

THE PSEUDOROTATIONAL ENERGY SPECTRUM OF AN
OCTAHEDRAL MOLECULE WITH $1/2$ -INTEGER SPIN

by

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Abstract

The Jahn-Teller effect, which underlies non-linear molecular energy spectra, has been the focus of many studies and measurements since its discovery in the 1930's. In this work we theoretically calculate the pseudorotational energy spectrum of an octahedral molecule using a two parameter fit. In particular we calculate the doubly degenerate energy levels belonging to the $\Gamma_8 \otimes (e \oplus t_{2g})$ problem. The Born-Oppenheimer Hamiltonian is constructed and solved on the canonical line bundle over $\mathbb{H}P(1)$. According to the strong Jahn-Teller approximation, the non-Jahn-Teller active vibrations are built upon the solutions to the Born-Oppenheimer Hamiltonian. This complete spectrum is compared to spectral data taken using IrF_6 .

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Chapter 1

Introduction

In 1937, H. A. Jahn and E. Teller [14] showed by exhaustive group theoretic calculation that any symmetric atomic configuration of a non-linear molecule is not at an energy minimum. The following year, H. A. Jahn [15] showed that the same is true for any non-linear molecule with spin. For each molecular symmetry group, Jahn and Teller calculated normal mode coordinates on which the molecule finds a minimum potential energy. These normal mode coordinates transform according to one or more irreducible representation of the symmetry group.

In particular, an octahedral molecule with half integer spin exhibiting four-fold degeneracy is referred to as the $\Gamma_8 \otimes (e_g \oplus t_{2g})$ problem. Γ_8 is the irreducible representation to which the potential energy transforms and e_g and t_{2g} are the two irreducible representations to which the normal mode coordinates transform. The Jahn-Teller effect has been studied extensively over the years, and both the $\Gamma_8 \otimes e_g$ and $\Gamma_8 \otimes t_{2g}$ problems have been solved exactly [3, 16, 19, 4]. However, the equal coupling case of $\Gamma_8 \otimes (e_g \oplus t_{2g})$ has only been approximated and modeled on computer. A complete solution has not been mathematically calculated to this date.

The goal of this work is to theoretically calculate the vibronic energy spectrum of an octahedral molecule with half integer spin and four-fold degeneracy, solving the $\Gamma_8 \otimes (e_g \oplus t_{2g})$ problem, and compare the result to existing data.

The Jahn-Teller normal mode coordinates determine a nuclear coordinate space in which the molecule's minimum potential energy submanifold exists. The Born-Oppenheimer approximation is applied in order to break the total molecular Hamiltonian into an electronic part which

is parametrically dependent on nuclear position and a nuclear part. The problem then becomes one of determining electronic eigenvalues on a four dimensional configuration space.

This calculation is carried out in the quaternion number field, which has been previously associated with physical problems involving half integer spins [7], in order to reduce the number of degrees of freedom. Furthermore, due to the global twisting of the electronic eigenspace, fibre bundles are employed to solve the eigenvalue problem in a more geometrically simple manner.

Pseudorotational oscillations occur when the nuclear coordinates remain on the previously determined minimal energy submanifold. Transverse oscillations occur when the molecule's nuclear positions cause it to oscillate in the configuration space perpendicular to the minimal submanifold. In the strong Jahn-Teller coupling approximation, the transverse oscillations are at high frequencies. Thus, their contribution to the total spectrum is solely in the high energy range. It has also been found that these transverse energy levels can be modeled well using computer algorithms [20]. This work, therefore, concentrates on determining the low energy pseudorotational spectrum only.

Finally, the solution to the electronic Hamiltonian is multiplied by a scale factor corresponding to the radius of the submanifold and added to an arbitrary zero point potential energy. This gives the pseudorotational energy levels which are fitted to known data [2] to determine these two parameters.

Chapter 2

The Born-Oppenheimer Approximation

2.1 The Total Hamiltonian

The Born-Oppenheimer approximation is useful when dealing with a many body problem with a very large mass ratio, such as that of nuclei to electrons. Rather than attempt to calculate the solution of a complex Schroedinger equation on a relatively straightforward Hilbert space, we will instead use a less complicated Born-Oppenheimer Hamiltonian consisting essentially of a Laplacian and an effective potential, on sections in a particular fibre bundle.

The total molecular Hamiltonian for a molecule with K nuclei of mass, M , and k electrons of mass, m , is,

$$H_{mol} = \frac{-1}{2M} \sum_{i=1}^K \Delta_{\rho_i} - \frac{1}{2m} \sum_{j=1}^k \Delta_{r_j} + V(\vec{\rho}, \vec{r}) + V_{nuc}(\vec{\rho}). \quad (2.1)$$

The coordinates are defined as follows:

$$\vec{\rho} = (\rho_1, \rho_2, \dots, \rho_K) \in N \subset \mathbb{R}^{3K}$$

$$\vec{r} = (r_1, r_2, \dots, r_k) \in X \subset \mathbb{R}^{3k}$$

where $\vec{\rho}$ is the position vector of all K nuclei in three dimensional Euclidean space and N is the subspace of nuclear configurations in \mathbb{R}^{3K} . Similarly, \vec{r} is the k -vector defining the configuration of the k electrons, and X is the subspace of \mathbb{R}^{3k} corresponding to electronic configurations. In Equation 2.1, $V(\vec{\rho}, \vec{r})$ is the potential function incorporating to all pairwise Coulomb interactions between two electrons or between a nucleus and an electron. $V_{nuc}(\vec{\rho})$ is the potential function corresponding to all nuclei-nuclei interactions.

Since we are using Euclidean spaces it is convenient to define the following metrics for the configuration spaces;

$$N \text{ has the metric } g_{ij} = 2M\delta_{ij}$$

$$X \text{ has the metric } h_{ij} = 2m\delta_{ij}.$$

Substituting the new metrics into Equation 2.1 we have,

$$H_{mol} = -\Delta_{(N)} - \Delta_{(X)} + V + V_{nuc}. \quad (2.2)$$

The Hamiltonian in Equation 2.2 acts on eigenfunctions, $\phi \in L^2(N \times X; \mathbb{C})$;

$$H_{mol} : L^2(N \times X; \mathbb{C}) \rightarrow L^2(N \times X; \mathbb{C}).$$

$L^2(N \times X; \mathbb{C})$ is defined as the set of all square integrable functions, $\phi : N \times X \rightarrow \mathbb{C}$. A function, f , with domain, D , is *square integrable* if $\int_D |f|^2 = 1$.

We are now in a position to separate the total Hamiltonian into a nuclear and an electronic component. The latter is denoted, H_{el} , and is parametrically dependent on nuclear coordinates;

$$H_{el}(\vec{\rho}) = -\Delta_{(X)} + V(\vec{\rho}, \cdot) : L^2(X; \mathbb{C}) \rightarrow L^2(X; \mathbb{C}). \quad (2.3)$$

Thus, H_{mol} has been decomposed into,

$$H_{mol} = -\Delta_{(N)} + V_{nuc} + \int_X^\oplus H_{el}(\vec{\rho}) d\vec{\rho} \quad (2.4)$$

where \int_X^\oplus refers to a direct integral over the electronic configuration space, X .

2.2 Redefine H_{mol} acting on bundle sections

We wish to define H_{mol} as acting on sections of a trivial fibre bundle. In order to accomplish this goal, first define the canonical isomorphism, h , between $L^2(N \times X; \mathbb{C})$ and $L^2(N; L^2(X; \mathbb{C}))$. For any function, $f \in L^2(N \times X; \mathbb{C})$ the isomorphism, $h : f \mapsto h(f)$ where $h(f) \in L^2(N; L^2(X; \mathbb{C}))$.

$h(f)$ is defined by $h(f) : x \mapsto f(x, \cdot) \quad \forall x \in N$ such that the inner product of $\langle f, g \rangle \in L^2(N; \mathbb{C})$ for all $g \in L^2(N; L^2(X; \mathbb{C}))$.

Second, define the trivial fibre bundle, ϵ :

$$\begin{array}{c} \epsilon : \quad L^2(X; \mathbb{C}) \times L^2(X; \mathbb{C}) \times N \\ \downarrow p \\ N \end{array}$$

Third, construct an isomorphism, \hat{h} , between square integrable functions in $L^2(N; L^2(X; \mathbb{C}))$ and square integrable sections of ϵ . Let σ be a square integrable section of ϵ ; $\sigma : x \mapsto (x, \hat{\sigma})$. For all $x \in N$, where $\hat{\sigma} \in p^{-1}(x)$ is some function in $L^2(X; \mathbb{C})$, define the isomorphism, $\hat{h} : \sigma \mapsto \hat{\sigma}$. Thus, there exists an isomorphism, $\hat{h} \circ h : L^2(N \times X; \mathbb{C}) \rightarrow L^2(\epsilon)$ and we can view H_{mol} as acting on square integrable sections of the the trivial bundle;

$$H_{mol} : L^2(\epsilon) \rightarrow L^2(\epsilon). \quad (2.5)$$

Next we wish to define a sub-bundle, $\eta \subset \epsilon$ which will be more topologically useful. Suppose that $H_{el}(\vec{\rho})$ has one or a direct sum of eigenspaces, $Z(\vec{\rho})$ with associated eigenvalues which are bounded away from the rest of the total spectrum. Then we can define a new fibre bundle, η :

$$\begin{array}{ccc} \eta : & Z(\cdot) & \hookrightarrow E \\ & & \downarrow p \\ & & N \end{array}$$

where $E = \{(\vec{\rho}, \phi) \in N \times L^2(X; \mathbb{C}) | \phi \in Z(\vec{\rho})\}$ and $p(\vec{\rho}, \phi) = \vec{\rho}$.

Each fibre of η is a subspace of a fibre of ϵ and thus η is a sub-bundle of ϵ , $\eta \subset \epsilon$. However, it is important to note that since N is not necessarily contractable and Z is assumed to be finite dimensional, η is in general a non-trivial finite dimensional fibre bundle. Since $\eta \subset \epsilon$, it follows that the set of square integrable sections over η is similarly, $L^2(\eta) \subset L^2(\epsilon)$.

2.3 The Born-Oppenheimer Hamiltonian

We know that H_{mol} acts on $L^2(\epsilon)$. The Born-Oppenheimer Approximation states that H_{mol} restricts to $L^2(\eta) \subset L^2(\epsilon)$. This means that if P is the orthogonal projection operator onto $L^2(\eta)$ then the construct, $P^\perp H_{mol} P$, will be small. There have been some approximations made of $P^\perp H_{mol} P$ by Hagedorn [12] for diatomic molecules, but it has been found that this approximation is valid at low energies and becomes increasingly worse at higher energies.

Assuming that the Born-Oppenheimer approximation is valid, we construct the Born-Oppenheimer Hamiltonian, H_{BO} ;

$$H_{BO} = PH_{mol}P : L^2(\eta) \rightarrow L^2(\eta). \quad (2.6)$$

where $P = \int_{\oplus} P(\vec{\rho}) d\vec{\rho}$ and H_{mol} is defined in Equation 2.2. Thus,

$$\begin{aligned} H_{BO} &= P(\vec{\rho})(-\partial_{\vec{\rho}}^2 - \partial_{\vec{r}}^2 + V + V_{nuc})P(\vec{\rho}) \\ &= P(\vec{\rho})(-\partial_{\vec{\rho}}^2 + 2P(\partial_{\vec{\rho}}P(\vec{\rho}))\partial_{\vec{\rho}} + \partial^2 P(\vec{\rho})) + H_{el} + V_{nuc} \end{aligned}$$

Thus, H_{BO} is a second order differential operator with leading symbol, $-g_{ij}$, (from the $-\partial_{\vec{\rho}}^2$ term) where g_{ij} is the metric on N .

