined, but any such $O$ will give the same result for $\phi_i(A, t)$, because the isotropy subgroup of the $O(3)$ action is the same for all $t \in [0, 1]$. Thus, $\phi_i$ is a well defined deformation. Furthermore, it is equivariant with respect to the action of $O(3)$ on $Herm_0(3, \mathbb{R})$. The retractions $r_i$ are now defined by $r_i(A) = \phi_i(A, 1)$. The homotopy types of the retracts $R_i$ follow from the isotropy subgroups of the $O(3)$ action on the diagonal matrices in $W_i$.

If $Z_1$ is the 1-dimensional eigenspace associated with $\mu_1$, then we may construct a real line bundle with fibre $Z_1$ over $W_1$ and total space

$$
X_1 = \{(v, A) \in \mathbb{R}^3 \times W_1 \mid Av = \mu_1 v\}. \quad (2.20)
$$

We denote this real line bundle by

$$
\xi_1 : \mathbb{R} \xrightarrow{\varphi_1} X_1 \xrightarrow{\phi_1} W_1 \quad (2.21a)
$$

where the projection operator is

$$
\varphi_1 : (v, A) \mapsto A. \quad (2.21b)
$$

Proving that $\xi_1$ satisfies the local triviality requirement of a vector bundle is not difficult. Similarly, the eigenspaces $Z_2$ and $Z_3$ for $\mu_2$ and $\mu_3$, respectively, may be used to construct real line bundles

$$
\xi_2 : \mathbb{R} \xrightarrow{\varphi_2} X_2 \xrightarrow{\phi_2} W_2 \quad (2.22)
$$

where

$$
\varphi_2 : (v, A) \mapsto A. \quad (2.21b)
$$
and
\[ \xi_3 : \mathbb{R} \xrightarrow{\varphi_3} X_3 \]
\[ \downarrow \]
\[ \varphi_3 \]
\[ W_3 \]
\[ \text{(2.23)} \]

**Proposition 2.2.** Over $\mathbb{R}P(2)$ is defined the canonical or tautological line bundle, $\tau$, and the bundles $\xi_1$ and $\xi_3$ are isomorphic to the pullback bundles $r_1^* \tau$ and $r_3^* \tau$, respectively. Over $\mathbb{R}F(1,1,1)$ are defined three canonical line bundles, $\tau_1$, $\tau_2$, and $\tau_3$, which are associated with the first, second, and third elements, respectively, in the triples of mutually orthogonal lines in $\mathbb{R}^3$. All three of these bundles are nontrivial, although their Whitney sum is isomorphic to the trivial $\mathbb{R}^3$ vector bundle over $\mathbb{R}F(1,1,1)$. The line bundle $\xi_2$ is isomorphic to the pullback bundle $r_2^* \tau_2$.

**Proof.** This proposition follows from the definition of the tautological bundles and the explicit construction of the line bundles, $\xi_i$, in terms of eigenspaces. □

We have established that none of the line bundles $\xi_1$, $\xi_2$, and $\xi_3$ are nontrivial because the maps $r_1$, $r_2$, and $r_3$ are deformation retractions. Furthermore, the first Stiefel-Whitney classes of $\xi_1$ and $\xi_3$ are the nontrivial elements in the cohomology groups
\[ H^1(W_1; \mathbb{Z}_2) = \mathbb{Z}_2 \quad \text{and} \quad H^1(W_3; \mathbb{Z}_2) = \mathbb{Z}_2, \]
respectively. The first Stiefel-Whitney class of $\xi_2$ is one of the three nontrivial elements of
\[ H^1(W_2; \mathbb{Z}_2) \cong \mathbb{Z}_2 \oplus \mathbb{Z}_2. \]
Precisely, it is the image of the first Stiefel-Whitney class of $\tau_2$ under $r_2^*$.

The usual Born-Oppenheimer approximation cannot be used to calculate the pseudorotational eigenvalues associated with each of the electronic eigenvalues $\lambda_1$, $\lambda_2$, and $\lambda_3$, because their corresponding real line bundles $\xi_1$, $\xi_2$, and $\xi_3$ are nontrivial. Instead, we must use a generalisation of the Born-Oppenheimer approximation to nontrivial vector bundles. To this end, we denote the intersection of $W_i \cap N'$ by $N_i$ and the restriction of $\xi_i$ to $N_i$ by $\eta_i$. The regions $N_i$ will be referred to as the similar degeneracy regions in $N'$. It follows from the Jahn-Teller Theorem that the electronic eigenvalue $\lambda_i(q)$ is minimised on a submanifold of $N_i$. Therefore, the molecular wavefunctions for low-energy pseudorotations associated with $\lambda_i$ are mostly supported on $N_i$. This leads us to make the approximation that these molecular wavefunctions lie in the Hilbert space $L^2(N_i \times \mathbb{R}^{3z}; \mathbb{R})$. By a standard construction \[58\], this Hilbert space is isomorphic to $L^2(N_i; L^2(\mathbb{R}^{3z}; \mathbb{R}))$. In order to define the Born-Oppenheimer

\[ \text{We remark that not only are each of the real line bundles } \xi_i \text{ nontrivial, but their complexifications are nontrivial complex line bundles. This contrasts with the } E \otimes e \text{ Jahn-Teller effect in which the the electronic eigenspaces form vector bundles which are isomorphic to the Möbius band. The complexification of the Möbius band is a trivial complex line bundle, which allows the Born-Oppenheimer Hamiltonian for the } E \otimes e \text{ Jahn-Teller effect to be written as a differential operator acting on complex-valued functions rather than sections of a nontrivial real line bundle. However, this approach to the } E \otimes e \text{ Jahn-Teller effect cannot be applied to the Jahn-Teller effect for orbital triplets.} \]
Hamiltonian associated with the \( i \)th electronic eigenspace, we shall view this Hilbert space in terms of the trivial vector bundle

\[
\epsilon_i : L^2(\mathbb{R}^3; \mathbb{R}) \xrightarrow{\cong} N_i \times L^2(\mathbb{R}^3; \mathbb{R}) \quad (2.26)
\]

Triviality of \( \epsilon_i \) implies that \( L^2(\epsilon_i) \), the Hilbert space of square integrable sections of \( \epsilon_i \), is canonically isomorphic to \( L^2(N_i; L^2(\mathbb{R}^3; \mathbb{R})) \). In light of these two isomorphism, the Hilbert space of molecular wavefunctions can be viewed as \( L^2(\epsilon_i) \) and the molecular Hamiltonian \( H_{\text{mol}} \) is therefore an operator on \( L^2(\epsilon_i) \).

The line bundle \( \eta_i \) is a sub-bundle of \( \epsilon_i \) and the Hilbert space \( L^2(\eta_i) \) is a subspace of \( L^2(\epsilon_i) \). We denote the projection operator onto \( L^2(\eta_i) \) by \( P_i \) and the projection operator onto the orthogonal complement of \( L^2(\eta_i) \) in \( L^2(\epsilon_i) \) by \( Q_i \). In terms of these vector bundles, the Born-Oppenheimer approximation states that the molecular Hamiltonian \( H_{\text{mol}} \) can be approximately restricted to \( L^2(\eta_i) \). Verifying this statement amounts to showing that \( Q_i H_{\text{mol}} P_i \) is small in some suitable sense. In the simplified context of diatomic molecules the accuracy of this approximation is analysed in \([17, 25, 26]\) and an expansion for higher order corrections is derived in \([25, 26]\). The approximate restriction of \( H_{\text{mol}} \) to \( L^2(\eta_i) \) is defined by

\[
B_i = P_i H_{\text{mol}} P_i : L^2(\eta_i) \rightarrow L^2(\eta_i) \quad (2.27)
\]

It is called the Born-Oppenheimer Hamiltonian.

Straightforward algebra establishes that \( B_i \) is a second order differential operator of the form

\[
B_i = -\nabla_i + V_i \quad (2.28)
\]

where the Laplacian \( \nabla_i \) is defined on the Hilbert space \( L^2(\eta_i) \) of square-integrable sections of \( \eta_i \) and the effective potential \( V_i \) is a bundle endomorphism of \( \eta_i \). The Laplacian acting on sections of a vector bundle is defined as follows.

**Definition 2.3 (Connection Laplacian).** Consider a vector bundle \( \xi \) over a Riemannian manifold \( \mathcal{M} \), with connection \( \nabla \). The tangent and cotangent bundles of \( \mathcal{M} \) are denoted by \( T\mathcal{M} \) and \( T^*\mathcal{M} \), respectively. The vector space of smooth sections of a vector bundle is denoted by \( C^\infty(\cdot) \). A connection on \( \xi \) is a bilinear map

\[
\nabla : C^\infty(T\mathcal{M}) \times C^\infty(\xi) \rightarrow C^\infty(\xi) \quad (2.29)
\]

This map, which is conventionally written as \( \nabla : (X, \sigma) \mapsto \nabla_X \sigma \), satisfies:

(i) \( \nabla_X(f \sigma) = (X \cdot f) \sigma + f \nabla_X \sigma \), where \( f \) is a function on \( \mathcal{M} \) and \( X \cdot f \) is the directional derivative of \( f \) in the direction \( X \).

(ii) \( X \cdot \langle \sigma, \omega \rangle = \langle \nabla_X \sigma, \omega \rangle + \langle \sigma, \nabla_X \omega \rangle \), where \( \langle \cdot, \cdot \rangle \) is the fibre-wise metric on \( \xi \).

Then on \( C^\infty(\xi) \), the covariant exterior differential relative to \( \nabla \),

\[
d : C^\infty(\xi) \rightarrow C^\infty(T^*\mathcal{M} \otimes \xi) \quad (2.30)
\]

is defined by \( d \sigma(X) = \nabla_X \sigma \). Note that \( C^\infty(T^*\mathcal{M} \otimes \xi) \) is simply the space of \( \xi \)-valued 1-forms.
The Connection Laplacian $\triangle : C^\infty(\xi) \rightarrow C^\infty(\xi)$ is defined by
\[
\triangle \sigma = -d^* d \sigma ,
\] (2.31)
where $d^*$ is the adjoint of $d$. In terms of the connection, it is given by $\triangle \sigma = \text{trace} \nabla^2 \sigma$. Finally, $\triangle$ is defined as a self-adjoint operator by a suitable extension of its domain to a Sobolev subspace of $L^2(\xi)$.

For the current situation in which $H_{\text{mol}}$ is time-reversal invariant and $\eta_i$ is a real line bundle, the connection $\nabla_i$ is the flat connection on $\eta_i$. Furthermore, a bundle endomorphism of a line bundle may be canonically identified with multiplication by a function on the base space. Therefore, $V_i$ is simply a potential function on $N_i$.

More generally, if $H_{\text{mol}}$ is not time-reversal invariant or if $\eta_i$ is a vector bundle with fibre dimension greater than or equal to 2, then the differential operator will contain derivatives of order one. However, the leading symbol of $B_i$ is the metric tensor of $N_i$ and therefore there exists a unique connection $\nabla$ on $\eta_i$ for which
\[
B_i = -\triangle \nabla_i + V_i ,
\] (2.32)
where $\triangle \nabla_i$ is the Laplacian with respect to $\nabla$ and $V_i$ is a bundle endomorphism [24, Lemma 4.8.1]. For the case in which $N_i$ is a region in Euclidean space, the connection $\nabla$ is the adiabatic connection described in [62].

The simplest approximation for the effective potential $V_i$ is
\[
V_i(q) = \lambda_i(q) + V_{\text{nuc}}(q) ,
\] (2.33)
where $V_{\text{nuc}}(q)$ is the nuclei-nuclei potential defined in (2.1) and $\lambda_i$ is an eigenvalue of $H_Z$ defined in (2.6).

It should be stressed that although the Hamiltonian (2.28) looks locally like the usual Born-Oppenheimer Hamiltonian, the global topology of a vector bundle is very important for any differential operator acting on sections of it. As an example, consider that the spectrum of the Laplacian acting on real-valued functions defined on the unit circle $S^1$ is \{n^2 \mid n = 0, 1, 2, \ldots \}, whereas the spectrum of the Laplacian acting on sections of the Möbius band over $S^1$ is \{n^2 \mid n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots \}.

We have chosen to make the nuclear mass implicit in the definition of $\triangle_i$ in (2.28) by including it in the definition of the Riemannian metric on $N_i$. In the normal mode coordinate system $(q_1, q_2, q_3, q_4, q_5)$, the covariant metric tensor on $N_i$ is defined to be
\[
g_{kl} = 2 \bar{M} \delta_{kl} ,
\] (2.34)
where $\delta_{kl}$ is the Kronecker delta tensor and $\bar{M}$ is the effective nuclear mass associated with the $e_g$ and $t_{2g}$ normal modes. In terms of these coordinates, the Laplacian $\triangle_i$ has the local form $\frac{1}{2\bar{M}} \sum_{k=1}^{5} \frac{\partial^2}{\partial q_k^2}$. Expressed in terms of the Hilbert-Schmidt inner product on $\text{Herm}_0(3, \mathbb{R})$ this Riemannian metric is
\[
g(A, B) = 2 \kappa^{-2} \bar{M} \text{ trace } (AB) ,
\] (2.35)
for $A$ and $B$ in $\text{Herm}_0(3, \mathbb{R})$.

The stable behaviour of the molecule is governed by the minima of the potentials $V_i$, which are bounded from below. The Jahn-Teller theorem implies that $V_i$ cannot be minimised at $q = 0$. Furthermore, the global minimum of $V_i$ is not an isolated point, but is a critical manifold $Y$, which is a compact submanifold of $N_i$. 
Note that the points \( q \in N' \) where two eigenvalues \( \lambda_i \) and \( \lambda_j \) cross transversally are singular points for the potentials \( V_i \) and \( V_j \), because the definition of these potentials incorporates the ordering (2.5). The potentials \( V_2 \) and \( V_3 \) may well be minimised at such singular points in \( N' \) and the Jahn-Teller theorem tells us nothing about such minima. However, depending on the molecular Hamiltonian and the details of the approximation used to derive \( V_i \), each of the effective potentials may also have differentiable local minima which correspond to some stable vibronic excitation of the molecule. The Jahn-Teller theorem does apply in this case and we can conclude that such minima cannot occur at \( q = 0 \). We will let \( Y \) denote any submanifold of \( N' \) on which one of the potentials \( V_i \) has a nonsingular minimum. The effective potential or Born-Oppenheimer Hamiltonian under consideration will be clear from context.

3. Foliations

In order to compute pseudorotational energy levels, we require detailed information about the geometry of \( Y \). We shall identify \( Y \) as a leaf of a foliation of a 4-dimensional sphere in the normal mode space \( N' \). As a consequence, we will be able not only to describe the geometry of \( Y \), but also precisely how \( Y \) is embedded in this sphere.

A foliation is a decomposition of a manifold into a layering of leaves. Any point in the manifold must be in exactly one leaf, which means that there can be no intersections between leaves and that the manifold must be completely filled by the leaves. We refer to [?] for the precise definition of a foliation and for an introduction to foliation theory.

Let \( S^4(r) \) denote the 4-dimensional sphere of radius \( r \) centred at the origin in \( N \). Under the identification of \( N \) with \( \text{Herm}_0(3, \mathbb{R}) \) we can view \( S^4(r) \) as being the sphere of radius \( r \) in \( \text{Herm}_0(3, \mathbb{R}) \). In this context, the sphere \( S^4(r) \) is invariant under the adjoint action of orthogonal group \( O(3) \). This action determines a decomposition of \( S^4(r) \) into orbits, where the orbit containing a matrix \( A \in S^4(r) \) is

\[
\{ B \in S^4(r) \mid B = O A O^t, \text{ for some } O \in O(3) \} .
\]  

(3.1)

The coordinate \( b \) introduced in (2.15) parameterises the orbit space of this action.

Note that the potential \( V_i \) depends on \( H_{el} \) only through the eigenvalue \( \lambda_i \). Both \( \lambda_i \) and the quadratic term \( s_0(q) \) are invariant under the adjoint action of \( O(3) \). Therefore, the minimising submanifold \( Y \) is entirely contained in a sphere \( S^4(r_0) \), where the radius \( r_0 \) depends on the physical parameters \( \kappa, \beta, \) and \( \bar{M} \). The similar degeneracy regions \( N_1, N_2, \) and \( N_3 \) each intersect this sphere \( S^4(r_0) \) and we denote the similar degeneracy regions in \( S^4(r_0) \) by

\[
\mathcal{W}_i = N_i \cap S^4(r_0) , \quad \text{for } i = 1, 2, 3 .
\]

(3.2)

The hierarchy of the submanifolds \( Y, S^4(r_0), \) and \( N' \) are shown in Figure [1]. Note that \( \mathcal{W}_2 = \mathcal{W}_1 \cap \mathcal{W}_3 \) and that \( \mathcal{W}_2 \) is the submanifold in \( S^4(r_0) \) where the three eigenvalues \( \mu_1, \mu_2 \) and \( \mu_3 \) are mutually distinct. Therefore, generically the minimising submanifold \( Y \) is contained in \( \mathcal{W}_2 \).
The open 5-dimensional manifold $N'$ is starlike about 0. The 4-dimensional sphere $S^4(r_0)$, which has radius $r_0$, is centred at 0 and is a submanifold of $N'$. The 3-dimensional submanifold $Y \subset S^4(r_0)$ is generically diffeomorphic to the real short flag manifold $\mathbb{RF}(1,1,1)$.

The restriction of the deformation retractions (2.14a) and (2.14c) to $S^4(r_0)$ are also deformation retractions. Although, it is not generally true that the restriction of a deformation retraction is also a deformation retraction, in this case each deformation retraction $r_i$ may be written as a composition of a deformation retraction of $W_i$ to $\mathcal{W}_i$ with a further retraction of $\mathcal{W}_i$. We denote $r_1(\mathcal{W}_1)$ by $\mathcal{R}_1$ and $r_3(\mathcal{W}_3)$ by $\mathcal{R}_3$. It follows from Proposition 2.1 that both $\mathcal{R}_1$ and $\mathcal{R}_3$ are diffeomorphic to the real projective space $\mathbb{RP}(2)$. However, the restriction of the deformation retraction (2.14b) to $S^4(r_0)$ implies that the similar degeneracy region $\mathcal{W}_2$ is diffeomorphic to $\mathbb{RF}(1,1,1) \times (0,1)$. This geometrical dichotomy suggests that the problem of calculating the pseudorotational spectra also divides into two cases. The pseudorotational spectra corresponding to $\lambda_1$ and $\lambda_3$ will be referred to as type I spectra, whereas the spectrum corresponding to $\lambda_2$ will be referred to as the type II spectrum. This terminology will also be used for the similar degeneracy regions associated with each of these eigenvalues.

The similar degeneracy regions $\mathcal{W}_i$ are open Riemannian submanifolds of the 4-dimensional sphere $S^4(r_0) \subset N$. They obtain their Riemannian metric from the restriction of the metric $g$ on $N$. It is important to note that the spectrum of the Born-Oppenheimer Hamiltonian $B_i$ depends crucially on the Riemannian geometry of $\mathcal{W}_i$. The first observation that we can make about the geometry of $\mathcal{W}_1$ and $\mathcal{W}_3$ is that they are isometric to each other as Riemannian manifolds. This follows from the inherent symmetry of the metric $g$.

For $0 < b < 1$, the orbits of the adjoint $O(3)$ action on $S^4(r_0)$ are diffeomorphic to the real flag manifold $\mathbb{RF}(1,1,1)$. These orbits, which we denote by $\mathfrak{S}(b)$, foliate the similar degeneracy region $\mathcal{W}_2$. The exceptional orbits when $b = 0$ and $b = 1$ are $\mathcal{R}_1$ and $\mathcal{R}_3$, respectively, because the deformation retractions $r_1$ and $r_3$ are
\( \mathfrak{W}_2 \approx \mathbb{R}F(1, 1, 1) \times (0, 1) \)

\[ \mathfrak{W}_1 \]

\[ \mathfrak{W}_3 \]

\[ \mathfrak{M}_1 = \mathfrak{F}(0) \approx \mathbb{R}P(2) \]

\[ \mathfrak{F}(b) \approx \mathbb{R}F(1, 1, 1) \]

\[ W_1 \approx \mathfrak{F}(b) \approx \mathbb{R}F(1, 1, 1) \times (0, 1) \]

\[ W_2 \approx \mathbb{R}F(1, 1, 1) \]

\[ W_3 \approx \mathbb{R}P(2) \]

Figure 2. Decomposition of \( S^4(r_0) \)

equivariant with respect to the \( O(3) \) action. Furthermore, \( \mathfrak{M}_1 \) and \( \mathfrak{M}_3 \) are isometric Riemannian manifolds. The decomposition of \( S^4(r_0) \) into similar degeneracy regions, which are in turn foliated into the orbits \( \mathfrak{F}(b) \), is shown in Figure 2.

Using a standard method for defining a coordinate system on a homogeneous space [29, Section II.4], we can construct coordinate systems on \( \mathfrak{F}(b) \) in terms of the Lie algebra of \( O(3) \). Specifically, define the diagonal matrix

\[
D(b) = \begin{pmatrix}
\frac{-r_0(1+b)}{(\sqrt{6})(\sqrt{1-b^2})} & 0 & 0 \\
0 & \frac{r_0(2b-1)}{(\sqrt{6})(\sqrt{1-b^2})} & 0 \\
0 & 0 & \frac{r_0(2-b)}{(\sqrt{6})(\sqrt{1-b^2})}
\end{pmatrix}
\]

and the following basis for the Lie algebra of \( O(3) \):

\[
E_1 = \begin{pmatrix}0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0\end{pmatrix}, \quad E_2 = \begin{pmatrix}0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0\end{pmatrix}, \quad E_3 = \begin{pmatrix}0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0\end{pmatrix}
\]

Then, terms of these matrices, a coordinate system for \( S^4(r_0) \) is

\[
A(b, x_1, x_2, x_3) = [\exp(x_2 E_2)]^t [\exp(x_1 E_1)]^t [\exp(x_3 E_3)]^t D(b) [\exp(x_3 E_3)] [\exp(x_1 E_1)] [\exp(x_2 E_2)]
\]

Using this coordinate system and related coordinate systems, it is straightforward to compute various geometrical quantities.

First, the Gaussian curvatures of \( \mathfrak{M}_1 \) and \( \mathfrak{M}_3 \) are constant and both equal to \((3r_0^2)^{-1}\). It is interesting to note that for \( r_0 = 1 \), the submanifolds \( \mathfrak{M}_1 \) and \( \mathfrak{M}_3 \) are both isometric to the image of the well-known Veronese embedding [3] [13] of \( \mathbb{R}P(2) \) into \( S^4 \). This embedding has also been studied by Massey [48] who called it the “canonical” embedding of \( \mathbb{R}P(2) \) into a sphere of minimum dimension. The lowest dimensional sphere into which \( \mathbb{R}P(2) \) can be embedded is \( S^4 \).
Consider now the generic leaves when $b \in (0, 1)$. The leaves $\mathfrak{F}(b)$ form a geodesically parallel family of submanifolds in $S^4(r_0)$. In terms of the coordinate system (3.3), the vector field $\frac{\partial}{\partial b}$ is a normal vector field to $\mathfrak{F}(b)$, which generates a geodesic flow from leaf to leaf. Furthermore, the adjoint action of $O(3)$ on $\text{Herm}_0(3, \mathbb{R})$ defines a connected closed subgroup of the isometry group of $\text{Herm}_0(3, \mathbb{R})$. Therefore, it follows from [3, Prop. 3.8.2] that for $b \in (0, 1)$, the orbits of this action form an isoparametric family of hypersurfaces in $S^4(r_0)$. Hence, the principal curvatures of $\mathfrak{F}(b)$ are constant. By direct computation, we find that they are

$$k_1(b) = \frac{1}{\sqrt{3} r_0} \frac{b - 2}{b} \quad (3.4a)$$
$$k_2(b) = \frac{1}{\sqrt{3} r_0} \frac{2b - 1}{1 - b} \quad (3.4b)$$
$$k_3(b) = \frac{1}{\sqrt{3} r_0} \frac{1 + b}{1 - b} \quad (3.4c)$$

Note that these principal curvatures are distinct, satisfying $k_1(b) < k_2(b) < k_3(b)$, for all $b \in (0, 1)$, and therefore, this is an isoparametric family of type 3. For $r_0 = 1$, it is isometric to Cartan’s isoparametric family in $S^4$. The focal submanifolds of this family are $\mathfrak{R}_1$ and $\mathfrak{R}_3$.

An $r$-dimensional submanifold is said to be minimal if its $r$-dimensional volume is locally extremal. It follows from results in [34] that $\mathfrak{R}_1$ and $\mathfrak{R}_3$ are minimal submanifolds of $S^4(r_0)$, because they are isolated orbits of the adjoint action of $O(3)$ on $S^4(r_0)$. Also, at least one of the submanifolds $\mathfrak{F}(b)$, for $b \in (0, 1)$, must be minimal. The submanifold $\mathfrak{F}(b)$ will be minimal if and only if its mean curvature vanishes. The mean curvature of $\mathfrak{F}(b)$ is

$$h(b) = \frac{1}{3} \sum_{i=1}^{3} k_i(b) = \frac{1}{3\sqrt{3} r_0} \frac{(2 - b)(2b - 1)(b + 1)}{(1 - b)b} \quad (3.5)$$

and the only value of $b \in (0, 1)$ for which $h(b)$ vanishes is $b = \frac{1}{2}$. Therefore, $\mathfrak{F}(\frac{1}{2})$ is a minimal submanifold.

The Gauss-Codazzi equations imply that for hypersurfaces in $S^4$, the scalar curvature is given by

$$\text{scal} = 6 - \sum_{i=1}^{3} k_i^2 + 9 h^2. \quad (3.6)$$

Substituting from (3.4), we find that the scalar curvature of $\mathfrak{F}(b)$ is $\text{scal}(b) = 0$, for all $b \in (0, 1)$.

The rejections $r_1$ and $r_3$ determine foliations of the similar degeneracy regions $\mathcal{W}_1$ and $\mathcal{W}_3$, respectively. These foliations will be useful in determining the

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1Isoparametric hypersurfaces in a manifold $\mathcal{M}$ are generally defined as the regular level hypersurfaces of an isoparametric function on $\mathcal{M}$. However, an equivalent definition for hypersurfaces in a sphere is that a family is isoparametric if and only if the hypersurfaces are geodesically parallel and have constant principal curvatures. See [3, Sect. 5.2.e] and [13, Sect. 3.1]. Such a family is said to be of type $n$ if there are $n$ distinct principal curvatures.
spectra of the Born-Oppenheimer Hamiltonians. The leaves of the foliation $\mathcal{F}_i$ of $\mathcal{W}_i$ are defined to be

$$\mathcal{L}_i(y) = r_i^{-1}(y),$$

for each $y \in \mathcal{R}_i$ and $i = 1, 3$. By construction there is a one-to-one correspondence between leaves of $\mathcal{F}_i$ and points in $\mathcal{R}_i$. Hence, we can view $\mathcal{R}_i$ as the leaf space of $\mathcal{F}_i$. Furthermore, the foliations $\mathcal{F}_1$ and $\mathcal{F}_3$ are isometric, with the substitution $b \mapsto 1 - b$ taking one to the other.