Lemma: [10] If $D : C^\infty(\xi) \rightarrow C^\infty(\xi)$ is a second order differential operator on sections of a bundle, ξ , and D has the leading symbol, g_{ij} , where g_{ij} is some Riemannian metric on the Base space, then there exists a unique connection, ω , on ξ such that

$$D = -\Delta_\omega + V.$$

V is locally an $n \times n$ matrix of potential functions if the fibres of ξ are n -dimensional.

By this lemma, it is clear that the Born-Oppenheimer Hamiltonian can be expressed as

$$H_{BO} = -\Delta_\omega + V_{eff} \quad (2.7)$$

Choose a local orthonormal basis for sections of η , $\{\phi_m\}$. Then the connection, ω , can be calculated;

$$\omega_i = \frac{1}{2}(g_{ij}A^j + g_{ij}g^{kl}\Gamma_{kl}^j)$$

where A^j is the $d \times d$ matrix whose elements are $\langle \phi_m, \frac{\partial}{\partial x^j} \phi_n \rangle_{L^2(X; \mathbb{C})}$ and ϕ_m, ϕ_n are eigenvalues of H_{el} . Γ_{kl}^j are Christoffel symbols of the base space of η which are for most smooth Base spaces, zero.

Thus, the effective potential in Equation 2.7, V_{eff} , is the sum:

$$V_{eff} = [H_{el}] + V_{nuc} + [-\frac{1}{2}g^{ij}\omega_j g^{-1}(\frac{\partial}{\partial \rho^i}g) - g^{ij} \langle \phi_m, \frac{\partial^2}{\partial \rho^i \partial \rho^j} \phi_n \rangle + g^{ij}(\frac{\partial}{\partial \rho^i}\omega_j) + g^{ij}\omega_i\omega_j] \quad (2.8)$$

where $[H_{el}] = \langle \phi_m, H_{el} \phi_n \rangle$ is a $d \times d$, ρ -dependent matrix, $g = \det[g_{ij}]$ and $\{\rho_i\}$ are the coordinates on N .

2.4 The Strong Jahn-Teller Approximation

We now apply the *strong Jahn-Teller approximation* to the problem, which means that we view the first term in Equation 2.8 as dominant, and V_{eff} becomes,

$$V_{eff} = [H_{el}(\vec{\rho})] \quad (2.9)$$

Let the symmetric nuclear configuration be $\vec{\rho}_0 \in N$. Then $[H_{el}(\vec{\rho}_0)] = \langle \phi_m(\vec{\rho}_0), H_{el}(\vec{\rho}_0) \phi_n(\vec{\rho}_0) \rangle$. If N is a contractable neighborhood of $\vec{\rho}_0$ then η over N is a trivial bundle. Note that $[H_{el}(\vec{\rho})]$ is not necessarily generally diagonalizable over N . Now we puncture N by removing $\vec{\rho}_0$ to get $N' = N - \{\vec{\rho}_0\} \subset N$.

V_{eff} will be minimized on a sub-manifold of non-zero dimension and non-trivial topology. A direct result of this non-trivial topology is the existence of pseudorotations on this minimum energy submanifold. It is these pseudorotational energy levels that this work attempts to calculate, and thus we wish to find the submanifold on which V_{eff} is minimized.

The strong Jahn-Teller approximation means that we find the minimum eigenvalue and thus the minimum V_{eff} and assume an infinite potential well elsewhere. Therefore, we have a successfully restated the problem of finding the spectrum corresponding to an octahedral molecule. We now wish to find the eigenvalues of the negative Laplacian, $-\Delta_\omega$, on the non-trivial fibre bundle

over the minimum energy submanifold. In this case V_{eff} is a constant zero point energy and can be easily added to the calculations in the final stage.

The solution to this simplified problem corresponds to the *pseudorotational spectrum*, referring to pseudorotations of the nuclear coordinates on the minimum energy submanifold. The remainder of the complete molecular spectrum is made up by the *transverse oscillations*, referring to nuclear coordinate oscillations perpendicular to the minimum energy submanifold.

However, the transverse oscillatory spectrum have been shown to be well modeled to a first order approximation by Simple Harmonic Oscillators [20], with characteristic frequency dependent on potential. In the strong Jahn-Teller approximation it is therefore reasonable to assume that there frequencies are quite large and thus the lower energy range is dominated by pseudorotational energy levels. The complete molecular energy spectrum is composed of the transverse oscillations built in SHO towers on each pseudorotational energy level.

Given that our two assumptions of the Born-Oppenheimer approximation and the strong Jahn-Teller approximation are valid, the solution to the problem of the molecular spectrum corresponds to finding eigenvalues of H_{BO} on the square integrable sections of η' over N' .

From Equation 2.7, H_{BO} is the sum of $-\Delta$ and an effective potential, V_{eff} . If we now separate our restricted nuclear configuration space, N' , into submanifolds on which the eigenvalues of H_{el} are constant, then from Equation 2.9 V_{eff} is also necessarily constant on each of these submanifolds.

In Chapter 3 the specific geometry of these submanifolds is determined for the problem of an octahedral molecule, by calculating the eigenvalues of the electronic Hamiltonian, H_{el} , and the manner in which the eigenvalues depend on nuclear coordinates.

Chapter 3

The Jahn-Teller Effect

In 1937 it was proven by Jahn and Teller [14] that a polyatomic molecule with orbital degeneracy arising solely from symmetry will not be energetically stable. Later that year H. A. Jahn generalized this theory [15] to include molecules with spin degeneracy. This section serves as a summary of their work.

Initially, it must be demonstrated that if the molecule's electronic energy is linearly dependent on nuclear displacement from symmetry in any direction, then the symmetric configuration cannot be stable. In other words, linear dependence on any spatial variable implies a non-zero slope of the energy curve at symmetry, and thus a perfectly symmetric molecule cannot be at minimum energy.

Let the nuclear configuration of the molecule be denoted $\vec{\rho}$, and the symmetric nuclear configuration, $\vec{\rho}_0$. $\vec{\rho}$ can then be expressed as a linear combination of displacements about $\vec{\rho}_0$;

$$\vec{\rho} = \vec{\rho}_0 + \sum_i \rho_i \eta_i, \quad (3.1)$$

where η_i are small normal displacements of the nuclei which can be chosen to transform according to irreducible representations of the molecular symmetry group [27].

A Taylor expansion of the electronic Hamiltonian from Equation 2.4 gives,

$$H_{\text{el}} = H_0 + \sum_i V_i(\vec{r})\eta_i + \sum_{ij} V_{ij}(\vec{r})\eta_i\eta_j + \cdots \quad (3.2)$$

where \vec{r} represents the electron coordinates, V_i and V_{ij} are entirely dependent upon electron

positions, and electronic kinetic energy is included in H_0 . H is, of course, dependent on nuclear configuration, $\vec{\rho}$ and $H_0 = H_{el}(\vec{\rho}_0)$.

At the degenerate symmetric state we have the following eigenvalue equation;

$$H_0\phi_\nu = E_0\phi_\nu, \quad (3.3)$$

where $\{\phi_\nu\}$ is a set of eigenfunctions for $H(\vec{\rho}_0)$.

At any nuclear configuration, $\vec{\rho} \neq \vec{\rho}_0$, the energy levels may be multiply degenerate, split into a set of energies, $\{E_\alpha\}$. The only way $\vec{\rho}_0$ will be stable is if every E_α has a minimum at $\vec{\rho} = \vec{\rho}_0$ in which case E_α becomes a perturbed energy level;

$$E_\alpha = E_0 + E_\alpha^1 + \dots \quad (3.4)$$

where the first order perturbation term, E_α^1 , is due to the linear terms, $\sum_i V_i(\vec{r})\eta_i$, in the total electronic energy.

It follows from perturbation theory [5] that these terms, E_α^1 , are the diagonal elements of the perturbation matrix;

$$M_{\nu\sigma} = \sum_i \eta_i \int \phi_\nu^* V_i \phi_\sigma d\tau, \quad (3.5)$$

or,

$$M_{\nu\nu} = \sum_i \eta_i \int V_i |\phi_\nu|^2 d\tau. \quad (3.6)$$

Unless the integrals in Equation 3.6 are zero, the perturbation energies will be linearly dependent on η_i . However, at a minimum energy, $\frac{\partial}{\partial \eta_i} H = 0$. Therefore, if the perturbation terms, $\{E_\alpha^j\}$ (and therefore the matrix elements, $M_{\nu\nu}$) are linearly dependent on some η_i the symmetric state is non-stable. By showing that the integrals in Equation 3.6 are non-zero, we prove that the symmetric state is non-stable and thus demonstrate the existence of the Jahn-Teller effect.

A background summary of the necessary group theory and derivations is provided in Appendix A. From [6, Chap. 5], if we have an integrand consisting of two factors,

$$\int f_A f_B d\tau, \quad (3.7)$$

the integral will be non-zero if it is invariant under all symmetry transformations which will be the case if it forms a basis for the totally symmetric representation of the group. It follows that the integrals in Equation 3.7 will be non-zero if the representation of the direct product, Γ_{AB} , contains the total symmetry representation.

We know from Equation A.6 that the number of times the total symmetry irreducible representation occurs in Γ_{AB} is,

$$a_1 = \frac{1}{h} \sum_R \chi_{AB}(R) \chi_1(R), \quad (3.8)$$

where h is the order of the group and $\chi_i(R)$ is the character of the group element, R , in the i^{th} irreducible representation. $\chi_1(R) = 1$ for all group operations, R , where χ_1 is a character of the totally symmetric representation.

Further, from Equation A.7;

$$\chi_{AB}(R) = \chi_A(R) \chi_B(R) \quad (3.9)$$

for direct product representations. Thus,

$$a_1 = \frac{1}{h} \sum_R \chi_A(R) \chi_B(R). \quad (3.10)$$

However, from Equation A.4,

$$\sum_R \chi_i(R) \chi_j(R) = h \delta_{ij} \quad (3.11)$$

and substituting Equation 3.11 into Equation 3.10 we find that,

$$a_1 = \delta_{AB} \quad (3.12)$$

Therefore, in order for the direct product, $f_A f_B$, to contain the total symmetry representation, the representation of one factor, Γ_A , must be or contain the same representation as Γ_B . We now apply this result to the matrix elements from Equation 3.6 which we wish to be non-zero.

In this case $|\phi|^2$ will transform as the symmetric product of the representation of ϕ with itself, $[\phi_\nu^2]$. Therefore, if $V_i(\vec{r})$ and $[\phi_\nu^2]$ contain the same irreducible representation then the

matrix elements are non-zero and the symmetric configuration is non-stable. In [14] all irreducible representations of $[\phi^2]$ are calculated, for ϕ transforming according to any irreducible representation of any molecular (point) symmetry group.

In the follow-up paper to [14], H. A. Jahn considers degeneracy arising from electron spin. It is shown that if the molecule has an even number of electrons then the above argument from [14] applies and the symmetric state is unstable. However, if the molecule has an odd number of electrons, degeneracy will still be broken by moving away from symmetry, unless the degeneracy is a twofold one of the sort introduced by Kramers [17], known as Kramers doublets.

The molecular symmetry group under study in this work is the double group, O'_h belonging to an octahedral molecule with spin. The addition of a group operation of a rotation by π generates the double group from O_h and corresponds to the operation of reversing spin. Table 3.1 is the complete character table for O_h [22].