**Proposition 3.1.** The foliations $\mathcal{F}_1$ and $\mathcal{F}_3$ are totally geodesic foliations\footnote{A submanifold $\mathcal{M} \subset \mathcal{M}'$ is said to be totally geodesic if every geodesic in $\mathcal{M}$ is also a geodesic in $\mathcal{M}'$. A foliation is totally geodesic if each leaf of the foliation is totally geodesic.} of $\mathcal{W}_1$ and $\mathcal{W}_3$, respectively.

**Proof.** It suffices to consider just $\mathcal{F}_1$, because the two foliations are isometric. The adjoint action of $O(3)$ on $\mathcal{W}_1$ is a transitive action on the leaf space of $\mathcal{F}_1$. This implies that any two leaves of $\mathcal{F}_1$ are isometric and we need only show that one of the leaves is totally geodesic.

A submanifold is totally geodesic if and only if its second fundamental form vanishes \cite[Theorem 4.1]{53}. In terms of the coordinate system in (3.3), the leaf corresponding to the diagonal matrix in the leaf space $\mathcal{R}_1$ is

$$\mathcal{L}_1(D) = \{ A(b, x_1, x_2, x_3) \mid b \in [0, 1), x_1 = 0, x_2 = 0, x_3 \in [0, \pi) \}. \quad (3.8)$$

An orthogonal frame field for the tangent bundle $T\mathcal{L}_1(D)$ is

$$\frac{\partial}{\partial x_0} = \frac{\partial A}{\partial b} \bigg|_{x_1=x_2=0} \quad \text{and} \quad \frac{\partial}{\partial x_3} = \frac{\partial A}{\partial x_3} \bigg|_{x_1=x_2=0} \quad (3.9)$$

In terms of this coordinate system, the second fundamental form of $\mathcal{L}_1(D)$ is

$$\Psi \left( \frac{\partial}{\partial x_i}, \frac{\partial}{\partial x_j} \right) = \sum_{l=1}^2 \Gamma^l_{ij} \frac{\partial}{\partial x_l}, \quad (3.10)$$

where $i, j = 0, 3$ and $\Gamma^l_{ij}$ are the Christoffel symbols of the second kind. Computing the relevant Christoffel symbols gives

$$\begin{align*}
\Gamma^1_{00} &= 0 & \Gamma^2_{00} &= 0 \\
\Gamma^1_{33} &= 0 & \Gamma^2_{33} &= 0 \\
\Gamma^1_{03} &= \Gamma^1_{30} = 0 & \Gamma^2_{03} &= \Gamma^2_{30} = 0
\end{align*} \quad (3.11)$$

on $\mathcal{L}_1(D)$. Therefore, $\Psi = 0$ on $\mathcal{L}_1(D)$. \[\square\]

In order to give a detailed description of the geometry of the leaves of $\mathcal{F}_1$ and $\mathcal{F}_3$, we first consider $S^2(r_0)$, the 2-dimensional sphere with the same radius as the ambient 4-sphere, $S^4(r_0)$. On $S^2(r_0)$ define geographical coordinates $(\varphi, \vartheta)$, where $\varphi \in [0, 2\pi)$ is the angle of longitude and $\vartheta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ is the angle of latitude. A straightforward computation using the coordinate system in (3.3) establishes the following result.
Proposition 3.2. For \( i = 1, 2 \), each leaf \( \mathcal{L}_i(y) \) of \( \mathcal{F}_i \) is isometric to the submanifold of \( S^2(r_0) \) which is defined by
\[
\left\{ (\varphi, \vartheta) \in S^2(r_0) \mid \frac{\pi}{6} < \vartheta \leq \frac{\pi}{2} \right\}.
\] (3.12)

In this coordinate system, the point \( y \in \mathcal{R}_1 \) corresponds to the north pole at \( \vartheta = \frac{\pi}{2} \). In other words, \( \mathcal{L}_i(y) \) is a 2-dimensional sphere of radius \( r_0 \), which has been truncated at 30° latitude. This truncated sphere is attached to \( \mathcal{R}_1 \) at \( y \), the north pole of \( \mathcal{L}_i(y) \).

On a leaf \( \mathcal{L}_1(y) \) of the foliation \( \mathcal{F}_1 \), the coordinate \( b \) is related to the latitude coordinate \( \varphi \) by
\[
\cos \varphi = \frac{\sqrt{3} b}{2 \sqrt{1 - b + b^2}}.
\] (3.13)

It follows that the leaves of the foliation \( \mathcal{F}_1 \) intersect \( \mathcal{F}(b) \) in circles of constant latitude on \( \mathcal{L}_1(y) \). This defines a foliation \( \mathcal{C}_1(b) \) of \( \mathcal{F}(b) \) by circles of radius \( r_0 \cos \varphi \). The leaves of this foliation are \( \mathcal{C}_1(y) = \mathcal{L}_1(y) \cap \mathcal{F}(b) \), for \( y \in \mathcal{R}_1 \), which implies that the leaf space of \( \mathcal{C}_1(b) \) is homeomorphic to \( \mathcal{R}_1 \). It follows from the Christoffel symbols calculated in (3.11) that the leaves of \( \mathcal{C}_1(b) \) are geodesics in \( \mathcal{F}(b) \), which means that \( \mathcal{C}_1 \) is a geodesic flow. Similarly, the intersection of the leaves of \( \mathcal{F}_3 \) with \( \mathcal{F}(b) \) give another geodesic flow, \( \mathcal{C}_3(b) \). Furthermore, the main theorem in [21] implies that \( \mathcal{C}_1(b) \) and \( \mathcal{C}_3(b) \) are Seifert fibrations of \( \mathcal{F}(b) \).

The leaves of the foliation \( \mathcal{F}_1 \) are also the fibres of the normal bundle of the embedding of \( \mathcal{R}_1 \) in \( S^4(r_0) \). We shall stretch our notation by using \( \mathcal{F}_1 \) to also denote this normal bundle. To understand \( \mathcal{F}_1 \) as a bundle, it is useful to compute its Euler class, which is an element the cohomology group \( H^2(\mathbb{R}P(2) ; \mathbb{Z}) \). It is necessary to use cohomology with twisted integer coefficients, denoted by \( \mathbb{Z} \), because \( \mathcal{R}_1 \) is a nonorientable manifold.

Proposition 3.3. The Euler class of \( \mathcal{F}_1 \) is \( e(\mathcal{F}_1) = \pm 2 \in H^2(\mathbb{R}P(2) ; \mathbb{Z}) \cong \mathbb{Z} \), where a choice of sign corresponds to a choice of orientation on \( S^4(r_0) \).

Proof. This follows directly from a general result that was conjectured by H. Whitney and proven by W. S. Massey [47]. Specifically, if \( \mathcal{M} \) is a closed, connected, nonorientable surface embedded in \( S^4 \), then the Euler class of the normal bundle has one of the following values:
\[
2\chi - 4, \ 2\chi, \ 2\chi + 4, \ldots, \ 4 - 2\chi,
\] (3.14)
where \( \chi \) is the Euler characteristic of \( \mathcal{M} \).

The Euler characteristic of \( \mathcal{R}_1 \) is \( \chi = \sum (-1)^q \dim H^q(\mathcal{R}_1 ; \mathbb{R}) = 1 \). \( \Box \)

Some additional insight can be gained by a more direct computation of \( e(\mathcal{F}_1) \). Consider the universal covering
\[
\mathbb{Z}_2 \hookrightarrow S^2(\sqrt{3} r_0) \rightarrow \mathcal{F}_1
\] (3.15)
The pullback by $p_1$ of the tangent bundle $T\mathfrak{N}_1$ is isomorphic to the tangent bundle $TS^2(\sqrt{3}r_0)$, because $p_1$ is a covering map. Therefore, the induced map on cohomology, $p_1^* : H^2(\mathfrak{N}_1; \mathbb{Z}) \rightarrow H^2(S^2; \mathbb{Z})$, must map the Euler class of $T\mathfrak{N}_1$ to the Euler class of $TS^2(\sqrt{3}r_0)$. This implies that the map $p_1^*$ above must be the multiplication by 2 map from $\mathbb{Z}$ to $\mathbb{Z}$, because the Euler characteristic of $S^2$ is 2.

Having identified the map $p_1^* : H^2(\mathfrak{N}_1; \mathbb{Z}) \rightarrow H^2(S^2; \mathbb{Z})$, we now consider the pullback bundle $p_1^*(\mathcal{F}_1)$. By looking directly at how $\mathcal{F}_1$ is constructed, it is apparent that $p_1^*(\mathcal{F}_1)$ is isomorphic to the associated projective tangent bundle over $PTS^2$. This bundle is constructed by considering the unit tangent bundle over $S^2$ and identifying each unit tangent vector with its negative. Therefore, the circle fibres of the unit tangent bundle double cover the $\mathbb{R}P(1)$ fibres of projective tangent bundle. Of course, $PTS^2$ is also an $S^1$ bundle over $S^2$. Furthermore, the Euler class of this bundle is $e(PTS^2) = 2e(TS^2) = 4$, which implies that the Euler class $e(p_1^*(\mathcal{F}_1))$ is equal to $\pm 4$, where the sign depends on whether our choice of orientation for $S^2$ is consistent with the orientation on $S^4(r_0)$. Recalling that we have already shown that $p_1^* : H^2(\mathfrak{N}_1; \mathbb{Z}) \rightarrow H^2(S^2; \mathbb{Z})$ is multiplication by 2, we conclude that the Euler class of $\mathcal{F}_1$ is $\pm 2$.

The nontriviality of the Euler class $e(\mathcal{F}_1)$ implies that $\mathfrak{M}_1$ is not simply a product of the leaf space $\mathfrak{N}_1$ with a generic leaf $\mathcal{L}_1(y)$, but rather, the leaves are twisted together in a complicated fashion. Note that up to sign, the Euler class $e(\mathcal{F}_3)$ is equal to the Euler class of $\mathcal{F}_1$.

We now examine further the geodesic flows $\mathcal{C}_i(b)$ in $\mathfrak{F}(b)$. The restriction of the deformation retraction $r_1$ to $\mathfrak{F}(b)$ is a submersion from $\mathfrak{F}(b)$ to $\mathfrak{N}_1$. The fibres of this submersion are the leaves of the geodesic flow $\mathcal{C}_1$. The manifold $\mathfrak{N}_1$ can be viewed as the leaf space of $\mathcal{C}_1(b)$. However, note that although $\mathfrak{N}_1$ carries a natural Riemannian metric when viewed as a submanifold of $S^4(r_0)$, this metric may not be the natural metric for $\mathfrak{N}_1$ when viewed as the leaf space of $\mathcal{C}_1(b)$. The tangent space $T_x \mathfrak{F}(b)$ decomposes into a 1-dimensional vertical subspace $T_x \mathcal{C}_1(b)$ and a 2-dimensional horizontal subspace $N_x \mathcal{C}_1(b)$. This decomposition allows us to decompose the measure on $\mathfrak{F}(b)$ into a leaf measure and an invariant transverse measure. With this decomposition we are able to compute the volume of $\mathfrak{F}(b)$.

**Proposition 3.4.** The volume of $\mathfrak{F}(b)$ is

$$\text{vol}(\mathfrak{F}(b)) = \frac{6\sqrt{3}b(1-b)\pi^2r_0^3}{(1-b+b^2)^{\frac{3}{2}}}. \quad (3.16)$$

Recall from (3.5) that $\text{vol}(\mathfrak{F}(b))$ must have a local extremum at $b = \frac{1}{2}$. From this proposition, we see that $\text{vol}(\mathfrak{F}(b))$ has a maximum at $b = \frac{1}{2}$, for $b \in (0, 1)$.

**Proof.** The principal curvatures in $\mathfrak{F}(b)$ are eigenvalues of the second fundamental form of the embedding of $\mathfrak{F}(b)$ in $S^4(r_0)$. Eigenvectors corresponding to these eigenvalues are called principal vector fields on $\mathfrak{F}(b)$. In can be verified by explicitly computing the second fundamental form that a tangent vector field to the leaves of $\mathcal{C}_1(b)$ is a principal vector field associated with the principal curvature $k_1(b)$. This implies that $\mathcal{C}_1(b)$ is a principal foliation of $\mathfrak{F}(b)$. Similarly, the foliation $\mathcal{C}_3(b)$ is the principal foliation associated with the principal curvature $k_3(b)$.
principal foliation, which is associated with \( k_2(b) \), shall be denoted by \( C_2(b) \). Although \( C_2(b) \) is also a circle foliation of \( \mathcal{F}(b) \), it does not arise from a deformation retraction in the same way as \( C_1 \) and \( C_3 \).

The horizontal subspaces define the normal bundle \( NC_1(b) \) and the tangent bundle \( T\mathcal{F}(b) \) decomposes into the Whitney sum \( TC_1(b) \oplus NC_1(b) \). Furthermore, \( dr_1 \), the differential of \( r_1 \), maps the normal bundle \( NC_1(b) \) to the tangent bundle \( T\mathcal{R}_1 \). In terms of the coordinate system \((3,3)\), orthonormal principal vector fields for \( C_2(b) \), and \( C_3(b) \), respectively, are

\[
V_2(r_0) = \frac{r_0 \sqrt{1 - b + b^2}}{\sqrt{3}(1 - b)} \left[ \cos x_3 \frac{\partial}{\partial x_1} + \frac{\sin x_3}{\cos x_1} \frac{\partial}{\partial x_2} + \frac{\sin x_1 \sin x_3}{\cos x_1} \frac{\partial}{\partial x_3} \right] \tag{3.17a}
\]

\[
V_3(r_0) = \frac{r_0 \sqrt{1 - b + b^2}}{\sqrt{3}} \left[ -\sin x_3 \frac{\partial}{\partial x_1} + \frac{\cos x_3}{\cos x_1} \frac{\partial}{\partial x_2} + \frac{\cos x_3 \sin x_1}{\cos x_1} \frac{\partial}{\partial x_3} \right] \tag{3.17b}
\]

These vector fields provide a frame for \( NC_1(b) \). Also, the vector fields

\[
X_1(r_0) = \frac{r_0}{\sqrt{3}} \frac{\partial}{\partial x_1} \bigg|_{b=0} \quad \text{and} \quad X_2(r_0) = \frac{r_0}{\sqrt{3} \cos x_1} \frac{\partial}{\partial x_2} \bigg|_{b=0}
\]

give an orthonormal frame for \( \mathcal{R}_1 \).

It follows from the definition of \( r_1 \) as a deformation retract that

\[
\begin{align*}
\frac{dr_1}{dx_1} &= \frac{\partial}{\partial x_1} \bigg|_{b=0} \\
\frac{dr_1}{dx_2} &= \frac{\partial}{\partial x_1} \bigg|_{b=0} \\
\frac{dr_1}{dx_3} &= 0
\end{align*}
\]

Therefore, the Jacobian of \( r_1 \) is \( \frac{1-b+b^2}{1-b} \). This implies that \( r_1 \) gives a decomposition of the measure on \( \mathcal{F}(b) \) into horizontal and vertical components if the leaf space is taken to be \( \mathbb{R}P(2) \) with constant Gaussian curvature

\[
K_1 = \frac{1-b}{3r_0^2(1-b+b^2)} \tag{3.20}
\]

The volume of \( \mathbb{R}P(2) \) with curvature \( K_1 \) is \( \frac{6\pi r_0^2 (1-b)}{1-b+b^2} \) and from equation \((3.13)\) the circumference of \( C_1(b) \) is \( \frac{\sqrt{3} \pi r_0 b}{2\sqrt{1-b+b^2}} \). The proposition then follows from Fubini’s theorem.

4. Covering Spaces

Recall that the Born-Oppenheimer Hamiltonian, \( B_i \), acts on \( L^2 \) sections of the line bundle \( \eta_i \). Furthermore, the effective potential, \( V_i \), is minimised on a submanifold \( Y \subset S^4(r_0) \), which corresponds to one of the leaves \( \mathcal{F}(b) \) of the isoparametric foliation of \( S^4(r_0) \). Molecular excitations may be viewed as motion on the energy minimising submanifold \( Y \) coupled with oscillations normal to \( Y \). If the quadratic Jahn-Teller coupling constant is large, then these two types of excitations will
be effectively decoupled. In this case, eigensections of $B_i$ are approximated by tensor products of sections in $\eta|_Y$, the restriction of the line bundle $\eta_i$ to $Y$, with functions of the coordinates for $N_2$ which are normal to $Y$. These sections of $\eta|_Y$ will be eigensections of the restriction of $B_i$ to $Y$, denoted by $R_i : L^2(\eta|_Y) \to L^2(\eta|_Y)$. This Schrödinger operator has the form

$$R_i = -\triangle_i(Y) + v_i,$$

where $\triangle_i(Y)$ is the Laplacian with respect to the flat connection on $L^2(\eta|_Y)$ and the constant $v_i$ is the value of $V_i$ on $Y$. Physically, the spectrum of the operator $R_i$ represents the quantum energy levels of a free particle on the compact manifold $Y$, with a state space twisted according to the line bundle $\eta$. A particle trajectory on $Y$ corresponds to a path of nuclear configurations within a compact submanifold of the nuclear configuration space of the molecule. Vibronic excitations of this nature are called pseudorotations, because they have the character of a generalised rotation. We remark that it is only in the context of the strong Jahn-Teller coupling approximation that it makes sense to interpret a special class of vibronic excitations as pseudorotations. If the Jahn-Teller coupling is not strong, then eigenvectors of the Born-Oppenheimer Hamiltonian cannot be decomposed into two types of excitations, pseudorotations and normal oscillations, which are effectively decoupled.

To find the spectrum of $R_i$, we will need to study its pullback over the universal covering projections of the leaves in our isoparametric foliation of $S^4(\tau_0)$. The fibre of the universal covering $p : \tilde{\mathcal{F}}(b) \to \mathcal{F}(b)$ is the fundamental group, $\pi_1(\tilde{\mathcal{F}}(b))$. For $b$ equal to either 0 or 1, we have that $\pi_1(\mathcal{F}_1) = \pi_1(\mathcal{F}_3) = \pi_1(\mathbb{R}P(2)) = \mathbb{Z}_2$. For $b \in (0, 1)$, the fundamental group of $\tilde{\mathcal{F}}(b)$ is isomorphic to $\pi_1(\mathbb{R}F(1, 1, 1))$. In the following proposition, we show that this is isomorphic to $Q_8$, the 8-element group of unit quaternions.

**Proposition 4.1.** The fundamental group of $\mathbb{R}F(1, 1, 1)$ is isomorphic to $Q_8$.

**Proof.** From Figure 2 we have that $\mathcal{M}_2 = \mathcal{M}_1 \cap \mathcal{M}_3$, where the homotopy types of these spaces are $\mathcal{M}_1 \simeq \mathbb{R}P(2)$, $\mathcal{M}_3 \simeq \mathbb{R}P(2)$, and $\mathcal{M}_2 \simeq \mathbb{R}F(1, 1, 1)$. The Mayer-Vietoris homology exact sequence for $\mathcal{M}_2 = \mathcal{M}_1 \cap \mathcal{M}_3$ gives $H_1(\mathbb{R}F(1, 1, 1); \mathbb{Z}) \simeq \mathbb{Z}_2 \oplus \mathbb{Z}_2$. Furthermore, the homotopy exact sequence for the fibre bundle

$$O(1) \times O(1) \times O(1) \xrightarrow{i} O(3) \xrightarrow{p} \mathbb{R}F(1, 1, 1)$$

implies that $\pi_1(\mathbb{R}F(1, 1, 1))$ is an 8-element group. In addition, the Hurewicz theorem implies that the commutator subgroup of $\pi_1(\mathbb{R}F(1, 1, 1))$ is $\mathbb{Z}_2$.

Up to isomorphism, there are only two nonabelian groups with 8 elements: the quaternion group $Q_8$ and the dihedral group $D_8$. Of these two groups, only $Q_8$ can be the fundamental group of a closed 3-manifold, $\mathcal{M}$. This is because the universal covering space of any closed 3-manifold with finite fundamental group has the homotopy type of $S^3$ [3, Thm. 3.6]. From this it follows that any element of order two in $\pi_1(\mathcal{M})$ must belong to the centre of $\pi_1(\mathcal{M})$ [?, Cor. 1]. However, $D_8$ contains an element of order two which is not in its centre. \qed
Over $p$ we have the following pullback square,

\[
\begin{array}{ccc}
\mathbb{R} & \xrightarrow{\pi_1(\mathbb{R})} & \mathbb{R} \\
\downarrow & & \downarrow \\
\tilde{X}_i(b) & \xrightarrow{\varphi_i} & X_i(b) \\
\downarrow & & \downarrow \\
\mathbb{R} & \xrightarrow{\pi_1(\mathbb{R})} & \mathbb{R} \\
\end{array}
\] (4.3)

for each of the real line bundles $\varrho_i(b) = \eta_i|\tilde{\mathbb{R}}(b)$. Note that $\varrho_1(b)$ is only well-defined for $0 \leq b < 1$, $\varrho_2(b)$ is only well defined for $0 < b < 1$, and $\varrho_3(b)$ is only well defined for $0 < b \leq 1$. The map $\tilde{\varphi}_i$ is the projection of the real line bundle $\tilde{\varrho}_i$, which is the pullback of $\varrho_i$ over $p$. The total space of $\tilde{\varrho}_i$ is defined as

\[
\tilde{X}_i(b) = \left\{(y, x) \in \tilde{\mathbb{R}}(b) \times X_i(b) \mid p(y) = \varphi_i(x)\right\}
\] (4.4)

and the projection $\tilde{\varphi}_i$ is defined by $\tilde{\varphi}_i : (y, x) \mapsto y$. Likewise, the map $\tilde{p}$, which is the pullback over $\varphi_i$ of $p$, is defined by $\tilde{p} : (y, x) \mapsto x$. Note that the diagram (4.3) is a commutative diagram in that $\varphi_i \circ \tilde{p} = p \circ \tilde{\varphi}_i$.

The universal covering space $\tilde{Y}$ has a Riemannian metric $\tilde{g}$, which is a lifting of the Riemannian metric $g$ on $Y$. Each of the Born-Oppenheimer Hamiltonians $R_i$, for $i = 1, 2, 3$, can be lifted to a Hamiltonian

\[
\tilde{R}_i = -\tilde{\Delta}_i + v_i,
\] (4.5)

where $\tilde{\Delta}_i$ is a Laplacian with respect to the Riemannian metric $\tilde{g}$. This operator acts on $L^2(\tilde{\eta}_i)$, the Hilbert space of $L^2$ sections of $\tilde{\eta}_i$. Note that an $L^2$ section of $\tilde{\eta}_i$ is a square integrable function $\sigma : \tilde{Y} \rightarrow \tilde{X}_i$ such that the composition $\tilde{\varphi}_i \circ \sigma$ is the identity almost everywhere on $\tilde{Y}$. This implies that $\sigma$ must be of the form

\[
\sigma : w \mapsto (w, \tilde{\sigma}(w))
\] (4.6)

where $\tilde{\sigma} = \tilde{p} \circ \sigma$ is a square integrable function from $\tilde{Y}$ to $X_i$, satisfying $\varphi_i \circ \tilde{\sigma} = p$.

Now consider a section $\phi \in L^2(\eta_i)$. This is a square integrable function $\phi : Y \rightarrow X_i$ such that $\varphi_i \circ \phi$ is the identity almost everywhere on $N_2$. From $\phi$, we construct a function $\tilde{\phi} : \tilde{Y} \rightarrow \tilde{X}_i$ by defining $\tilde{\phi} = \phi \circ p$. The pullback of $\phi$ is then $\tilde{\phi} : \tilde{Y} \rightarrow \tilde{X}_i$, defined by $\tilde{\phi}(w) = (w, \phi(w))$. This construction of pulling back a section from $\eta_i$ to $\tilde{\eta}_i$ constitutes a one-to-one linear map $\Upsilon$ of $L^2(\eta_i)$ into $L^2(\tilde{\eta}_i)$, because $p$ is a finite-to-one covering projection.

Each element $g \in \pi_1(Y)$ defines a deck transformation\footnote{A deck transformation $D$ of the universal covering space projection $p$ is a homeomorphism $D : \tilde{Y} \rightarrow \tilde{Y}$ satisfying $p \circ D = p$. For more details on deck transformations, see Section III.6 of [11].} $D(g) : \tilde{Y} \rightarrow \tilde{Y}$, because the group $D$ of all deck transformations on $\tilde{Y}$ is canonically isomorphic to $\pi_1(Y)$. Each deck transformation $D_g \in D$ induces a linear operator $\Lambda(g)$ on $L^2(\tilde{\eta}_i)$, defined by mapping the section

\[
\sigma : w \mapsto (w, \tilde{\sigma}(w))
\]
to the section
\[ \Lambda(g) \sigma: w \mapsto (w, \tilde{\sigma}(D_g^{-1}(w))). \] 
(4.7)

To compute the spectrum of \( R_i \), we will use the following lemma.

**Lemma 4.2.** Suppose that \( p: \tilde{M} \to M \) is a cover map and that \( \eta \) is a vector bundle over \( M \). Let \( \tilde{\eta} \) denote the pullback of \( \eta \) over \( p \). If \( \phi \in L^2(\eta) \) is an eigenvector for a differential operator \( R: L^2(\eta) \to L^2(\eta) \) with eigenvalue \( \lambda \), then the pullback section \( \tilde{\phi} = \Upsilon(\phi) \) is an eigenvector of the pullback operator \( \tilde{R} \) with eigenvalue \( \lambda \). Conversely, if \( \tilde{\phi} \in L^2(\tilde{\eta}) \) is an eigenvector of \( \tilde{R} \) with eigenvalue \( \lambda \) and \( \tilde{\phi} \) is in the image of \( \Upsilon \), then \( \tilde{\phi} \) is the pullback of an eigenvector of \( R \) with eigenvalue \( \lambda \).

We remark that this result for the special case of Laplacians acting on functions is given in [2, Section III.A.II] and [16, pp. 27–28].