	$4C_3$ $4C_3^2$ $3C_2$ $3C_4$ $3C_4^3$ $6C_2'$							
O'	E	R	$4C_3^2R$	$4C_3R$	$3C_2R$	$3C_4^3R$	$3C_4R$	$6C_2'R$
A_1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	1	-1	-1	-1
E	2	2	-1	-1	2	0	0	0
T_1	3	3	0	0	-1	1	1	-1
T_2	3	3	0	0	-1	-1	-1	1
Γ_6	2	-2	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0
Γ_7	2	-2	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0
Γ_8	4	-4	-1	1	0	0	0	0
$(\chi_{\Gamma_8}(g))^2$	16	16	1	1	0	0	0	0
$\chi_{\Gamma_8}(g^2)$	4	4	1	1	-4	0	0	-4
$\{\chi(g)^2\}$	6	6	0	0	2	0	0	2
$A_1 + E + T_2$	6	6	0	0	2	0	0	2

Table 3.1: Character table of O'

The integrand of the perturbation matrix elements (Equation 3.6) are found to transform according to $V[\phi^2]$ for an even number of electrons, and as $V\{\bar{\phi}^2\}$ for an odd number of electrons, where $\{\bar{\phi}^2\}$ refers to the antisymmetric product of $\bar{\phi}$'s representation with itself. Eigenfunctions of a molecule with spin, $\{\bar{\phi}\}$, are not L^2 functions like $\{\phi\}$. The Hilbert space containing $\{\bar{\phi}\}$ is anticommuting. From Equation A.9, the antisymmetric product of an irreducible representation, Γ , with itself is defined by its characters as;

$$\{\chi(g)^2\} = \frac{1}{2}[(\chi(g))^2 - \chi(g^2)] \quad (3.13)$$

for any group element, g .

Since we are interested in the molecule, IrF_6 , and Ir has atomic number, 77, IrF_6 has an odd number of electrons. Thus we need to find the antisymmetric product of greater than twofold degenerate representations of the octahedral double group. We want more than twofold degenerate representations since unsplitable Kramers doublets may well exist.

It should be noted here that O'_h is O' with a center of inversion, thus the total number of classes of O'_h is 16, the second 8 of which are simply the first 8 followed by an inversion, i . In the irreducible representations, Γ_1 through Γ_8 of O'_h , the characters of the second 8 classes are duplicates of the characters of Γ_1 through Γ_8 for O' . Also, since performing the operation of inversion twice is equal to E , the identity element, the following calculations on O' apply identically to O'_h .

The characters of the square of the group elements ($\chi_{\Gamma_8}(g^2)$) are found using the g^2 's determined in Table 3.2. The group element, R , refers to a rotation by 2π radians, which is differentiated from the identity element, E , which refers to a rotation by 0 or 4π radians. For each group element, g , in a given class, Table 3.2 determines g' where,

$$g' = g^2$$

by calculating the total rotation of g^2 and any integer number of 4π rad rotations.

g^2	total rotation (rad)	reduced rotation (rad)	resulting g'
E^2	8π	0	E
R^2	4π	0	E
$(C_3)^2$	$\frac{4\pi}{3}$	$\frac{4\pi}{3}$	C_3^2
$(C_3^2)^2$	$\frac{8\pi}{3}$	$2\pi + \frac{2\pi}{3}$	C_3R
$(C_2)^2$	2π	2π	R
$(C_4)^2$	π	π	C_2
$(C_4^3)^2$	3π	$2\pi + \pi$	C_2R
$(C_2')^2$	2π	2π	R

Table 3.2: Determining $g' = g^2$

$\{\Gamma_8^2\}$ is thus calculated in Table 3.1 and is found to be reducible to;

$$\{\Gamma_8'^2\} = A_{1g} + E_g + T_{2g}. \quad (3.14)$$

as shown by the equality of the last two lines of Table 3.1.

Therefore, if $V_i(\vec{r})$ transforms according to any of these irreducible representations contained in $\{\phi^2\}$ then the integrals in Equation 3.6 are non-zero and the symmetric molecule is unstable. However, since $V_i(\vec{r})$ transforms according to the molecular symmetry group, if $\{\phi^2\}$ contains one of the irreducible representations of the molecular group then the integral is non-zero.

Equation 3.14 shows that this is the case. Furthermore, the above calculation determines the normal mode coordinates which span a configuration space in which the molecule may reach a lower energy level than that at symmetry. For an octahedral molecule with spin, this space is a 5 dimensional nuclear configuration space with two coordinates, ϵ_1 and ϵ_2 transforming according to the two dimensional representation, E_g , and three coordinates, τ_1 , τ_2 , and τ_3 transforming according to the three dimensional representation, T_{2g} .

Chapter 4

Analyzing the electronic Hamiltonian

We have already determined in Chapter 2 that an octahedral molecule will lower its potential energy by distorting along normal mode coordinates which transform according to the 2-dimensional E and 3-dimensional T_2 representations. Octahedral molecules with spin still vibrate along these normal coordinates, however, we are now concerned with a four-fold degeneracy of two unsplittable Kramers doublets.

This is known as the $\Gamma_8 \otimes (e \oplus t_2)$ problem referring to the Jahn-Teller effect for an electronic Hamiltonian transforming according to the Γ_8 representation with coupled linear vibronic interactions between the E and T_2 representations.

Let us denote the symmetrized normal coordinates transforming according to the E and T_2 representations as $\{Q_{\Gamma_i}\}$ where each coordinate possesses the following transformation properties [3];

$$Q_\theta \sim \frac{1}{\sqrt{3}}(3z^2 - r^2), \quad Q_\epsilon \sim x^2 - y^2,$$

$$Q_\xi \sim 2yz, \quad Q_\eta \sim 2xz, \quad Q_\zeta \sim 2xy.$$

Figure 4.1 displays corresponding cartesian coordinates as follows; (i) E_g displacements (Q_θ), (ii) E_g displacements (Q_ϵ), (iii) T_{2g} displacements (Q_ξ), (iv) T_{2g} displacements (Q_η), (v) T_{2g} displacements (Q_ζ).

We recombine the total Hamiltonian from Equation 2.2 in the following form;

$$H_{mol} = \hat{H}(\vec{r}) + \hat{V}(\vec{r}, \vec{\rho}) + \hat{T}(\vec{\rho}) \quad (4.1)$$

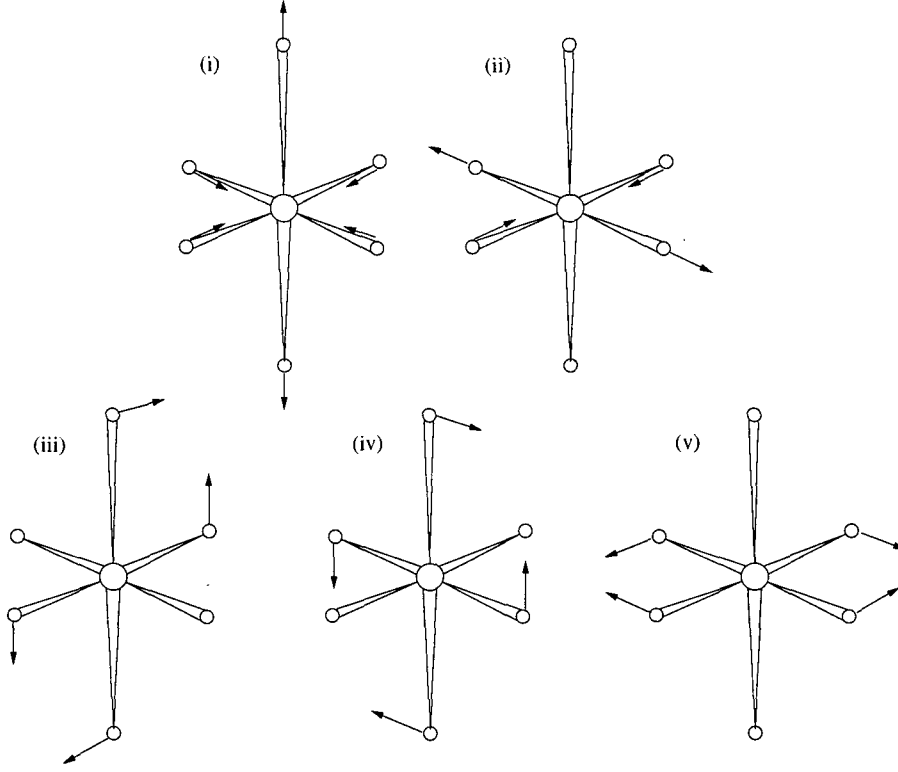


Figure 4.1: Octahedral normal mode coordinates.

where $\hat{H}(\vec{r})$ includes electronic kinetic and electron-electron potential terms, $V(\vec{r}, \vec{\rho})$ now contains electron-nuclei and nuclei-nuclei Coulomb interactions, and $\hat{T}(\vec{\rho})$ is the nuclear kinetic energy term, $-\Delta_{(N)}$.

Now we expand $\hat{V}(\vec{r}, \vec{\rho})$ in terms of the symmetrized displacements, $\{Q_{\Gamma_\gamma}\}$, to second order;

$$V(\vec{r}, \vec{\rho}) \simeq V(\vec{r}, \vec{\rho}_0) + \sum_i \left(\frac{\delta V}{\delta \rho_i} \right)_0 (\rho_i - \rho_{0i}) + \frac{1}{2} \sum_{ij} \left(\frac{\delta^2 V}{\delta \rho_i \delta \rho_j} \right)_0 (\rho_i - \rho_{0i}) (\rho_j - \rho_{0j}) \quad (4.2)$$

where the zero subscript means evaluate at the symmetric nuclear configuration.

By substituting Equation 4.2 into Equation 4.1, H_{mol} becomes,

$$H_{mol} = \hat{T}(\vec{\rho}) + U(\vec{r}, \vec{\rho}) \quad (4.3)$$

$$U(\vec{r}, \vec{\rho}) = \hat{H}(\vec{r}, \vec{\rho}_0) + \sum_{\Gamma_\gamma} V_{\Gamma_\gamma}(\vec{r}) Q_{\Gamma_\gamma} + \frac{1}{2} \sum_{\Gamma_1 \gamma_1} \sum_{\Gamma_2 \gamma_2} W_{\Gamma_1 \gamma_1 \Gamma_2 \gamma_2}(\vec{r}) Q_{\Gamma_1 \gamma_1} Q_{\Gamma_2 \gamma_2} \quad (4.4)$$

where $\hat{H}(\vec{r}, \vec{\rho}_0) = \hat{H}(\vec{r}) + \hat{V}(\vec{r}, \rho_0)$, $V_{\Gamma_\gamma}(\vec{r}) = \frac{\delta \hat{V}(\vec{r}, \vec{\rho}_0)}{\delta Q_{\Gamma_\gamma}}$ and $W_{\Gamma_1 \gamma_1 \Gamma_2 \gamma_2}(\vec{r}) = \frac{\delta^2 \hat{V}(\vec{r}, \vec{\rho}_0)}{\delta Q_{\Gamma_1 \gamma_1} \delta Q_{\Gamma_2 \gamma_2}}$.