**Proof.** Denote the projection map and total space of \( \eta \) by \( q \) and \( E \), respectively. Then, the total space of \( \tilde{\eta} \) is
\[ \{(x, y) \in \tilde{M} \times E \mid p(x) = q(y)\} \] 
(4.8)

and the projection map is \( \tilde{q}: (x, y) \to x \).

Suppose that \( \phi \in L^2(\eta) \) satisfies \( R\phi = \lambda \phi \). Then the pullback section is \( \tilde{\phi}(x) = (x, \phi \circ p(x)) \). It follows from the definition of \( \tilde{R} \) that
\[ \tilde{R}\tilde{\phi} = (x, R \phi \circ p) = (x, \lambda \phi \circ p) = \lambda \tilde{\phi}. \] 
(4.9)

Now consider \( \tilde{\phi} \in \text{Image}(\Upsilon) \) satisfies \( \tilde{R}\tilde{\phi} = \lambda \tilde{\phi} \). There exists a unique \( \phi \in L^2(\eta) \) such that \( \Upsilon(\phi) = \tilde{\phi} \). From the construction of \( \tilde{R} \), we have
\[ \tilde{R}\tilde{\phi} = (x, R \phi(p(x))) \quad \text{and} \quad \tilde{R}\tilde{\phi} = (x, \lambda \phi(p(x))). \] 
(4.10)

Therefore, \( R \phi = \lambda \phi \), because \( p \) is a covering.

Note that the image of the map \( \Upsilon: L^2(\eta_i) \to L^2(\tilde{\eta}_i) \) is the fixed point set of the group action
\[ \Lambda: \pi_1(Y) \times L^2(\tilde{\eta}_i) \to L^2(\tilde{\eta}_i). \] 
(4.11)

Therefore, we may use the action \( \Lambda \) of the group \( \pi_1(Y) \) on \( L^2(\tilde{\eta}_i) \) and Lemma 4.2 to obtain the spectrum of \( B_i \) from the spectrum of \( \tilde{B}_i \).

The real line bundle \( \tilde{\eta}_i \) is isomorphic to the trivial line bundle, because \( \tilde{Y} \) is simply connected. Therefore, it has a smooth globally-defined normalised section. In fact, there exist exactly two normalised sections and we chose one to denote by \( \tau \). Of course, the other section will then be \( -\tau \) and the set of normalised sections is \( \Gamma(\tilde{\eta}_i) = \{\tau, -\tau\} \). Nontriviality of \( \eta_i \) implies that the action of \( \Lambda \) on \( \Gamma(\tilde{\eta}_i) \) must be transitive. Otherwise, \( \tau \) would be invariant under \( \Lambda \) and could be pushed down to give a normalised section of \( \eta_i \), which is contrary \( \eta_i \) being nontrivial. Thus, the action \( \Lambda \) is
\[ \Lambda_1 \tau = \tau \quad \Lambda_{-1} \tau = -\tau. \] 
(4.12)
Using the section $\tau$, we are able to represent $L^2$ sections of $\tilde{\eta}_i$ as elements of $L^2(\tilde{Y}; \mathbb{R})$, the real Hilbert space of real-valued square-integrable functions on $\tilde{Y}$. A section $\sigma : \tilde{Y} \to \tilde{X}_1$ is represented by the function

$$f : \tilde{Y} \to \mathbb{R}, \quad \text{defined by } \quad f(w) = \langle \tau(w), \sigma(w) \rangle,$$

where $\langle \cdot, \cdot \rangle$ is the fibre-wise inner product on $\tilde{\eta}_i$. This correspondence is a Hilbert space isomorphism from $L^2(\tilde{\eta}_i)$ to $L^2(\tilde{Y}; \mathbb{R})$. It follows from (4.12) and (4.13) that $\sigma$ is a $\Lambda$-invariant section of $\tilde{\eta}_i$ if and only if the function $f$ corresponding to $\sigma$ satisfies

$$\Lambda_1 f = f \quad \Lambda_{-1} = -f. \quad (4.14)$$

Now consider the case when $b_0 \in (0, 1)$. Before computing the action $\Lambda$ of $\pi_1(Y) \cong Q_8$ on each of the Hilbert spaces $L^2(\tilde{\eta}_i)$, some basic facts about $Q_8$ will be reviewed. The nonabelian group $Q_8$ has an order two commutator subgroup. We label the unit in $Q_8$ by $1$ and the nontrivial element in the commutator subgroup by $-1$. Following convention, the other six elements of $Q_8$ are denoted by $\pm i$, $\pm j$, and $\pm k$. The nontrivial proper subgroups of $Q_8$ are the commutator subgroup $\{\pm 1\}$ and the three abelian subgroups of order four, $\{\pm 1, \pm i\}$, $\{\pm 1, \pm j\}$, and $\{\pm 1, \pm k\}$. Each of the latter three subgroups is isomorphic to the cyclic group $\mathbb{Z}_4$, because each contains an element of order four.

Note that each of the three real line bundles $\tilde{\eta}_i$ is isomorphic to the trivial real line bundle over $\tilde{Y}$, because $\tilde{Y}$ is simply connected. Therefore, there exists a smooth globally-defined normalised section for $\tilde{\eta}_i$. As before, there are exactly two such sections, related by multiplication by $-1$ and the group $\pi_1(Y)$ acts on $\Gamma(\tilde{\eta}_i)$, the set of normalised sections. Nontriviality of $\eta_i$ implies that $\Lambda$ must be a transitive group action of $\pi_1(Y)$ on the set $\Gamma(\tilde{\eta}_i)$. Therefore, the isotropy subgroup of this action must be one of the three order four subgroups of $Q_8$. Each of these isotropy subgroups corresponds to one of the three line bundles $\eta_i$, for $i = 1, 2, 3$.

The precise correspondence between the line bundle $\eta_i$ and the order four subgroups of $\pi_1(Y)$ can be determined from the the classification theorem for covering projections [65, Section 2.5]. This theorem states that there is a one-to-one correspondence between covering projections from a connected covering space to $Y$ and subgroups of $\pi_1(Y)$, where two subgroups are considered as equivalent if they are conjugate to each other. Therefore, $\tilde{Y}$ has exactly three 2-fold covering projections, corresponding to the three inequivalent order four subgroups of $\pi_1(Y)$. Now consider that associated with the real line bundles $\eta_i$ are three principal $O(1)$ bundles, $P(\eta_i)$, for $i = 1, 2, 3$. These principal bundles are inequivalent 2-fold coverings of $Y$, and therefore, they must correspond to the three order four subgroups of $\pi_1(Y)$. This correspondence identifies the fundamental group of the total space $P(X_i)$ of $P(\eta_i)$ with one of the order four subgroups of $\pi_1(Y)$.

It remains to verify that this identification of the line bundles $\eta_i$ with the order four subgroups of $\pi_1(Y)$ is reflected in the isotropy subgroup of the action $\Lambda$ on $\Gamma(\tilde{\eta}_i)$. We denote the pullback of each of the line bundles $\eta_i$ over the projection $P(\tilde{\eta}_i)$ of its associated principal bundle $P(\eta_i)$ by $\eta'_i$. As remarked above, each $\eta'_i$ is isomorphic to the trivial real line bundle over $P(X_i)$. In the same vein as the action $\Lambda$ constructed above, there is an action of $O(1)$ on $\Gamma(\eta'_i)$, the two element set of
normalised sections in $\eta'_i$. Furthermore, this action must be transitive because $\eta_i$ is a nontrivial line bundle. From each of the 2-fold covering spaces $P(X_i)$, we obtain the universal covering space $Y$ by taking a further 4-fold covering with projection $c_i$. The fibre of this 4-fold covering is the fundamental group of $P(X_i)$. The three distinct ways of obtaining the universal covering projection $p: \tilde{Y} \to Y$ as the composition of a 4-fold covering projection and a 2-fold covering projection are shown in the diagram below.

Note that the pullback of $\eta'_i$ over $c_i$ is the pullback of a trivial line bundle. Therefore, sections in $\Gamma(\tilde{\eta}_i)$ are invariant under the action $\Lambda$ induced by the deck transformations of this covering projection. Thus, the deck transformations corresponding to the order four subgroup of $\pi_1(Y)$ which is associated with $\eta_i$ is the isotropy subgroup of the action $\Lambda$ on $\Gamma(\tilde{\eta}_i)$.

It is simply a matter of labelling convention how we chose to designate the isotropy subgroups of $\Lambda$ as order four subgroups in $Q_8$. We shall denote the isotropy subgroup of $\Lambda$ on $\Gamma(\tilde{\eta}_1)$ by $\{\pm 1, \pm i\}$, the isotropy subgroup of $\Lambda$ on $\Gamma(\tilde{\eta}_2)$ by $\{\pm 1, \pm j\}$ and the isotropy subgroup of $\Lambda$ on $\Gamma(\tilde{\eta}_3)$, and $\{\pm 1, \pm k\}$. Therefore, any normalised section $\tau$ in $\Gamma(\tilde{\eta}_i)$ transforms according to

$$
\begin{align*}
\Lambda_{\pm 1} \tau &= \tau \\
\Lambda_{\pm j} \tau &= -\tau
\end{align*}
$$

There are similar transformation equations for sections in $\Gamma(\tilde{\eta}_2)$ and $\Gamma(\tilde{\eta}_3)$.

Given a choice of normalised section $\tau \in \Gamma(\tilde{\eta}_i)$, $L^2$ sections of $\tilde{\eta}_i$ are represented as functions by equation (4.13).

It follows from (4.16) that $\sigma$ is a section in $\tilde{\eta}_1$ satifying $\Lambda_g \sigma = \sigma$ for all $g \in \pi_1(N_2)$ if and only if the associated function $f$ satisfies

$$
\begin{align*}
\Lambda_{\pm 1} f &= f \\
\Lambda_{\pm j} f &= -f
\end{align*}
$$

Similary, a section $\sigma$ in $\tilde{\eta}_2$ or $\tilde{\eta}_3$ satisfies $\Lambda_g \sigma = \sigma$ for all $g \in \pi_1(N_2)$ if and only if the associated function satisfies

$$
\begin{align*}
\Lambda_{\pm 1} f &= f \\
\Lambda_{\pm j} f &= f
\end{align*}
$$

and

$$
\begin{align*}
\Lambda_{\pm 1} f &= f \\
\Lambda_{\pm j} f &= f
\end{align*}
$$
respectively.

Under the Hilbert space isomorphism (4.13), the Schrödinger operators \( \tilde{B}_i \), for \( i = 1, 2, 3 \), correspond to the operators

\[
\hat{B}_i = -\hat{\triangle}_2 + \hat{V}_i,
\]

acting on the function space \( L^2(\tilde{N}_2; \mathbb{R}) \). The Laplacian \( \hat{\triangle}_2 \) is defined with respect to the Riemannian metric \( \tilde{g} \). Viewed as a function on \( \tilde{N}_2 \), the potential function \( \hat{V}_i \) is the same as \( \tilde{V}_i \); however, they should be distinguished as operators because \( \tilde{V}_i \) acts on \( L^2(\tilde{\eta}_i) \), whereas \( \hat{V}_i \) acts on \( L^2(N_2; \mathbb{R}) \). The spectrum of the Born-Oppenheimer Hamiltonian \( B_i \) will be obtained by finding all eigenfunctions of \( \hat{B}_i \) which have the transformation properties in (4.17) for \( H_1 \), or corresponding transformation properties for \( H_2 \) and \( H_3 \).

Recall that the potential \( V_i \) is minimised on the submanifold \( Y = \mathfrak{F}(b_0) \). Therefore, the potential \( \hat{V}_i \) is minimised on the covering space \( \tilde{Y} = p^{-1}(Y) \). The submanifold \( \tilde{Y} \subset \tilde{N}_2 \) is diffeomorphic to the 3-dimensional sphere \( S^3 \). The Riemannian metric on \( \tilde{Y} \) is \( \tilde{g} \), which has the same local curvature as \( Y \) with Riemannian metric \( g \), because \( \tilde{Y} \) is a covering space of \( Y \).

5. Spectrum on the Projective Spaces

In this section we calculate the spectrum of the Laplacian with respect to the flat connection on the line bundles \( \eta_1 \) and \( \eta_3 \), restricted to \( \mathfrak{R}_1 \) and \( \mathfrak{R}_3 \), respectively. The fundamental group \( \pi_1(Y) \) is now \( \mathbb{Z}_2 \) and the pullback square (4.3) becomes

\[
\begin{array}{c}
\mathbb{R} \\
\uparrow \\
X_i \\
\downarrow \quad p_i \\
\mathbb{R}
\end{array}
\Rightarrow
\begin{array}{c}
\tilde{\mathbb{R}}_i \\
\uparrow \quad \tilde{\varphi}_i \\
\tilde{X}_i \\
\downarrow \quad \hat{p}_i \\
\mathbb{R}_i
\end{array}
\Rightarrow
\begin{array}{c}
\mathbb{Z}_2 \\
\uparrow \\
\hat{\mathbb{R}}_i \\
\downarrow \quad \hat{p}_i \\
\mathbb{Z}_2
\end{array} \quad \text{(5.1)}
\]

where \( i = 1, 3 \). The line bundles \( \varphi_i \) are isomorphic to the canonical line bundle over \( \mathbb{R}P(2) \). Its pullback \( \tilde{\eta}_1 \) is easily seen to be isomorphic to the trivial line bundle, because \( \tilde{N}_1 \) is simply connected. However, it will be useful to note that the bundle \( p_1 \) is isomorphic to the associated principal bundle for the real line bundle \( \varphi_1 \). It is generally true that the pullback of a vector bundle over its associated principal bundle is isomorphic to the trivial bundle.