Suppose now that we classify the electronic basis states, $\psi_n(\vec{r})$, by the irreducible representations, Γ_γ where the total eigenvalues are made up by,

$$\Psi_n(\vec{r}, \vec{\rho}) = \sum_{k=1}^f \psi_k(\vec{r}) \xi_k(\vec{\rho}).$$

In the case where all f electronic wave functions belong to the same irreducible representation, the Wigner-Eckart theorem states that matrix elements of any operator with these functions are not independent. Thus,

$$\langle \psi_{\Gamma_{\gamma_1}}(\vec{r}) | V_{\Gamma_\gamma}(\vec{r}) | \psi_{\Gamma_{\gamma_2}}(\vec{r}) \rangle = \langle \bar{\Gamma} | V_{\Gamma} | \bar{\Gamma} \rangle \langle \Gamma_\gamma \bar{\Gamma}_{\gamma_2} | \Gamma_{\gamma_1} \rangle \quad (4.5)$$

where $\langle \bar{\Gamma} | V_{\Gamma} | \bar{\Gamma} \rangle$ is the reduced matrix element independent of γ_1 , γ_2 , or γ , which shall be denoted, V_{Γ} , for convenience. $\langle \Gamma_\gamma \bar{\Gamma}_{\gamma_2} | \Gamma_{\gamma_1} \rangle$ are the Clebsch-Gordan coefficients.

Substituting Equation 4.5 into Equation 4.4 and summing over the appropriate normal mode coordinate representations;

$$U = \sum_{\Gamma_\gamma} V_{\Gamma} Q_{\Gamma_\gamma} \hat{C}_{\Gamma_\gamma} + \frac{1}{2} \sum_{\Gamma_1 \Gamma_2} \sum_{\Gamma_\gamma} W_{\Gamma}(\Gamma_1 \times \Gamma_2) \{Q_{\Gamma_1} \times Q_{\Gamma_2}\}_{\Gamma_\gamma} \hat{C}_{\Gamma_\gamma} \quad (4.6)$$

where \hat{C}_{Γ_γ} are matrices composed of the Clebsch-Gordan coefficients, $W_{\Gamma}(\Gamma_1 \times \Gamma_2)$ is the reduced matrix element of the operator, $W_{\Gamma_1 \gamma_1 \Gamma_2 \gamma_2}$ from Equation 4.4, and the zero point energy is taken from Equation 4.4, $\langle \psi_{\Gamma_\gamma} | H(\vec{r}, \vec{\rho}_0) | \psi_{\Gamma_\gamma} \rangle = 0$.

Separating the totally symmetric tensors from Equation 4.6, i.e. those proportional to \hat{C}_{A_1} , and adding them to the kinetic term from Equation 4.4 we get the totally symmetric part of the Hamiltonian;

$$H_0 = \left(\sum_{\Gamma_\gamma} \frac{1}{2M(\Gamma)} \partial_{\Gamma_\gamma}^2 + \frac{1}{2} \sum_{\Gamma_\gamma} \sum_{\Gamma_1 \Gamma_2} W_{A_1}(\Gamma_1 \times \Gamma_2) Q_{\Gamma_1} Q_{\Gamma_2} \right) \hat{C}_{A_1}. \quad (4.7)$$

Changing to mass weighted coordinates to remove the $M(\Gamma)$'s and denoting the eigenvalue of $||W_{A_1}(\Gamma_1 \times \Gamma_2)||$ in the new coordinates by ω_Γ we obtain,

$$H_0 = \frac{1}{2} \sum_{\Gamma_\gamma} (\Delta_{(X)_{\Gamma_\gamma}} + \omega_\Gamma Q_{\Gamma_\gamma}^2) \hat{C}_{A_1}. \quad (4.8)$$

Finally, adding the totally symmetric term from Equation 4.8 to the rest of the Hamiltonian from Equation 4.6 and taking into account only linear vibronic couplings we find the electronic Hamiltonian,

$$H_{el} = \frac{1}{2} \sum_{\Gamma_\gamma} (\Delta_{(X)\Gamma_\gamma} + \omega_\Gamma^2 Q_{\Gamma_\gamma}^2) \hat{C}_{A_1} + \sum_{\Gamma_\gamma} V_\Gamma Q_{\Gamma_\gamma} \hat{C}_{\Gamma_\gamma} \quad (4.9)$$

The Clebsch-Gordan coefficients given by a basis of electronic states of the Γ_8 term have been determined as follows [3]. The basis of states are:

$$\begin{aligned} |e_1\rangle &= \frac{1}{\sqrt{2}}(\psi_{1/2} + i\psi_{-3/2}) \\ |e_2\rangle &= \frac{1}{\sqrt{2}}(-\psi_{-1/2} - i\psi_{3/2}) \\ |e_3\rangle &= \frac{1}{\sqrt{2}}(-\psi_{1/2} + i\psi_{-3/2}) \\ |e_4\rangle &= \frac{1}{\sqrt{2}}(\psi_{-1/2} - i\psi_{3/2}) \end{aligned} \quad (4.10)$$

and the Clebsch-Gordan coefficients are,

$$\begin{aligned} \hat{C}_1 &= \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} & \hat{C}_2 &= \begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} \\ \hat{C}_3 &= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{bmatrix} & \hat{C}_4 &= \begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{bmatrix} \\ \hat{C}_5 &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} & \hat{C}_A &= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \end{aligned} \quad (4.11)$$

It has been demonstrated [7] that time-reversal invariant fermionic systems have a natural quaternion basis, and thus we wish to make the following basis change [23]. If $|J, m\rangle$ is the

basis for a spin J multiplet, $m = -J \dots J$, then the time reversal operator acts as follows:

$$\Theta[\alpha|J, m \rangle] = (-1)^{J-m} \alpha^* |J, -m \rangle \quad \forall \alpha \in \mathbb{C} \quad (4.12)$$

which leads to a canonical quaternion basis of the Hilbert space with half-odd integer spin, J ;

$$e_l = |J, J - 2l + 2 \rangle \quad \forall l = 1, 2 \dots J + \frac{1}{2}. \quad (4.13)$$

For example, if we wish to study a Hilbert space of a molecule with spin $J = \frac{3}{2}$, then $l = 1, 2$ and the quaternion basis is;

$$e_1 = |\frac{3}{2}, \frac{3}{2} \rangle, \quad e_2 = |\frac{3}{2}, -\frac{1}{2} \rangle \quad (4.14)$$

where,

$$\begin{aligned} \Theta e_1 &= \Theta |\frac{3}{2}, \frac{3}{2} \rangle = |\frac{3}{2}, -\frac{3}{2} \rangle \\ \Theta e_2 &= \Theta |\frac{3}{2}, \frac{1}{2} \rangle = -|\frac{3}{2}, \frac{1}{2} \rangle. \end{aligned} \quad (4.15)$$

Therefore, we now change from the $\{|e_i \rangle\}$ basis, to a basis consisting of $\{\psi_{3/2}, \psi_{-1/2}\}$ along with the Time Reversal Operator, Θ . In this way we have $\psi_{1/2} = \Theta \psi_{-1/2}$ and $\psi_{-3/2} = \Theta \psi_{3/2}$.

From Equation 4 we have the new basis in terms of four-vectors in $\{|e_i\rangle\}$,

$$\begin{aligned}
 \psi_{3/2} &= \frac{1}{\sqrt{2}}(|e_2\rangle + |e_4\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \\
 \psi_{1/2} &= \frac{1}{\sqrt{2}}(|e_1\rangle - |e_3\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \\ 0 \end{bmatrix} \\
 \psi_{-1/2} &= \frac{1}{\sqrt{2}}(|e_4\rangle - |e_2\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ -1 \\ 0 \\ 1 \end{bmatrix} \\
 \psi_{-3/2} &= \frac{1}{\sqrt{2}}(|e_1\rangle + |e_3\rangle) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}.
 \end{aligned} \tag{4.16}$$

Now, using Equation 4.11 and Equation 4.16 we change bases of the Clebsch-Gordan coefficients in the following manner:

$$\begin{aligned}
 \hat{C}_1 \psi_{3/2} &= \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ -1 \\ 0 \\ -1 \end{bmatrix} = -\psi_{3/2} \\
 \hat{C}_1 \psi_{-1/2} &= \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ -1 \\ 0 \\ 1 \end{bmatrix} = \psi_{-1/2}.
 \end{aligned}$$

Thus, in the new basis we have,

$$C_1 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \in Herm_0(2, \mathbb{H}) \quad (4.17)$$

where $Herm_0(2, \mathbb{H})$ is the set of 2×2 Hermitian quaternion matrices with zero trace.

Following the example of Equation 4.17, the remaining four Clebsch-Gordan matrices are calculated in the new basis and are all elements of $Herm_0(2, \mathbb{H})$:

$$\begin{aligned} C_2 &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} & C_3 &= \begin{bmatrix} 0 & k \\ -k & 0 \end{bmatrix} \\ C_4 &= \begin{bmatrix} 0 & j \\ -j & 0 \end{bmatrix} & C_5 &= \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}. \end{aligned}$$

It is easily verified that in both the quaternion and real bases, the Clebsch-Gordan coefficients behave consistently. That is, $\hat{C}_i \psi_j = C_i \psi_j$ for all $i \in \{1, 2, 3\}$ and $j = 3/2, 1/2$.

The span of the Clebsch-Gordan matrices over \mathbb{R} is now,

$$\sum_{i=1}^5 q_i C_i = \begin{bmatrix} q_1 & q_2 + q_3 i + q_4 j + q_5 k \\ q_2 - q_3 i - q_4 j - q_5 k & -q_1 \end{bmatrix}$$

which is the general form of any element of $Herm_0(2, \mathbb{H})$.

Constructing the Hamiltonian now from Equation 4.9 we have,

$$H_{el} = \begin{bmatrix} \frac{1}{2}\omega_E^2(q_1^2 + q_2^2) + \frac{1}{2}\omega_T^2(q_3^2 + q_4^2 + q_5^2) + q_1 & V_E q_2 + V_T(q_3 i + q_4 j + q_5 k) \\ V_E q_2 - V_T(q_3 i + q_4 j + q_5 k) & \frac{1}{2}\omega_E^2(q_1^2 + q_2^2) + \frac{1}{2}\omega_T^2(q_3^2 + q_4^2 + q_5^2) \end{bmatrix} \quad (4.18)$$

When one coupling constant is dominant, the calculation is carried out assuming the dominant constant is one, and the other is zero. However, it has been found that equal Jahn-Teller coupling holds true for many systems [20];

$$\omega_E = \omega_T = \omega \quad \text{and} \quad V_E = V_T = V.$$

Once the equal coupling calculation is successfully carried out, it is assumed that further results between equal and zero coupling can be extrapolated from the existing calculations.

The eigenvalues from Equation 4.18 are now

$$\lambda = \frac{1}{2}\omega^2 \sum_{i=1}^5 q_i^2 \pm V \sqrt{\sum_{i=1}^5 q_i^2}.$$

Thus, with the eigenvalues depending solely on $\sum_{i=1}^5 q_i^2$, or the radius of an S^4 , we have a configuration space of $S^4 \subset \text{Herm}_0(2, \mathbb{H})$. Further, S^4 is isometric to $\mathbb{HP}(1)$, which is the quaternion Grassmanian manifold, consisting of one-dimensional quaternion lines in \mathbb{H}^2 . Also, $\text{Herm}_0(2, \mathbb{H}) \simeq \mathbb{R}^5$, and so we have a configuration space of a round $\mathbb{HP}(1)$ with a variable radius canonically embedded in \mathbb{R}^5 .

Chapter 5

The Spectrum of the Laplacian over certain Bundles

It has been determined in Chapter 1 that we wish to find the eigenvalues of the Laplacian, Δ , where the eigenfunctions are sections of the canonical quaternion line bundle, η , over the quaternion Projective Space, $\mathbb{HP}(n)$.

Initially the necessary steps towards the solution of this problem will be taken using the canonical line bundle over the Complex Projective Space, $\mathbb{CP}(n)$, since this is a somewhat simpler task. Also the spectrum of the Laplacian on $\mathbb{CP}(1)$ itself, can be compared to known results on the isomorphic space, S^2 and the spectrum over the canonical bundle may be compared with calculated spherical harmonics and their eigenvalues, known as Monopole Harmonics.

The first step to solving the eigenvalue problem is to pullback η over its associated principal bundle and prove that the resulting line bundle, η^* is equivalent to a trivial bundle. (For an explanation of the terms pullback, or principal bundle see Appendix B.) Sections on η^* are then associated with real functions on its base space, S^{2n+1} in the Complex case and S^{4n+3} in the quaternion case, with respect to a choice of a basis frame of sections.

We begin by finding all $U(1)$ or $SP(1)$ invariant functions on the spheres, S^{2n+1} or S^{4n+3} , and then determine the transformation properties of the pullback connection on η . It then becomes possible to construct eigenfunctions which are non-invariant in such a way that they cancel the non-invariance of the chosen frame of sections and thus push down to sections on η with eigenfunctions making up the spectrum of the Laplacian on η .

In Section 6.1 we perform the above calculations in the Complex case and compare to known results, and in Section 6.2 we complete these calculations in the quaternion case.

5.1 The Complex Projective Space

5.1.1 The Pullback of a vector bundle over its principal bundle

We seek first to prove that the pullback of the canonical line bundle, η , over its associated principal bundle results in a line bundle, denoted η^* , which is identical to a trivial bundle;

$$\begin{array}{ccccc}
 & \mathbb{C}^2 & & \mathbb{C}^2 & \\
 \eta^* : & \downarrow & & \downarrow & : \eta \\
 & \tilde{E} & \xrightarrow{\tilde{q}} & E & \\
 & \downarrow (\tilde{\sigma} \uparrow) \tilde{p} & & \downarrow p (\uparrow \sigma) & \\
 U(1) & \hookrightarrow S^{2n+1} & \xrightarrow{q} & \mathbb{CP}(n) &
 \end{array}$$

In this case, sections on η^* , which solve the Laplacian may be “pushed down” by the projection map, q , to sections on η which are solutions to the Laplacian and thus are the desired eigenfunctions.

Lemma 1: The pullback of a vector bundle over its associated principal bundle is equivalent to a trivial bundle [25].

Proof: The following diagram depicts a vector bundle, η , pulled back over its associated principal bundle, where G is the structure group of η ;

$$\begin{array}{ccccc}
 & & \eta : & F & \\
 & & & \downarrow & \\
 & & & E & \\
 & & & \downarrow p & \\
 G & \hookrightarrow & \tilde{E} & \longrightarrow & B
 \end{array}$$

Consider the trivial bundle, η^* , over the principal total space and construct the following pullback square:

$$\begin{array}{ccccc}
 \eta^* : & F & & F & : \eta \\
 & \downarrow & & \downarrow & \\
 & \tilde{E} \times F & \xrightarrow{\tilde{q}} & E & \\
 & \downarrow \tilde{p} & & \downarrow p & \\
 G & \hookrightarrow & \tilde{E} & \xrightarrow{q} & B
 \end{array}$$

We wish to define the *Principal Map*, $P : \tilde{E} \times F \rightarrow E$ which will make η^* the trivial pullback of η over its associated principal bundle. If $b \in V_i \subset B$ where $b = q(e)$, $e \in \tilde{E}$, then define for all $y \in F$, $P_i(e, y) = \phi_i(b, q_i(e) \cdot y)$ where $\{q_i\}$ are functions with range in the subset $V_i \subset B$ and $\{\phi_i\}$ are the coordinate functions (defined in Appendix B). Now, for all $b \in V_i \cap V_j$ we have

$$\phi_i(b, q_i(e) \cdot y) = \phi_j(b, g_{ji}(b) \cdot q_i(e) \cdot y) = \phi_j(b, q_j(e) \cdot y).$$

where g_{ij} are the change of coordinate functions (defined in Appendix B). Thus, $\{P_i\}$ is continuous on the intersections of two coordinate subsets of B and a unique function, P , is defined as the union of $\{P_i\}$.

Commutivity in the pullback square is then straightforward;

$$p \circ P(e, y) = b = q(e) = q \circ \pi(e, y) \blacksquare$$

5.1.2 Two Theorems

Theorem 1: Let f be a homogeneous harmonic polynomial of degree k on \mathbb{R}^{n+1} , where a harmonic function is one which satisfies, $\Delta f = 0$. Then $f|_{S^n}$ is an eigenfunction of the Laplacian on the sphere, with eigenvalue $k(k+n-1)$.

Proof: Let p be any point on S^n with associated unit vector, $x_p \in \mathbb{R}^{n+1}$. Then let $\{x_2, \dots, x_{n+1}\}$ be a frame of unit vectors forming a basis for the tangent space, $T_p(S^n)$.

Define a set of geodesics based on the frame of vectors,

$$\tilde{\gamma}_i(\alpha) = (\cos \alpha)\vec{x} + (\sin \alpha)\vec{x}_i, \quad (5.1)$$

where each $\tilde{\gamma}_i$ is a great circle around S^n in the \vec{x}_i direction and α is the angle.

Now take a function on \mathbb{R}^{n+1} , f , with partial derivatives with respect to the basis, $\left(\frac{\partial f}{\partial x_i}\right)$, $i = 1, \dots, n+1$ where $x_1 = x_p$. The first derivative of $f \circ \gamma_i$ with respect to α is then,

$$\frac{\partial(f \circ \gamma_i)}{\partial \alpha} = -\sin \alpha \frac{\partial f}{\partial x_1} + \cos \alpha \frac{\partial f}{\partial x_i} \quad (5.2)$$

and the second derivative evaluated at the point, $q = \gamma_i(0)$;

$$\frac{\partial^2(f \circ \gamma_i)}{\partial^2 \alpha(0)} = -\frac{\partial f}{\partial x_1}(q) + \frac{\partial^2 f}{\partial x_i^2}(q). \quad (5.3)$$

Thus we can calculate,

$$\Delta^{S^n}(f|_{S^n})(q) = -\sum_{i=2}^{n+1} \frac{d^2}{d\alpha^2}(f \circ \gamma_i)(0) = -\sum_{i=2}^{n+1} \frac{\partial^2 f}{\partial x_i^2}(q) + n \frac{\partial f}{\partial x_1}(q) \quad (5.4)$$

$$(\Delta^{\mathbb{R}^{n+1}} f)(q) = -\sum_{i=1}^{n+1} \frac{\partial^2 f}{\partial x_i^2}(q) = -\sum_{i=2}^{n+1} \frac{\partial^2 f}{\partial x_i^2}(q) - \frac{\partial^2 f}{\partial x_1^2}(q)$$

and therefore,

$$(\Delta^{\mathbb{R}^{n+1}} f)(q) - \Delta^{S^n}(f|_{S^n})(q) = -\frac{\partial^2 f}{\partial x_1^2}(q) - n \frac{\partial f}{\partial x_1}(q)$$

or, since x_1 is in fact a radial vector of S^n ,

$$(\Delta^{\mathbb{R}^{n+1}} f)|_{S^n} = \Delta^{S^n}(f|_{S^n}) - \frac{\partial^2 f}{\partial r^2}|_{S^n} - n \frac{\partial f}{\partial r}|_{S^n} \quad (5.5)$$

Now, suppose that f is a homogeneous harmonic polynomial of degree k on \mathbb{R}^{n+1} . This means that f can be written as a sum of terms of the following form;

$$x_0^{m_0} x_1^{m_1} \cdots x_n^{m_n}$$

where for each term, $\sum_{i=0}^n m_i = k$. By changing to spherical coordinates it follows that from each term there may be factored r^k , leaving a multiplication of sin's and cos's. Thus, f can be written as $r^k f|_{S^n}$ and Equation 5.5 becomes,

$$0 = \Delta^{S^n}(f|_{S^n}) - k(k-1)f|_{S^n} - nk(f|_{S^n}).$$

Therefore,

$$\Delta^{S^n}(f|_{S^n}) = k(k+n-1)f|_{S^n}, \quad (5.6)$$

and it is proven that $f|_{S^n}$ is an eigenfunction of Δ^{S^n} with eigenvalue, $k(k+n-1)$ ■

Theorem 2: For all $k \geq 0$, the following orthogonal decomposition holds:

$$\mathcal{P}_{2k} = \mathcal{H}_{2k} \oplus r^2 \mathcal{H}_{2k-2} \oplus \cdots \oplus r^{2k} \mathcal{H}_0 \quad (5.7)$$

$$\mathcal{P}_{2k+1} = \mathcal{H}_{2k+1} \oplus r^2 \mathcal{H}_{2k-1} \oplus \cdots \oplus r^{2k} \mathcal{H}_1 \quad (5.8)$$

where \mathcal{P}_k is the set of all homogeneous polynomials of degree k on \mathbb{R}^{n+1} and \mathcal{H}_k is the set of all homogeneous harmonic polynomials of degree k on \mathbb{R}^{n+1} .

Proof: It is clear that Theorem 2 holds for \mathcal{P}_0 and \mathcal{P}_1 since $\mathcal{P}_0 = \mathcal{H}_0$ and $\mathcal{P}_1 = \mathcal{H}_1$. By induction, if we show that for all $k \geq 0$, $\mathcal{P}_k = \mathcal{H}_k \oplus r^2 \mathcal{P}_{k-2}$ then it follows that $\mathcal{P}_{k+2} = \mathcal{H}_{k+2} \oplus r^2 \mathcal{P}_k$ and so on, built up from \mathcal{P}_0 and \mathcal{P}_1 .

To prove Theorem 2 inductively, it is sufficient to show that if there exists an element, $P \in \mathcal{P}_{k+2}$ which is orthogonal to \mathcal{P}_k then P must be harmonic. P is a harmonic function if and only if $\Delta P = 0$. However, since $P \in \mathcal{P}_{k+2}$, $\Delta P \in \mathcal{P}_k$, and ΔP is therefore equal to zero if and only if it is orthogonal to all $r^{2l} \mathcal{H}_{k-2l}$ ($0 \leq 2l \leq k$) or, identically, if ΔP is orthogonal to all $\tilde{\mathcal{H}}_{k-2l}$. Here, $\tilde{\cdot}$ refers to restriction to S^n . Let Δf refer to $\Delta^{\mathbb{R}^{n+1}} f$ and $\Delta \tilde{f}$ refer to $\Delta^{S^n} f|_{S^n}$.

Suppose there exists some $P \in \mathcal{P}_{k+2}$ and $H \in \mathcal{H}_{k-2l}$ for some l . As well, suppose that P is orthogonal to \mathcal{P}_k and thus also to $\tilde{\mathcal{P}}_k$. Then,

$$\Delta \widetilde{PH} = (\Delta \tilde{P})\tilde{H} + 2 \langle d\tilde{P} | d\tilde{H} \rangle + \tilde{P}(\Delta \tilde{H}). \quad (5.9)$$

Integrating Equation 5.9 over the S^n sphere,

$$0 = \int_{S^n} \Delta \widetilde{PH} = \int_{S^n} (\Delta \tilde{P})\tilde{H} + 2 \int_{S^n} \langle d\tilde{P} | d\tilde{H} \rangle + \int_{S^n} \tilde{P}(\Delta \tilde{H}). \quad (5.10)$$

Since $H \in \mathcal{H}_{k-2l}$,

$$\Delta \tilde{H} = (k - 2l)(k - 2l + n - 1)\tilde{H}, \quad (5.11)$$

(from the results of Theorem 1). Therefore the third term becomes,

$$\int_{S^n} \tilde{P}(\Delta \tilde{H}) = (k - 2l)(k - 2l + n - 1) \int_{S^n} \tilde{P}\tilde{H} = 0,$$

the last integral being equal to zero since P is assumed to be orthogonal to $\tilde{\mathcal{P}}_k$.