We will refer to the trivial element in \( \pi_1(Y) = \mathbb{Z}_2 \) by \( 0 \) and the nontrivial element by \( 1 \). The fact that the action \( \Lambda \) defined in (4.11) is a group action implies that \( \Lambda_0 \tau = \tau \), and that \( \Lambda_1 \tau \) is either \( \tau \) or \( -\tau \). Observe that if \( \Lambda_1 \tau \) were equal to \( \tau \), then \( \tau \) would be a normalised section in \( \tilde{\eta}_1 \), which could be obtained as the pullback of a normalised section in \( \eta_1 \). However, this is impossible because \( \eta_1 \) is a nontrivial
real line bundle. In summary, nontriviality of $\eta_1$ implies that $\Lambda$ must be a transitive group action of $\mathbb{Z}_2$ on the set $\{\tau, -\tau\}$. Therefore,

$$\Lambda_0 \tau = \tau \quad \text{and} \quad \Lambda_1 \tau = -\tau. \quad (5.2)$$

It follows from (4.13) and (5.2) that $\psi$ is a section of $\widetilde{\eta}_1$ satisfying $\Lambda_g \psi = \psi$ for all $g \in \mathbb{Z}_2$, if and only if

$$\Lambda_0 f = f \quad \text{and} \quad \Lambda_1 f = -f. \quad (5.3)$$

where the function $f$ is associated to $\psi$ by (4.13) and the action $\Lambda$ on functions is defined by $\Lambda f(w) = f(D^{-1}g(w))$.

**Theorem 5.1.** The eigenvalues of $-\nabla_1(\mathcal{R}_1)$ are

$$\lambda_n = \frac{n(n+1)}{3r_0^2}, \quad \text{for } n = 1, 3, 5, \ldots. \quad (5.4a)$$

The multiplicities of these eigenvalues are

$$\text{mult}(\lambda_n) = 2n + 1. \quad (5.4b)$$

The spectrum of $-\nabla_3(\mathcal{R}_3)$ is the same as the spectrum of $-\nabla_1(\mathcal{R}_1)$. 

**Proof.** Considering first $\eta_1|_{\mathcal{R}_1}$, the associated principal bundle is the nontrivial $\mathbb{Z}_2$-bundle

$$\mathbb{Z}_2 \rightarrow S^2(\sqrt{3} r_0) \rightarrow \mathcal{R}_1 \quad (5.5)$$

The pullback of $\eta_1|_{\mathcal{R}_1}$ over its associated principal bundles is $\widetilde{\eta}_1|_{\mathcal{R}_1}$, which is isomorphic to the trivial line bundle of $\mathcal{R}_1$. It follows from Lemma 4.2 that the eigenvalues of $\nabla_1$ correspond to the eigenfunctions of the pullback Laplacian $\widetilde{\nabla}_1$ on $S^2(\sqrt{3}r_0)$, which transform according to (5.3).

The Laplacian $\widetilde{\nabla}_1$ is the standard Laplacian on $S^2(\sqrt{3}r_0)$, because $\nabla_1$ is the Laplacian with respect to the flat connection on $\eta_1|_{\mathcal{R}_1}$. Therefore, the eigenvectors of $-\widetilde{\nabla}_1$ are the restrictions to $S^2(\sqrt{3}r_0)$ of the harmonic polynomials in $\mathbb{R}^3$ [73]. These polynomials constitute the kernel of the usual Laplacian on $\mathbb{R}^3$. The eigenvalue associated to a harmonic polynomial of degree $n$ is

$$\lambda_n = \frac{n(n+1)}{3r_0^2}, \quad \text{for } n = 0, 1, 2, \ldots. \quad (5.6a)$$

The multiplicity of $\lambda_n$ is

$$\text{mult}(\lambda_n) = 2n + 1 \quad (5.6b)$$

The transformation properties in (5.3) imply that the eigenvalues of $\nabla_1$ correspond to the harmonic polynomials of odd degree.

The spectrum of the Laplacian on $\eta_3|_{\mathcal{R}_3}$ is the same as the spectrum on $\eta_1|_{\mathcal{R}_1}$, because the two bundles are isometric. □
6. Spectrum with Constant Curvature

Although the universal covering space of \( Y = \tilde{Y}(b) \), for \( b \in (0, 1) \), is diffeomorphic to \( S^3 \), it is not isometric to a standard sphere \( S^3(r) \) with constant curvature \( \frac{1}{r^2} \). This may be verified by calculating \( K_i \), the sectional curvature of \( \tilde{Y}(b) \) in planes orthogonal to the principal foliation \( C_i(b) \). These sectional curvatures are

\[
K_1^S = \frac{2(1 - b + b^2)}{3(1 - b) r_0^2}, \quad K_2^S = \frac{2(1 - b + b^2)}{3b(1 - b) r_0^2}, \quad \text{and} \quad K_3^S = \frac{2(1 - b + b^2)}{3br_0^2}.
\]

(6.1)

The universal covering space would have constant curvature if and only if \( Y \) had constant curvature. However, because it is covered by a sphere, \( Y \) does admit a constant curvature Riemannian structure [76, Thm. 5.1.2]. The notation \( Y_K \) will be used to denote the manifold \( Y \) with curvature \( K \). The universal covering space, \( \tilde{Y}_K \), of \( Y_K \) is isometric to the 3-sphere of radius \( r = \frac{1}{\sqrt{K}} \). It is instructive to first carry out the computation of the spectra of the bundle Laplacians \( \triangle_i(Y_K) \), for \( i = 1, 2, 3 \), on \( Y_K \), before confronting this problem for \( Y \) with the more complicated isoparametric Riemannian structure.

The pullback of \( \triangle_i(Y_K) \) with respect to the flat connection on \( \eta_i \), is \( \triangle(S^3(r)) \), the standard Laplacian on the 3-sphere. All of the eigenvalues of \( \triangle(S^3(r)) \) are obtained as the restrictions to \( S^3(r) \) of the harmonic polynomials in \( \mathbb{R}^4 \). We denote the vector space of harmonic polynomials of degree \( n \) on \( \mathbb{R}^4 \) by \( H_n \). This is the eigenspace of \( -\triangle(S^3(r)) \) with eigenvalue \( \lambda_n = \frac{n(n+2)}{r^2} \) [73]. To determine the dimensions of the eigenspaces of \( \triangle(S^3(r)) \), we first consider the vector space \( P(n) \), consisting of all degree \( n \) homogeneous polynomials on \( \mathbb{R}^4 \). The dimension of \( P(n) \) is

\[
\dim(P(n)) = \binom{n+3}{n}.
\]

(6.2)

The Laplacian on \( \mathbb{R}^4 \) is an onto linear map

\[
\triangle(\mathbb{R}^4) : P(n) \rightarrow P(n-2),
\]

(6.3)

where \( P(n) \) is interpreted as the 0-dimensional vector space when \( n < 0 \). Recalling that \( H(n) \) is the kernel of the map in (6.3), we obtain that the multiplicity of \( \lambda_n \) is

\[
\dim(\mathcal{H}(n)) = \dim(P(n)) - \dim(P(n-2)) = (n+1)^2, \quad \text{for } n = 0, 1, 2, \ldots.
\]

(6.4)

Using Lemma 4.2 we obtain the eigensections of \( -\triangle_i(Y_K) \), by finding all harmonic polynomials in \( \mathbb{R}^4 \) which transform accordingly under the action of \( \Lambda \) in (4.17).

To explicitly construct the action \( \Lambda \), use the fact that a vector \((x_0, x_1, x_2, x_3) \in \mathbb{R}^4\) can be represented as a quaternionic number \( x \in \mathbb{H} \) by setting

\[
x = x_0 + x_1i + x_2j + x_3k
\]

(6.5)
The group $Q_8$ acts on the sphere $S^3(r) \subset \mathbb{R}$ by left multiplication. This action of $Q_8$ on $S^3(r)$ induces the action $\Lambda$ that is defined in Section 4. Specifically,

\[
\begin{align*}
\Lambda_{\pm 1} & : f(x_0, x_1, x_2, x_3) \mapsto f(\pm x_0, \pm x_1, \pm x_2, \pm x_3) \\
\Lambda_{\pm 1} & : f(x_0, x_1, x_2, x_3) \mapsto f(\pm x_1, \mp x_0, \pm x_3, \mp x_2) \\
\Lambda_{\pm j} & : f(x_0, x_1, x_2, x_3) \mapsto f(\pm x_2, \mp x_3, \mp x_0, \mp x_1) \\
\Lambda_{\pm k} & : f(x_0, x_1, x_2, x_3) \mapsto f(\pm x_3, \pm x_2, \mp x_1, \mp x_0)
\end{align*}
\] (6.6a-d)

Comparing this action to the transformation properties in (4.17) allows us to prove the following theorem.

**Theorem 6.1.** The three Laplacians $\triangle_i(Y_K)$, $i = 1, 2, 3$, have the same spectrum. The eigenvalues of $-\triangle_i(Y_K)$ are

\[
\lambda_n = r^{-2}(n + 1)(n + 2), \quad \text{for } n = 0, 1, 2, \ldots \] (6.7a)

The multiplicity of $\lambda_n$ is

\[
\text{mult}(\lambda_n) = (n\backslash 2 + 1)(2n + 3),
\] (6.7b)

where $\backslash$ is the integer division operator.

**Proof.** In order to find a basis of harmonic polynomials on $\mathbb{R}^4$ which have the required transformation properties under $\Lambda$, we first note that the action $\Lambda$ commutes with the Laplacians. Therefore, we can proceed by first finding the subspace of homogeneous polynomials which have the transformation properties given by (4.17) and then find the harmonic polynomials within this subspace.

Begin by considering the subspace $P_1(n)$, which is defined as the subspace of all degree $n$ polynomials that transform according to (4.17a). The invariance of $f \in P_1(l)$ under $\Lambda_{-1}$ implies that the degree of $f$ must be even. To consider the remaining elements of $Q_8$, it will suffice to check only $\Lambda_1$ and $\Lambda_2$, because $k = 1j$.

Our analysis will be organised according to the number of distinct exponents in the homogeneous polynomials $f(x_0, x_1, x_2, x_3) = x_0^{n_0} x_1^{n_1} x_2^{n_2} x_3^{n_3}$, where $l = n_0 + n_1 + n_2 + n_3$ is even. First, consider polynomials for which the exponent of $x_i$ is the same for each $i = 1, 2, 3$. A polynomial of the form $f(x_0, x_1, x_2, x_3) = x_0^n x_1^l x_2 x_3^n$ is invariant under both $\Lambda_j$ and $\Lambda_k$, which is inconsistent with (4.17). Therefore, there are no nontrivial polynomials of this form in $P_1(l)$.

Next we consider homogeneous polynomials for which two of the variables have one exponent $n_1 \geq 0$ and the other two variables have a distinct exponent $n_2 \geq 0$. The transformation of such polynomials in $P_1'(l)$ is given in tabular form.

---

10Our choice of left multiplication rather than right multiplication is simply a matter of convention.
The transformations \( \Lambda \) and the subspace of polynomials that transform according to (4.17a) in \( P \) is

\[
\begin{array}{c|ccc}
 & \Lambda_i & \Lambda_j & \Lambda_k \\
\hline
f_1 = (x_0 x_1)^{n_1} (x_2 x_3)^{n_2} & (-1)^{n_1+n_2} f_1 & (-1)^{n_1+n_2} f_6 & f_6 \\
\hline
f_2 = (x_0 x_2)^{n_1} (x_1 x_3)^{n_2} & f_5 & (-1)^{n_1+n_2} f_2 & (-1)^{n_1+n_2} f_5 \\
f_3 = (x_0 x_3)^{n_1} (x_1 x_2)^{n_2} & (-1)^{n_1+n_2} f_4 & f_4 & (-1)^{n_1+n_2} f_3 \\
f_4 = (x_1 x_2)^{n_1} (x_0 x_3)^{n_2} & (-1)^{n_1+n_2} f_3 & f_3 & (-1)^{n_1+n_2} f_4 \\
f_5 = (x_1 x_3)^{n_1} (x_0 x_2)^{n_2} & f_2 & (-1)^{n_1+n_2} f_5 & (-1)^{n_1+n_2} f_2 \\
f_6 = (x_2 x_3)^{n_1} (x_0 x_1)^{n_2} & (-1)^{n_1+n_2} f_6 & (-1)^{n_1+n_2} f_1 & f_1
\end{array}
\] (6.8)

The subspace \( \mathcal{P}'(l) \subset \mathcal{P}(l) \), defined as the span of all polynomials of this form for any values of \( n_1 \) and \( n_2 \) has dimension

\[
\dim(\mathcal{P}'(l)) = \begin{cases} 
\frac{3l}{2}, & \text{if } l \equiv 0 \pmod{4} \\
\frac{3(l+2)}{2}, & \text{if } l \equiv 2 \pmod{4}
\end{cases}
\] (6.9)