Thus,

$$0 = \int_{S^n} (\Delta \tilde{P})\tilde{H} + 2 \int_{S^n} \langle d\tilde{P} | d\tilde{H} \rangle. \quad (5.12)$$

However, from Equation 5.4,

$$\begin{aligned} \Delta \tilde{P} &= \widetilde{\Delta P} + \frac{\partial^2 \tilde{P}}{\partial r^2} + n \frac{\partial \tilde{P}}{\partial r} \\ &= \widetilde{\Delta P} + (k + 2)(n + k + 1)\tilde{P}, \end{aligned} \quad (5.13)$$

and the first term in Equation 5.12 becomes,

$$\int_{S^n} (\Delta \tilde{P})\tilde{H} = \int_{S^n} \widetilde{\Delta P}\tilde{H} + (k + 2)(n + k + 1) \int_{S^n} \tilde{P}\tilde{H} = \int_{S^n} \widetilde{\Delta P}\tilde{H}, \quad (5.14)$$

again, since P is orthogonal to $\tilde{\mathcal{P}}_k$. Therefore, Equation 5.12 is rewritten as,

$$\begin{aligned} \int_{S^n} \widetilde{\Delta P}\tilde{H} &= -2 \int_{S^n} \langle d\tilde{P} | d\tilde{H} \rangle = -2 \langle \tilde{P} | \Delta \tilde{H} \rangle \\ &= -2(k - 2l)(k - 2l + n - 1) \langle \tilde{P} | \tilde{H} \rangle = 0, \end{aligned} \quad (5.15)$$

from Equation 5.11 and the fact that P is orthogonal to $\tilde{\mathcal{P}}_k$.

We have shown that $\int_{S^n} \widetilde{\Delta P} \tilde{H} = 0$ and thus, that ΔP is orthogonal to \mathcal{P}_k for all $k \geq 0$ and therefore, $\Delta P = 0$ ■

5.1.3 The Spectrum of the Laplacian on $\mathbb{CP}(n)$

Consider once more the pullback of η , the canonical line bundle over $\mathbb{CP}(n)$, over its associated principal bundle:

$$\begin{array}{ccc}
 & \mathbb{C}^2 & \mathbb{C}^2 \\
 \eta^* : \downarrow & & \downarrow : \eta \\
 \tilde{E} & \xrightarrow{\tilde{q}} & E \\
 (\tilde{\sigma} \uparrow) \tilde{p} \downarrow & & \downarrow p(\uparrow \sigma) \\
 U(1) \hookrightarrow S^{2n+1} & \xrightarrow{q} & \mathbb{CP}(n)
 \end{array}$$

From Lemma 1, proved in Sec. 4.1.1, we know that $\tilde{\eta}$ is identical to a trivial complex line bundle whose fibres are great circles, and thus its sections $\tilde{\sigma}$ can be represented by complex functions on S^{2n+1} . The projection function, q , takes the great circles in S^{2n+1} to the complex line in $\mathbb{CP}(n)$ in which the circle lies. Thus, q is invariant under unit complex ($U(1)$) multiplication.

In order to determine the spectrum of the Laplacian on η we first wish to determine the spectrum of the Laplacian on functions on $\mathbb{CP}(n)$. To find these functions, we initially construct the spectrum of the Laplacian on functions on S^{2n+1} and then q projects these functions down to $\mathbb{CP}(n)$.

Consider the set of homogeneous, harmonic polynomials of degree k on \mathbb{R}^{2n+2} . From Theorem 1, these polynomials are eigenfunctions of the Laplacian on S^{2n+1} with known eigenvalues. If we then determine those homogeneous harmonic polynomials which are also invariant under unit complex multiplication, the projection map, q , takes these functions to eigenfunctions on $\mathbb{CP}(n)$ with the same eigenvalues.

Homogeneous polynomials of degree k in \mathbb{R}^{2n+2} are in $2n+2$ real variables, $(x_0, x_1 \dots x_{2n+1})$.

Now construct $n+1$ complex variables from pairs of these real variables as follows:

$$z_0 = x_0 + ix_1$$

$$z_1 = x_2 + ix_3$$

$$z_n = x_{2n} + ix_{2n+1}$$

$$z = (z_0, z_1 \dots z_n)$$

Let $\mathcal{P}_{k,l}$ be the set of polynomials of degree k in z and degree l in \bar{z} , where $\bar{z} = (\bar{z}_0, \bar{z}_1 \dots \bar{z}_n)$ is the complex conjugate of z . Since all z_i 's commute, we can classify polynomials by degrees of z and \bar{z} rather than worry about individual z_i 's.

If $P \in \mathcal{P}_{k,l}$ and we multiply z by a unit complex number, $e^{i\theta}$;

$$P(z, \bar{z}) \rightarrow P(e^{i\theta}z, e^{i\bar{\theta}}\bar{z}) = P(e^{i\theta}z, e^{-i\theta}\bar{z}) = e^{i(k-l)\theta}P(z, \bar{z}).$$

Therefore, P will be an invariant polynomial if $k = l$.

Now we have $\mathcal{P}_{k,k}$, the set of bihomogeneous polynomials of degree k in z and \bar{z} (which are also invariant under $U(1)$ multiplication). Let $\mathcal{H}_{k,k}$ be the set of harmonic polynomials satisfying the above conditions.

From Theorem 2 we have,

$$\mathcal{P}_{2k} = \mathcal{H}_{2k} \oplus r^2 \mathcal{P}_{2k-2}.$$

Thus, by turning these polynomials into bihomogenous polynomials of complex degree k we have,

$$\mathcal{P}_{k,k} = \mathcal{H}_{k,k} \oplus r^2 \mathcal{P}_{k-1,k-1},$$

and then restricting all of these polynomials to the sphere, S^{2n+1} :

$$\tilde{\mathcal{P}}_{k,k} = \tilde{\mathcal{H}}_{k,k} \oplus r^2 \tilde{\mathcal{P}}_{k-1,k-1}. \quad (5.16)$$

Therefore,

$$\dim \tilde{\mathcal{H}}_{k,k} = \dim \tilde{\mathcal{P}}_{k,k} - \dim \tilde{\mathcal{P}}_{k-1,k-1} = \dim \mathcal{P}_{k,k} - \dim \mathcal{P}_{k-1,k-1}. \quad (5.17)$$

It follows from Equation 5.16,

$$\bigoplus_k \tilde{\mathcal{P}}_{k,k} = \bigoplus_k \tilde{\mathcal{H}}_{k,k}. \quad (5.18)$$

It only remains to show that $\bigoplus_k \tilde{\mathcal{P}}_{k,k}$ is dense in $C^\infty(\mathbb{CP}(n))$, or dense up to unit complex multiplication in $C^\infty(S^{2n+1})$. Then, by the Stone-Weierstrass theorem and Equation 5.18, $\bigoplus_k \tilde{\mathcal{H}}_{k,k}$ is the complete set of eigenfunctions on $\mathbb{CP}(n)$. This is proven in Section 6.1.4. The following is a determination of the spectrum of the Laplacian on $\mathbb{CP}(n)$ assuming the Stone-Weierstrass proof.

The dimension of $\mathcal{P}_{k,k}$ will be the square of the dimension of \mathcal{P}_k , which is simply the number of polynomials of degree k in $n+1$ variables. Thus, from Equation 5.17,

$$\dim \tilde{\mathcal{H}}_{k,k} = \binom{n+k}{k}^2 - \binom{n+k-1}{k-1}^2. \quad (5.19)$$

Therefore, we have found the spectrum of the Laplacian on $\mathbb{CP}(n)$ whose eigenfunctions are harmonic, bihomogeneous polynomials of degree k in $z, \bar{z} \in \mathbb{C}^{n+1}$, restricted to S^{2n+1} . The eigenvalues are from Equation 5.6,

$$\lambda_k = 2k(2k + (2n+1) - 1) = 4k(k+n), \quad (5.20)$$

with multiplicity, m_k equal to the dimension of $\tilde{\mathcal{H}}_{k,k}$ which is simplified from Equation 5.19;

$$m_k = n(n+2k) \left(\frac{n(n+1) \dots (n+k-1)}{k!} \right)^2. \quad (5.21)$$

5.1.4 Completeness of the spectrum on $\mathbb{CP}(n)$

To prove that we have constructed a complete set of eigenfunctions on $\mathbb{CP}(n)$ we use the Stone-Weierstrass Theorem which states that if the calculated functions on S^{2n+1} separate points on

$\mathbb{C}P(n)$ then the set of eigenfunctions is complete. Separation of points on $\mathbb{C}P(n)$ is equivalent to separation of points on S^{2n+1} up to unit complex multiplication (or $U(1)$) invariance.

Suppose z and z' are two non-identical points on S^{2n+1} . Separation of points means that if $z \neq z' \cdot u$ for some $u \in U(1)$ then there must exist some function, $f \in \mathcal{H}_{k,k}$ for some k , such that $f(z) \neq f(z')$.

Let us define the points as follows;

$$z = (z_0, z_1, \dots, z_n)$$

$$z' = (z'_0, z'_1, \dots, z'_n)$$

where $z_k = \rho_k e^{i\theta_k}$ and $z'_k = \rho'_k e^{i\theta'_k}$.

One of the following three cases will hold:

1) There exists some $i \in \{0 \dots n\}$ such that $\rho_i \neq \rho'_i$.

2) $\rho_i = \rho'_i$ for all $i \in \{0 \dots n\}$ and,

$$\theta'_i - \theta_i = \theta \tag{5.22}$$

is true for all $i \in \{0 \dots n\}$ and for some constant θ .

3) $\rho_i = \rho'_i$ for all $i \in \{0 \dots n\}$ and Equation 5.22 is not true for all $i \in \{0 \dots n\}$. Then there exists some $j, k \in \{0 \dots n\}$ such that $\theta_j - \theta_k \neq \theta'_j - \theta'_k$.

If case (1) is true, then the function,

$$f = z_i \bar{z}_i \in \mathcal{H}_{1,1}$$

will separate the points, z and z' , even if $\theta_i = \theta'_i \ \forall i$ since in that case, $z_i \bar{z}_i = \sum_{j=1}^n |\rho_j|^2$ and there is some i such that $\rho_i \neq \rho'_i$ so $f(q_1) \neq f(q_2)$.

If case (2) is true, then $z' \cdot e^{i\theta} = z$ and the two points differ only by a unit complex and are therefore the same point on $\mathbb{C}P(n)$.

If case (3) is true, then $f = z_i \bar{z}_j$ separates the points since,

$$f(q_1) = \rho_i e^{i\theta_i} \rho_j e^{-i\theta_j} = \rho_i \rho_j e^{i(\theta_i - \theta_j)}$$

$$f(q_2) = \rho'_i e^{i\theta'_i} \rho'_j e^{-i\theta'_j} = \rho_i \rho_j e^{i(\theta'_i - \theta'_j)}$$

and thus $f(z) \neq f(z')$.

5.1.5 Comparison of the spectrum on $\mathbb{CP}(1)$ with that on S^2

For $n = 1$, $\mathbb{CP}(1)$ is the sphere, S^2 , therefore the previous calculation of the spectrum with $n = 1$ must agree with the known spectrum of the Laplacian on S^2 . The spectrum of the Laplacian on S^n with radius 1 has been calculated in Sec. 4.1.2 to be:

$$\lambda_k = k(k + n - 1), \quad (5.23)$$

with multiplicity,

$$m_k = \frac{(n + k - 2)(n + k - 3) \cdots (n + 1)n}{k!} (n + 2k - 1). \quad (5.24)$$

However, since $\mathbb{CP}(1)$ and S^2 do not have the same radius the following calculations determine the relative radius of $\mathbb{CP}(1)$.

We define the complex projective plane, $\mathbb{CP}(n)$, in terms of the bundle,

$$\begin{array}{ccc} U(1) & \hookrightarrow & S^{2n+1} \\ & & \downarrow q \\ & & \mathbb{CP}(n) \end{array}$$

where the projection, q , takes great circles in S^{2n+1} to the plane (or complex line) in $\mathbb{CP}(n)$ in which they lie.

If $\vec{q} \in S^{2n+1}$ such that $p(\vec{q}) = m \in \mathbb{CP}(n)$ then decompose the tangent plane, $T_q(S^{2n+1})$ into two orthogonal subspaces; the first subtended by $i \cdot \vec{q}$ which p projects entirely to zero in $T_m(\mathbb{CP}(n))$, and the second orthogonal to the first subspace. p will thus project the second

subspace isometrically onto $T_m(\mathbb{CP}(n))$. We now have an almost complex structure on $\mathbb{CP}(n)$ created by multiplying by i in the second subspace.

Definition: An almost hermitian manifold with a complex structure, J , which is invariant under parallel translation is known as a *Kähler manifold*.

It is possible to show [1, F.34] that a Kähler manifold with constant holomorphic curvature has sectional curvature described by,

$$R(\vec{x}, \cdot)\vec{x} = \begin{cases} 0 & \text{for } \mathbb{R} \cdot \vec{x}, \\ 4k \times Id & \text{for } \mathbb{R} \cdot J\vec{x}, \\ k \times Id & \text{for vectors } \perp \text{ to } \vec{x} \text{ and } J\vec{x}. \end{cases} \quad (5.25)$$

Clearly, the almost complex structure previously constructed on $\mathbb{CP}(n)$ respects parallel displacement and thus $\mathbb{CP}(n)$ with this structure is a Kähler manifold. The group of unitary transformations on \mathbb{C}^{n+1} , $U(n+1)$, is transitive and isometric on $\mathbb{CP}(n)$. That is, for any two points, $m, n \in \mathbb{CP}(n)$ with associated 2-planes, T_m and T_n , there exists an element, $u \in U(n+1)$ which takes $(m, T_m) \mapsto (n, T_n)$ isometrically. It follows that $\mathbb{CP}(n)$ has constant holomorphic sectional curvature, since sectional curvature on a 2-plane is invariant under isometric unitary transformations. Therefore, we may suppose that this constant holomorphic curvature of $\mathbb{CP}(n)$ is equal to $4k$ for some k .

Definition: A continuous vector-valued function, Y , along a geodesic, $c : [a, b] \rightarrow M$ (where $a, b \in \mathbb{R}$ and M is the manifold in question) is a *Jacobi Section* if

$$(D_{\dot{c}})^2 Y + R(\dot{c}, Y)\dot{c} = 0, \quad (5.26)$$

where, once again, R is the sectional curvature.

Let $\{e_1(s) \dots e_n(s)\}$ be a set of vector-valued functions ($s \in [a, b]$) parallel along c which form a basis for each $T_{c(s)}M$. If we now express Y as a linear combination of functions:

$$Y(s) = Y_i(s)e_i(s),$$

then Equation 5.26 becomes

$$\frac{d^2 Y_i}{ds^2} + a_j^i Y_j = 0, \quad (5.27)$$

where a_j^i is the sectional curvature of $e_j(s)$ with respect to $e_i(s)$:

$$R(\dot{c}(s), e_j(s))\dot{c}(s) = a_j^i e_i(s).$$

Now, let \vec{x} be a tangent vector to $\mathbb{CP}(n)$ at the point m , and let $\gamma(t)$ be the associated geodesic along \vec{x} . Define a Jacobi section, Y , along γ , such that,

$$Y(0) = 0 \text{ and } Y'(0) = \vec{y}$$

where \vec{y} is orthogonal to \vec{x} . We can decompose \vec{y} into y_1 and y_2 , where y_1 is the projection of \vec{y} onto $J \cdot \vec{x}$ and y_2 is orthogonal to $J \cdot \vec{x}$ (and to \vec{x}).

Since Y must satisfy Equation 5.27 where the sectional curvature is already known from Equation 5.25 we may express Y as,

$$Y_1(t) = y_1 \sin(t(2\sqrt{k})) \quad (5.28)$$

$$Y_2(t) = y_2 \sin(t\sqrt{k}) \quad (5.29)$$

$Y_1(t)$ has one half the period of $Y_2(t)$, and since they are orthogonal to each other, they meet at zero for the first time when $t = \pi/\sqrt{k}$.

However, it has been shown [1, C.IV.11] that any two geodesics, c_x and c'_x , along two tangent vectors to $\mathbb{CP}(n)$, x and x' , meet for the value π if x and x' do not lie in the same orthogonal complex line. Thus, from Equation 5.29, Y_1 and Y_2 should meet at $t = \pi$ and k must equal 1. Therefore, the holomorphic curvature of $\mathbb{CP}(n)$ is 4.

Since the square of the radius of a sphere is proportional to its holomorphic curvature, and the S^2 mentioned previously has radius 1, we may consider $\mathbb{CP}(1)$ to be an S^2 with radius 2. We must, therefore, divide its spectrum calculated in Sec. 4.1.3 by the square of its radius, 4.

From Eqns 5.20 and 5.21 the spectrum of the Laplacian on $\mathbb{CP}(1)$ is,

$$\lambda_k(\mathbb{CP}(1)) = 4k(k+1), \quad (5.30)$$

$$m_k(\mathbb{CP}(1)) = (2k+1).$$

Dividing these eigenvalues by 4 we get,

$$\lambda'_k = k(k+1), \quad (5.31)$$

$$m'_k = (2k+1).$$

From Eqns 5.23 and 5.24 the spectrum of the Laplacian on S^2 is,

$$\lambda_k(S^2) = k(k+1) \quad (5.32)$$

$$m_k(S^2) = (2k+1)$$

which is identical to the eigenvalues and multiplicities calculated in Equation 5.31 which are those of $\mathbb{CP}(1)$, adjusted for the radius difference.

5.1.6 The Pullback of a connection over $\mathbb{CP}(n)$

Consider the pullback square from Sec. 4.1.1 where $n = 1$:

$$\begin{array}{ccccc} & \mathbb{C}^2 & & \mathbb{C}^2 & \\ & \downarrow & & \downarrow & \\ \eta^* : & \tilde{E} & \xrightarrow{\tilde{q}} & E & : \eta \\ & \downarrow \tilde{p} & & \downarrow p & \\ U(1) & \hookrightarrow S^3 & \xrightarrow{q} & \mathbb{CP}(1) & \end{array}$$

The canonical line bundle over $\mathbb{CP}(1)$, η , is pulled back over its principal bundle to get the bundle, η^* , which was shown to be equivalent to a trivial bundle in Sec. 4.1.1.

$\mathbb{CP}(1)$ is the set of all complex lines (or planes) through the origin in \mathbb{C}^2 (or \mathbb{R}^4). $E = \{(l, z) \in \mathbb{CP}(1) \times \mathbb{C}^2 | z \in l\}$. The projection, $p : (l, z) \mapsto l$. The projection, q takes $x \in S^3$ to the plane

through the origin which is defined by the great circle on which x lies. Clearly, different points which lie on the same great circle of S^3 will be projected by q to the same complex line in $\mathbb{CP}(1)$, thus the fibre of this bundle is $U(1)$, representing multiplication by unit complex numbers, $e^{i\theta}$, around the given great circle.

$$\tilde{E} = \{(x, (l, z)) \in S^3 \times E \mid p \circ \tilde{q} = q \circ \tilde{p}\} \text{ or, } \tilde{E} = \{(x, q(x), z) \in S^3 \times \mathbb{CP}(1) \times \mathbb{C}^2 \mid z \in q(x)\}.$$

The projection map, $\tilde{p} : (x, q(x), z) \mapsto x$ and the projection map, $\tilde{q} : (x, q(x), z) \mapsto (q(x), z)$.

Therefore, sections of η^* behave as,

$$\hat{\sigma} : x \mapsto (x, q(x), z)|_{z \in q(x)} \text{ for all } x \in S^3. \quad (5.33)$$

Thus, sections on η^* are equivalent to functions from S^3 to \mathbb{C} where \mathbb{C} is the complex line, $q(x)$.

We wish to find sections, σ , on η which are eigenfunctions of the Laplacian. However, since η^* is equivalent to a trivial bundle, it is far easier to find sections, $\hat{\sigma}$, on η^* which push down to appropriate sections on η .

We have found in Sec. 4.1.3 $U(1)$ invariant functions mapping $S^3 \rightarrow \mathbb{C}$ which are eigenfunctions of the Laplacian. Since the map, q , is invariant under unit complex multiplication, these $U(1)$ invariant functions push down to form the eigenspace of the Laplacian on $\mathbb{CP}(1)$. However, a function which maps $S^3 \rightarrow \mathbb{C}$ is not equivalent to its corresponding section. For any trivial bundle there exists an orthonormal frame of sections, (ϕ_1, \dots, ϕ_m) . In this case, $m = 2$, and the functions are of the form, $f : S^3 \rightarrow \mathbb{C} \simeq \mathbb{R}^2$. Each function can be expressed as $f = (f_1, f_2)$ where $f_i : S^3 \rightarrow \mathbb{R}$ and $f_i : x \mapsto \langle \phi_i(x), \sigma(x) \rangle$. Thus a section on η^* corresponding to the function, f , may be expressed as

$$\sigma = \sum_{i=1}^2 f_i \cdot \phi_i.$$

For this reason we must determine how a normalized basis of sections on η^* transforms under $U(1)$ multiplication. Clearly, this frame cannot be invariant under $U(1)$ multiplication, otherwise the frame would push down to a continuous frame of sections on η , implying that η be a trivial bundle, which it is not. Once it is understood how the sections on η^* transform, it will

be apparent how to construct non-invariant functions on S^3 which cancel the non-invariance of the frame of sections and thus push down to eigensections of the Laplacian on η .