It follows from (6.8) that if \( n_1 + n_2 \) is odd, then a basis of polynomials with the transformation properties (4.17) is \( \{f_2 + f_5, f_3 - f_4\} \). If \( n_1 + n_2 \) is even, then a basis for the polynomials which transform as required is \( \{f_1 - f_6\} \). Therefore, the dimension of \( \mathcal{P}'(l) \cap \mathcal{P}_1(l) \) is

\[
d_1(l) = \begin{cases} 
\frac{l}{2}, & \text{for } l = 0, 2, 4, \ldots \\
\frac{l+2}{2}, & \text{for } l = 1, 3, 5, \ldots
\end{cases}
\] (6.10)

Finally, consider \( \mathcal{P}''(l) \), the vector space complement of both of the two subspaces of \( \mathcal{P}(l) \) already considered. The dimension of \( \mathcal{P}''(l) \) is

\[
\dim(\mathcal{P}''(l)) = \begin{cases} 
\frac{(l+3)}{2} - \frac{3l+2}{4}, & \text{if } l \equiv 0 \pmod{4} \\
\frac{(l+3)}{2} - \frac{3l+6}{4}, & \text{if } l \equiv 2 \pmod{4}
\end{cases}
\] (6.11)

The transformations \( \Lambda_1, \Lambda_j, \) and \( \Lambda_k \) all act on \( \mathcal{P}''(l) \) without nontrivial fixed points and the subspace of polynomials that transform according to (4.17a) in \( \mathcal{P}''(l) \) can be constructed by noting that for any \( f \in \mathcal{P}''(l) \), the polynomial \( f + \Lambda_1 f - \Lambda_j f - \Lambda_k f \) transforms as required. Therefore, the dimension of \( \mathcal{P}''(l) \cap \mathcal{P}_1(l) \) is

\[
d_2(l) = \frac{1}{4} \dim(\mathcal{P}''(l)) = \begin{cases} 
0, & \text{for } m = 0 \\
2 \left( \frac{m+2}{3} \right) - \frac{m+1}{2}, & \text{for } m = 1, 3, 5, \ldots \\
2 \left( \frac{m+2}{3} \right) - \frac{m}{2}, & \text{for } m = 2, 4, 6, \ldots
\end{cases}
\] (6.12)

where \( l = 2m \) and \( m = 0, 1, 2, \ldots \)

Combining the results from (6.10) and (6.12), we calculate that the dimension of the subspace \( \mathcal{P}_1(2m) \) is

\[
d_1(2m) + d_2(2m) = \begin{cases} 
0, & \text{for } m = 0 \\
2 \left( \frac{m+2}{3} \right) + \frac{m+1}{2}, & \text{for } m = 1, 3, 5, \ldots \\
2 \left( \frac{m+2}{3} \right), & \text{for } m = 2, 4, 6, \ldots
\end{cases}
\] (6.13)

The vector subspace of degree \( l \) harmonic polynomials which transform according to (4.17a) is \( \mathcal{H}_1(l) = \mathcal{P}_1(l) \cap \mathcal{H}(l) \). Using the fact that \( \triangle(\mathbb{R}^4) : \mathcal{P}_1(l) \to \mathcal{P}(l-2) \)
is an onto linear map, we obtain that the dimension of \( \mathcal{H}_1(2m) \) is

\[
\dim (P_1(2m)) - \dim (P_1(2m - 2)) = \begin{cases} 
\frac{m(2m+1)}{2}, & \text{for } m = 0, 2, 4, \ldots \\
\frac{(m+1)(2m+1)}{2}, & \text{for } m = 1, 3, 5, \ldots 
\end{cases}
\]

(6.14)

Notice that each of the eigenspaces, \( \mathcal{H}(l) \), is nontrivial, except for \( l = 0 \). This implies that the spectrum of \(-\triangle_1(Y_K)\) consists of all eigenvalues of \(-\triangle(S^3(r))\), except for the zero eigenvalue. Re-indexing (6.14) in terms of \( n = m - 1 \) completes the proof for \(-\triangle_1(Y_K)\). The results for \(-\triangle_2(Y_K)\) and \(-\triangle_3(Y_K)\) are obtained by simply permuting \( i, j, \) and \( k \) in the above calculation. □

### 7. Spectrum with Isoparametric Geometry

To compute the spectra of the line bundle Laplacians on \( \mathcal{F}(b) \) with the isoparametric metric, \( g_b \), we shall make use of the fact that the 3-dimensional unit sphere may be viewed as \( \mathbb{Sp}(1) \), the Lie group of unit quaternions in \( \mathbb{H} \). Note that this Lie group is isomorphic to \( SU(2) \), should the reader prefer to view it in that guise.

The Lie algebra, \( \mathfrak{sp}(1) \), of \( \mathbb{Sp}(1) \) is a 3-dimensional real vector space. This Lie algebra may be viewed as the tangent space at the identity and in this context it is a vector space generated by \{\( i, j, k \)\}. For \( x = x_1 i + x_2 j + x_3 k \) and \( y = y_1 i + y_2 j + y_3 k \), we define the inner product

\[
x \cdot y = \frac{1}{2} \sum_{i=0}^{3} x_i y_i .
\]

(7.1)

With this inner product, the adjoing representation of \( \mathbb{Sp}(1) \) on \( \mathfrak{sp}(1) \) defines a map

\[
\text{Ad} : \mathbb{Sp}(1) \longrightarrow \mathbb{SO}(3) \subset \mathbb{GL}(\mathfrak{sp}(1)) ,
\]

(7.2)

which is a 2-fold covering. In the 3-fold coverings of (4.15), \( P(X_i) \cong \frac{O(3)}{O(1) \times O(1)} \) and \( \mathfrak{f}(b) \cong \frac{O(3)}{O(1) \times O(1) \times O(1)} \) are homogeneous spaces. The projections

\[
P(\varphi_i) : P(X_i) \longrightarrow \mathfrak{f}(b)
\]

(7.3)

correspond to factoring out one of the \( O(1) \) factors, for each of \( i = 1, 2, 3 \), respectively. The remaining 4-fold covering projections is

\[
c_i = \text{Ad} \circ a_i , \quad \text{for } i = 1, 2, 3 .
\]

(7.4)

The 2-fold covering projection \( a_i \) is defined as

\[
a_i : \mathbb{SO}(3) \longrightarrow P(X_i) \cong \frac{O(3)}{O(1) \times O(1)} = \frac{\mathbb{SO}(3)}{S(O(1) \times O(1))} ,
\]

(7.5)

where \( S(O(1) \times O(1)) = \{(1, 1), (-1, -1)\} \).

We shall define the Riemannian metric on \( \mathbb{Sp}(1) \) to be \( p^*g_b \), the pull up of the Riemannian metric from \( \mathfrak{f}(b) \). Recall that \( g_b \) is invariant with respect to the adjoint action of \( O(3) \) on \( \mathfrak{f}(b) \). Therefore, \( p^*g_b \) is also an invariant metric and the Laplacian with respect to \( p^*g_b \) is an invariant differential operator. An invariant differential operator on a compact Lie group is completely determined by its form on the Lie
algebra [68]. Specifically, if \{x_1, x_2, x_3\} is an orthonormal basis for \((\mathfrak{sp}(1), p^*g_b)\), then
\[
\triangle(\mathfrak{sp}(1), p^*g_b) = \sum_{i=1}^{3} x_i^2, \tag{7.6}
\]
where the tangent vector \(x_i\) acts on functions as a directional derivative.

The differential of the projection \(p\) is
\[
dp: \mathfrak{sp}(1) \longrightarrow T_{D(b, r)}\mathbb{B}(b), \quad x \longmapsto [\text{ad}(x), D(b, r)], \tag{7.7}
\]
where \(\text{ad}\), the adjoint representation of \(\mathfrak{sp}(1)\), is the differential of \(\text{Ad}\) in equation (7.2). It follows that the metric \(p^*g_b\) on \(\mathfrak{sp}(1)\) is
\[
p^*g_b(x, y) = \text{trace} ([\text{ad}(x), D(b, r) [\text{ad}(y), D(b, r)]), \tag{7.8}
\]
where \(D(b, r)\) is defined in equation (2.16). Therefore, an orthonormal basis for \((\mathfrak{sp}(1), p^*g_b)\) is
\[
x_1 = \frac{\sqrt{1-b+b^2}}{\sqrt{3}r(1-b)} i, \quad x_2 = \frac{\sqrt{1-b+b^2}}{\sqrt{3}r} j, \quad \text{and} \quad x_3 = \frac{\sqrt{1-b+b^2}}{\sqrt{3}rb} k \tag{7.9}
\]
In terms of this basis, the Laplacian is
\[
\triangle(\mathfrak{sp}(1), p^*g_b) = \frac{1-b+b^2}{3r^2} \left( (1-b)^{-2} i^2 + j^2 + b^{-2}k^2 \right) \tag{7.10}
\]
Our approach to determining the spectrum of \(\triangle(\mathfrak{sp}(1), p^*g_b)\) will be to utilize the Peter-Weyl theorem as in [68]. The set of all equivalence classes of irreducible representations of \(\mathfrak{sp}(1)\) is
\[
\mathcal{R}(\mathfrak{sp}(1)) = \{(\rho_m, Q_m) \mid m = 0, 1, 2 \ldots \} \tag{7.11}
\]
where \(Q_m\) is the vector space of homogeneous polynomials in two complex variables [66]. For \(x = x_0 + x_1i + x_2j + x_3k \in \mathbb{H}\), we define two maps from \(\mathbb{H}\) to \(\mathbb{C}\) by \(h_1(x) = x_0 + ix_2\) and \(h_2(x) = x_1 + ix_3\). In terms of \(h_1\) and \(h_2\), a right action of \(\mathbb{H}\) on \(\mathbb{C}^2\) is given by
\[
[z_1 z_2] \longmapsto [z_1 z_2] \begin{bmatrix}
h_1(x) & -h_2(x) \\
h_2(x) & h_1(x) \end{bmatrix} \tag{7.12}
\]
We then define the action of \(\rho_m\) on \(Q_m\) by
\[
\rho_m(x)f(z_1, z_2) = f(\overline{h_1(x)} z_1 + \overline{h_2(x)} z_2, h_1(x) z_2 - h_2(x) z_1). \tag{7.13}
\]

On \(Q_m\), we define the \(\mathfrak{sp}(1)\)-invariant inner product
\[
((f_1, f_2)) = \sum_{k=0}^{m} a_k b_k k! (m-k)!, \tag{7.14}
\]
where \(f_1 = \sum_{k=0}^{m} a_k z_1^k z_2^{m-k}\) and \(f_1 = \sum_{k=0}^{m} b_k z_1^k z_2^{m-k}\).
With respect to this inner product, an orthonormal basis for $Q_m$ is
\[
\left\{ u^m_k = [k!(m-k)!]^{-\frac{1}{2}} z_1^k z_2^{m-k} \mid k = 0, 1, 2, \ldots m \right\} .
\] (7.15)
The matrix elements of $\rho_m(x)$ are
\[
[\rho_m(x)]_{ij} = ((u^m_i, \rho_m(x) u^m_j)).
\] (7.16)
It follows directly from the Peter-Weyl theorem that
\[
\left\{ \sqrt{m+1} [\rho_m]_{ij} \mid i, j = 0, 1, 2, \ldots m \quad \text{and} \quad m = 0, 1, 2, \ldots \right\}
\] (7.17)
is an orthonormal basis for $L^2(Sp(1); \mathbb{C})$. The Hilbert space inner product on $L^2(Sp(1); \mathbb{C})$ is
\[
\langle f, g \rangle = \int f(x) \overline{g(x)} \, dx,
\] (7.18)
where $dx$ is the usual normalised bi-invariant Haar measure on $Sp(1)$. Note that this measure is proportional to the measure induced by the Riemannian metric $p^*g_b$.

The representation $(\rho_m, Q_m)$ of $Sp(1)$ induces an infinitesimal representation $(\rho'_m, Q_m)$ of the Lie algebra $sp(1)$. In terms of the basis polynomials $u_{mk}$ for $Q_m$, this representation is given by
\[
\rho'_m(i) u^m_k = ku^m_{k-1} - (m-k)u^m_{k+1}
\] (7.19a)
\[
\rho'_m(j) u^m_k = i(m-2k)u^m_k
\] (7.19b)
\[
\rho'_m(k) u^m_k = -i(ku^m_{k-1} + (m-k)u^m_{k+1})
\] (7.19c)
Utilizing (7.10), the Casimir operator for $-\Delta(Sp(1), p^*g_b)$ is
\[
\rho'_m(-\Delta(Sp(1), p^*g_b)) = \frac{1-b+b^2}{3r^2} \left( (1-b)^2 \rho'_m(i)^2 + \rho'_m(j)^2 + b^{-2} \rho'_m(k)^2 \right),
\] (7.20)
for the representation $(\rho_m, Q_m)$. Writing this as an $(m+1) \times (m+1)$ matrix with respect to the basis $\{u_i\}$, we define
\[
[\Omega_m]_{ij} = ((u^m_i, \rho'_m(-\Delta(Sp(1), p^*g_b)) u^m_j)), \quad \text{for } i, j = 0, 1, 2, \ldots, m.
\] (7.21)
It follows from the Peter-Weyl theorem that the eigenvalues of the Laplacian $-\Delta(Sp(1), p^*g_b)$ are given by all of the eigenvalues of the matrices $\Omega_m$, for $m = 0, 1, 2, 3, \ldots$. Furthermore, if $\lambda^m$ is an eigenvalue of $\Omega_m$, then the multiplicity of $\lambda^m$ as an eigenvalue of $-\Delta(Sp(1), p^*g_b)$ is $\dim(Q_m) = m + 1$.

Note that the restriction of the action $\rho_m$ to the unit quaternions $Q_8 \subset \mathbb{H}$ corresponds to the action $\Lambda$ defined in (6.3) where we identify functions of two complex variables with functions of four real variables by
\[
f(z_1, z_2) = f(\Re(z_1), \Re(z_2), \Im(z_1), \Im(z_2)) .
\] (7.22)
The real and imaginary parts of a complex number are denoted by $\Re$ are $\Im$, respectively.
The action $\Lambda$ of $Q_8$ on $Q_m$ is simply the restriction of $\rho_m$ to $Q_8 \subset \mathbb{H}$. Therefore,

\begin{align*}
\Lambda_{\pm 1} & : f(z_1, z_2) \mapsto f(\pm z_1, \pm z_2) \\
\Lambda_{\pm 1} & : f(z_1, z_2) \mapsto f(\pm z_2, \mp z_1) \\
\Lambda_{\pm j} & : f(z_1, z_2) \mapsto f(\mp i z_1, \pm i z_2) \\
\Lambda_{\pm k} & : f(z_1, z_2) \mapsto f(\mp z_2 i, \mp z_1 i)
\end{align*}

(7.23a-d)

This action commutes with the endomorphism $\rho_m'(-\Delta (Sp(1), p^* g_b))$, because it is an isometry with respect to the inner product $(\cdot, \cdot)$. Therefore, by considering the subspace of $Q_m$ that transforms according to 4.17a under the action $\Lambda$, we obtain the Casimir matrices $\Omega^1_m$ of $-\triangle_1 (\mathfrak{g}(b))$. The result is summarised in the following theorem.

**Theorem 7.1.** For $m = 1, 3, 5, \ldots$, the Casimir matrix $\Omega^1_m$ is an $\frac{m+1}{2} \times \frac{m+1}{2}$ matrix. It’s entries, which are labelled by $i, j = 0, 1, 2, \ldots, \frac{m-1}{2}$, are

\[
[\Omega^1_m]_{ij} = \begin{cases} 
\frac{1-b+b^2}{3} \left[ \frac{(m-1)(m+2)}{4b^2} + \frac{3m^2+3m-2}{4(1-b)^2} + 1 \right], & \text{for } i = j = \frac{m-1}{2} \\
\frac{1-b+b^2}{3} \left[ \frac{1-2b+2b^2}{2b^2(1-b)^2} (4i(m-i) + m) + (2i-m)^2 \right], & \text{for } i = j < \frac{m-1}{2} \\
\frac{(1-b+b^2)(1-2b)}{6b^2(1-b)^2} \sqrt{(i+1)(m-i)(2i+1)(2m-2i-1)}, & \text{for } i = j - 1 \\
\frac{(1-b+b^2)(1-2b)}{6b^2(1-b)^2} \sqrt{(i)(m-i+1)(2i-1)(2m-2i+1)}, & \text{for } i = j + 1 \\
0, & \text{otherwise}
\end{cases}
\]

(7.24)
For \( m = 2, 4, 6, \ldots \), the Casimir matrix \( \Omega_1^m \) is an \( \frac{m}{2} \times \frac{m}{2} \) matrix. For \( i, j = 0, 1, \ldots, \frac{m-2}{2} \), it entries are

\[
\frac{1 - b + b^2}{3} \left[ 3m^2 + 3m - 2 \right] \left( \frac{1}{4 b^2} + \frac{(m - 1)(m + 2)}{4 (1 - b)^2} + 1 \right),
\]

for \( i = j = \frac{m - 2}{2} \)

\[
\frac{1 - b + b^2}{3} \left[ \frac{1 - 2b + 2b^2}{2 b^2 (1 - b)^2} \left( (2i + 1)(2m - 2i + 1) + m \right) + (2i + 1 - m)^2 \right],
\]

for \( i = j < \frac{m - 2}{2} \)

\[
\frac{(1 - b + b^2)(1 - 2b)}{6 b^2 (1 - b)^2} \sqrt{(i + 1)(m - i - 1)(2i + 3)(2m - 2i - 1)},
\]

for \( i = j - 1 \)

\[
\frac{(1 - b + b^2)(1 - 2b)}{6 b^2 (1 - b)^2} \sqrt{(i)(m - i)(2i + 1)(2m - 2i + 1)},
\]

for \( i = j + 1 \)

\[
0,
\]

otherwise (7.25)

Note that matrices \( \Omega_1^m \) are tridiagonal in that only the diagonal, super-diagonal, and sub-diagonal entries are non-zero. This makes a numerical computation of the eigenvalues quite computationally inexpensive. Furthermore, At \( b = \frac{1}{2} \) the matrices \( \Omega_1^m \) are diagonal and explicit formulae for the eigenvalues of \( -\Delta_1 \left( G \left( \frac{1}{2} \right) \right) \) are easily obtained. After some simplification, the eigenvalues are

\[
\lambda_{m,l} = \frac{1}{4} m^2 + 3 l m - 3 l^2 + m,
\]

for \( m = 1, 3, 5, \ldots \) and \( l = 0, 1, 2, \ldots, \frac{m-1}{2} \). Also,

\[
\lambda_{m,l} = \frac{1}{4} m^2 + 3 l m - 3 l^2 + \frac{5}{2} m - 3 l - \frac{3}{4}
\]

(7.27)

for \( m = 2, 4, 6, \ldots \) and \( l = 0, 1, 2, \ldots, \frac{m-2}{2} \).

The Casimir matrices for the Laplacian \( -\Delta_3 (G(b)) \) on the line bundle \( \eta_3 |_{G(b)} \) are obtained from the Casimir matrices for \( -\Delta_1 (G(b)) \) by substituting \( 1 - b \) for \( b \).

The Casimir matrices of \( -\Delta_2 (G(b)) \) are obtained from the subspace of \( Q_m \) that transforms as \[4.17b\] under the action \( \Lambda \). The result is given in the following theorem.
Theorem 7.2. For $m = 1, 2, 3, \ldots$, the $ij$ entry of the $\frac{m+1}{2} \times \frac{m+1}{2}$ matrix $\Omega_m^2$ is

$$
[\Omega_m^2]_{ij} = \begin{cases}
\frac{1 - b + b^2}{3} \left[ ((4i)(m - i) + 3m - 1) \left( \frac{1 - 2b + b^2}{2b^2(1-b)^2} \right) 
+ (m - 2i - 1)^2 \right], & \text{for } i = j = \frac{m-1}{2} \\
\frac{(1 - b + b^2)(1-2b)}{6b^2(1-b)^2} \sqrt{(i+1)(2i+1)(m-i)(2m-2i-1)}, & \text{for } j = i + 1 \leq \frac{m-3}{2} \\
\frac{(1 - b + b^2)(1-2b)}{6b^2(1-b)^2} \sqrt{(i)(2i+1)(m-i)(2m-2i+1)}, & \text{for } j = i - 1 \leq \frac{m-5}{2} \\
\frac{(1 - b + b^2)(1-2b)}{6\sqrt{2}b^2(1-b)^2} \sqrt{(m-1)(m+1)(m+2)}, & \text{for } j = i = \frac{m-1}{2} \text{ or } j = i - 1 = \frac{m-3}{2} \\
0, & \text{otherwise}
\end{cases}
$$

(7.28)

For $m = 2, 4, 6, \ldots$, the $ij$ entry of the $\frac{m}{2} \times \frac{m}{2}$ matrix $\Omega_m^2$ is

$$
[\Omega_m^2]_{ij} = \begin{cases}
\frac{1 - b + b^2}{3} \left[ ((4i)(m - i) + m) \left( \frac{1 - 2b + b^2}{2b^2(1-b)^2} \right) 
+ (m - 2i)^2 \right], & \text{for } i = j = 0, 1, 2, \ldots, \frac{m-2}{2} \\
\frac{(1 - b + b^2)(1-2b)}{6b^2(1-b)^2} \sqrt{(i+1)(2i+1)(m-i)(2m-2i-1)}, & \text{for } j = i + 1 \\
\frac{(1 - b + b^2)(1-2b)}{6b^2(1-b)^2} \sqrt{(i)(2i-1)(m-i+1)(2m-2i+1)}, & \text{for } j = i - 1 \\
0, & \text{otherwise}
\end{cases}
$$

(7.29)

At $b = \frac{1}{2}$ the eigenvalues of $-\triangle_2(\mathbf{\Omega}(b))$ can be given explicitly because the matrices $\Omega_m^2\left(\frac{1}{2}\right)$ are diagonal. For $m = 1, 3, 5, \ldots$ the eigenvalues are

$$
\lambda_{m,l}^2 = \frac{1}{4} m^2 + 3l m - 3l^2 + \frac{5}{2} m - 3l - \frac{3}{4},
$$

where $l = 0, 1, 2, \ldots, \frac{m-1}{2}$. Also, for $m = 2, 4, 6, \ldots$ the eigenvalues are

$$
\lambda_{m,l}^2 = \frac{1}{4} m^2 + 3l m - 3l^2 + m,
$$

where $l = 0, 1, 2, \ldots, \frac{m-2}{2}$. 
8. Spectral Flow

The spectra of the tridiagonal Casimir matrices $\Omega_{m}^{1}$ and $\Omega_{m}^{2}$ have been numerically computed as a function of $b$ and the results plotted in Figures 3 and 4 respectively. These plots show the spectral flow of $-\triangle_{1}(\mathfrak{F}(b))$ and $-\triangle_{2}(\mathfrak{F}(b))$ with $b$. The eigenvalues of $-\triangle_{i}(\mathfrak{F}(b))$ are denoted by $\lambda_{m,l}^{i}$, which is the $l$th eigenvalue of $\Omega_{m}^{i}$.

First consider the spectral flow of $-\triangle_{1}(\mathfrak{F}(b))$ shown in Figure 3. As $b$ goes to 0, the singular foliation $\mathfrak{F}(b)$ flows to the sphere $\mathfrak{R}_{1}$. Under this flow, most of the eigenvalues of $-\triangle(\mathfrak{F}(b))$ blow-up to infinity. However, the eigenvalues $\lambda_{m,0}^{1}$ for $m = 1, 3, 5, \ldots$ flow to the eigenvalues of $-\triangle_{1}(\mathfrak{R}_{1})$ calculated in Theorem 5.1. As $b$ goes to 1, all eigenvalues of $-\triangle_{1}(\mathfrak{F}(b))$ blow up. This is to be expected, because the line bundle $\eta_{1}$ is not defined on $\mathfrak{R}_{3}$.

Now consider the spectral flow of $-\triangle_{2}(\mathfrak{F}(b))$, shown in Figure 4. The line bundle $\eta_{2}$ is not defined in either of the $b \to 0$ or $b \to 1$ limits. This results in the all eigenvalues of $-\triangle_{2}(\mathfrak{F}(b))$ blowing up to infinity as $b$ goes to either 0 or 1.

9. Conclusions

An electronic triplet, $\{\lambda_{1}, \lambda_{2}, \lambda_{3}\}$ has three Born-Openheimer Hamiltonians, $B_{i}$, associated with each of the three eigenvalues on the triplet. The potential function for each of these Hamiltonians is minimised on one of isoparametric submanifolds $\mathfrak{F}(b)$. Therefore, up to a constant, the spectrum of $B_{i}$ is given by the spectrum of $-\triangle_{i}(\mathfrak{F}(b))$, for $b = \lambda_{2}-\lambda_{1} \lambda_{3}-\lambda_{1}$. These eigenvalues are given by the eigenvalues of the Casimir matrices in Theorems 7.1 and 7.2. They are plotted in Figures 3 and 4.

Although we have specifically considered the $T \otimes (e_{g} \oplus t_{2g})$ Jahn-Teller effect of octahedral molecules, our results also apply to pseudorotational excitations of electronic triplet states for any molecule. This includes the $T \otimes h_{g}$ Jahn-Teller effect of icosahedral molecules. Evidence for this Jahn-Teller effect in the icosahedral molecule $C_{60}$ has been reported in [23]. As well, molecules with icosahedral symmetry also exhibit a Jahn-Teller effect for electronic quadruplets.

We remark on the relationship between our work and Berry phases in Jahn-Teller problems. Berry phases appearing in the $T \otimes (e_{g} \oplus t_{2g})$ and $T \otimes h_{g}$ Jahn-Teller problems have been studied in [15] and [1, 45], respectively. The topological results in this paper can also be used to compute Berry phases and we refer to [19] for a description of how this is done. However, it is apparent from the results in this paper that the full geometrical content of the Jahn-Teller effect exceeds that which can be determined by Berry phases alone.

To summarise, the primary contribution of our work has been to supply a rigorous basis for the topological and geometrical aspects of Jahn-Teller computations for electronic triplets. We initially reported on the connection between isoparametric geometry and the Jahn-Teller effect in [60]. In pursuing this relationship, we have demonstrated that the connection Laplacian on the tautological lines bundles over Cartan’s isoparametric foliation of type 3 in $S^{3}$ exhibit interesting spectral flow properties.
Figure 3. The eigenvalues of $-\Delta_1(\mathfrak{f}(b))$ plotted against $b$. The eigenvalue $\lambda_{m,j}^1$ is labelled by $m, j$ on the graph.
Figure 4. The eigenvalues of $-\triangle_2(\mathcal{F}(b))$ plotted against $b$. The eigenvalue $\lambda_{m,l}^2$ is labelled by $l, m$ on the graph.
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