Lemma 2: For an arbitrary normalized real section, $\hat{\sigma}_R$ on η^* the following equation is true:

$$\hat{\sigma}_R(ux) = u\hat{\sigma}_R(x) \text{ for all } x \in S^3, u \in U(1). \quad (5.34)$$

Proof: We modify the definition of a section on η^* from Equation 5.33 to the following definition of a normalized real section;

$$\hat{\sigma}_R(x) = (x, q(x), ax) \text{ where } a \in \mathbb{R}, |a| = 1.$$

Beginning with the left hand side of Equation 5.34,

$$\hat{\sigma}_R(ux) = (ux, q(ux), a(ux)).$$

Let $u = e^{i\theta}$ for some $0 \leq \theta < 2\pi$. Multiplication by $e^{i\theta}$ will move the point x to a different point of S^3 on the same great circle. $q(ux) = q(x)$ by its fundamental $U(1)$ invariance. $a(ux) = e^{i\theta}x$, and thus,

$$\hat{\sigma}_R(ux) = (ux, q(x), u \cdot ax)$$

Now, assuming we define multiplication by unit complex numbers in \tilde{E} as multiplication in the great circle, we may quickly evaluate the right hand side of Equation 5.34,

$$u\hat{\sigma}_R(x) = u(x, q(x), a\vec{x}) = (ux, uq(x), ua\vec{x}) = (ux, q(x), u \cdot a\vec{x}),$$

since multiplication by $e^{i\theta}$ in the great circle which defines the plane, $q(x)$, will not change the plane ■

Thus, Equation 5.34 is correct and real sections of η^* will transform by one full rotation for every full $U(1)$ rotation on S^3 . As a result, we must construct functions which rotate once in the opposite direction for every rotation on S^3 , i.e.:

$$f(e^{i\theta}x) = e^{-i\theta}f(x) \text{ for all } x \in S^3, 0 \leq \theta < 2\pi. \quad (5.35)$$

5.1.7 The Spectrum of the Laplacian on the canonical bundle

As determined in Sec 6.1.6, the spectrum of the Laplacian on the canonical line bundle, η , will consist of those sections on $\hat{\eta}$ which are not pullback sections, but instead satisfy the following,

$$\sigma(uz) = u^{-1}\sigma(z) \text{ for all } u \in U(1).$$

That is, the corresponding functions on S^{2n+1} will be non-invariant under unit complex multiplication and will instead satisfy Equation 5.35. The set of functions satisfying Equation 5.35 will consist of an *invariant* harmonic bihomogenous function as defined in Sec 6.1.3, multiplied by a single factor of \bar{z}_i . This set of functions is simply the set of all bihomogenous harmonic functions with one more factor of \bar{z} than z , $\{\oplus_k \mathcal{H}_{k,k+1}\}$.

From Theorem 1, the eigenvalues of these functions will be once again, $\hat{k}(\hat{k} + \hat{n} - 1)$ where in this case, \hat{k} is odd and \hat{n} is the dimension of S^{2n+1} ,

$$\hat{k} = 2k + 1,$$

$$\hat{n} = 2n + 1.$$

The possible eigenvalues of the Laplacian on η are therefore,

$$E_k = (2k + 1)(2k + 2n + 1), \quad k = 0, 1, 2, \dots \quad (5.36)$$

The solution to this problem relates to the physical problem of monopole harmonics on the S^2 sphere. Wu and Yang [28] calculated the eigenvalues of these harmonics to be,

$$E_l = l(l + 1), \quad l = 0, 1, 2, \dots \quad (5.37)$$

In comparison, we may substitute $n = 1$ into Equation 5.36 (since $\mathbb{CP}(1)$ is homomorphic to S^2) and divide by the square of the relative radius of $\mathbb{CP}(1)$ which is 2 (determined in Sec. 4.1.5).

These energy levels become:

$$E'_k = \frac{1}{4}(2k + 1)(2k + 3) = \left(\frac{2k + 1}{2}\right) \left(\left(\frac{2k + 1}{2}\right) + 1\right), \quad k = 0, 1, 2, \dots \quad (5.38)$$

which match the monopole harmonic eigenvalues in Equation 5.37 exactly.

In order to determine the multiplicity of non-invariant harmonic functions on $\mathbb{CP}(1)$, we return to the number of invariant $2k$ dimensional polynomials in $n + 1$ variables,

$$\dim \mathcal{P}_{k,k} = \binom{n+k}{k}^2.$$

These polynomials are multiplied by one complex factor of \bar{z}_0 or \bar{z}_1 and the dimension is thus multiplied by 2. If we denote the set of non-invariant $2k + 1$ dimensional functions as $\mathcal{P}_{k,k+1}$ then,

$$\dim \mathcal{P}_{k,k+1} = 2 \binom{n+k}{k}^2$$

and thus,

$$\dim \mathcal{H}_{k,k+1} = 2 \binom{n+k}{k}^2 - 2 \binom{n+k-1}{k-1}^2. \quad (5.39)$$

For $\mathbb{CP}(1)$ we substitute $n = 1$ into Equation 5.39 and find the multiplicity of the spectrum of the Laplacian on η ,

$$m_k^\eta(1) = 2m_k(1) = 2(2k + 1).$$

5.1.8 Completeness of the spectrum over the canonical bundle

In the same manner as Sec. 4.1.4, we seek to prove that the spectrum determined for the Laplacian on the canonical complex line bundle over $\mathbb{CP}(n)$ is complete. The Stone-Weierstrass theorem states that the spectrum is complete if and only if the eigenfunctions separate points on $\mathbb{CP}(n)$. The set of eigenvectors in question is, $\{\tilde{\mathcal{H}}_{k,k+1}\}$.

Suppose that $z, z' \in S^{2n+1} \subset \mathbb{C}^{n+1}$, where

$$\begin{aligned} z &= (z_0, \dots, z_n) = (\rho_0 e^{i\theta_0} \dots \rho_n e^{i\theta_n}) \\ z' &= (z'_0, \dots, z'_n) = (\rho'_0 e^{i\theta'_0} \dots \rho'_n e^{i\theta'_n}). \end{aligned}$$

Then one of the following cases must be true:

1) There exists some $i \in \{0 \dots n\}$ such that $\rho_i \neq \rho'_i$. Then the function, $f = z_i \bar{z}_i \bar{z}_i$ separates the points, z and z' .

2) $\rho_i = \rho'_i$ for all $i \in \{0 \dots n\}$ and there exists some $j \in \{0 \dots n\}$ such that $\theta_j - \theta_0 \neq \theta'_j - \theta'_0$. Then the function, $f = (z_j \bar{z}_0) \bar{z}_j$ separates the points, z and z' .

3) $\rho_i = \rho'_i$ and $\theta_i - \theta_0 = \theta'_i - \theta'_0$ for all $i \in \{0 \dots n\}$, in which case there exists an α , with $0 \leq \alpha < 2\pi$, such that $z' = ze^{i\alpha}$, thus the projection, q , projects z and z' to the same point in $\mathbb{CP}(n)$ and need not be separated.

The details of the calculations of $f(z)$ and $f(z')$ for the above three cases is left out as they are essentially identical to those carried out in Sec. 4.1.4.

5.2 The quaternion Projective Space

5.2.1 The Spectrum of the Laplacian on $\mathbb{HP}(n)$

As in the Complex case we construct invariant functions on S^{4n+3} which are harmonic, and thus determine the spectrum of the Laplacian on $\mathbb{HP}(n)$.

Homogeneous polynomials in \mathbb{R}^{4n+4} are in real variables, $(x_0, x_1, \dots, x_{4n+3})$. We equate groups of four real variables with quaternion variables as follows;

$$q_0 = x_0 + ix_1 + jx_2 + kx_3$$

$$q_1 = x_4 + ix_5 + jx_6 + kx_7$$

.

.

.

$$q_n = x_{4n} + ix_{4n+1} + jx_{4n+2} + kx_{4n+3}$$

Now we seek homogeneous quaternion polynomials in $(q_0, q_1, \dots, q_n) \in \mathbb{HP}^{n+1}$ which are invariant under unit quaternion multiplication.

For any pair of quaternion variables, q_m and q_l , there are six invariant terms with which to construct invariant polynomials:

$$q_m \bar{q}_m, \quad q_l \bar{q}_l, \quad q_m \bar{q}_l, \quad q_l \bar{q}_m, \quad \hat{q}_m \bar{\hat{q}}_l, \quad \tilde{q}_m \bar{\tilde{q}}_l.$$

We are using the notation, \hat{q} and \tilde{q} in order to create a fully one to one correspondence between $(x_0 \dots x_{4n+3})$ and $(q_0 \dots q_n)$. To define these terms, let $q = x + iy + jz + kw$. Then,

$$\bar{q} = x - iy - jz - kw,$$

$$\hat{q} = x - iy + jz + kw,$$

$$\tilde{q} = x + iy - jz + kw,$$

and thus,

$$\bar{\tilde{q}} = x + iy + jz - kw.$$

The terms, $\hat{q}_l \bar{\hat{q}}_m$ and $\tilde{q}_l \bar{\tilde{q}}_m$ are not included in the list of invariant terms since they are not independent of the six invariant terms;

$$\begin{aligned} \hat{q}_l \bar{\hat{q}}_m &= \overline{\tilde{q}_m \bar{\tilde{q}}_l}, \\ \tilde{q}_l \bar{\tilde{q}}_m &= \overline{\hat{q}_m \bar{\hat{q}}_l}. \end{aligned}$$

Thus the number of possible invariant pairs of $(q_0 \dots q_n)$ is $6 \binom{n+1}{2}$. Since the number of polynomials of degree k in M variables is $\binom{M-1+k}{k}$.

It is also important to note that all terms including,

$$q_i \bar{q}_j q_j \bar{q}_i = q_i \bar{q}_i \bar{q}_j q_j = q_i \bar{q}_i q_j \bar{q}_j$$

are redundant since $q_i \bar{q}_i = \bar{q}_i q_i = |q_i|^2$ which is a real number, and thus $q_i \bar{q}_i q_j \bar{q}_j$ is also a real number.

The dimension of all degree $2k$ polynomials in $(q_0 \dots q_n)$ which are invariant under unit quaternion multiplication, (denoted N_k), is the number of degree k polynomials in the allowed pairs

of q_i 's minus the number of redundant degree $k - 2$ polynomials in the same pairs:

$$N_k = \binom{6\binom{n+1}{2} - 1 + k}{k} - \binom{6\binom{n+1}{2} - 3 + k}{k-2} \quad (5.40)$$

which simplifies to,

$$N_k = \frac{(a + 2k - 1) \cdot (a + k - 2)(a + k - 3) \cdots (k + 1)}{(a - 1)!}$$

where $a = 3n(n+1) - 1$. The number of harmonic homogeneous invariant quaternion polynomials in \mathbb{H}^{n+1} is therefore, $\dim \mathcal{H}_{k,k}^Q = N_k - N_{k-1}$.

From Theorem 1, the spectrum of the Laplacian on $\mathbb{HP}(n)$ is $k'(n' + k' - 1)$ where k' is even and $n' = 4n + 3$. So the eigenvalues and multiplicities are;

$$\begin{aligned} E_k &= 4k(k + 2n + 1) \quad k = 1, 2, 3 \dots \\ m_k &= N_k - N_{k-1} = \frac{(a + k - 3)(a + k - 4) \cdots (k + 1)}{(a - 1)!} [a^2 - 3a + 2ak - 2k + 2] \end{aligned} \quad (5.41)$$

where $a = 3n(n + 1) - 1$.

5.2.2 Completeness of the spectrum on $\mathbb{HP}(n)$

The Stone-Weierstrass argument proving that $\{\oplus_k \tilde{\mathcal{H}}_{k,k}^Q\}$ is the complete spectrum of the Laplacian on $\mathbb{HP}(n)$ runs along similar lines as that of the Laplacian on $\mathbb{CP}(n)$.

Since the sets of (quaternion) functions restricted to the sphere are equal; $\oplus_k \tilde{\mathcal{P}}_{k,k}^Q = \oplus_k \tilde{\mathcal{H}}_{k,k}^Q$ we wish to show that $\{\oplus_k \tilde{\mathcal{P}}_{k,k}^Q\}$ separates points on the base space, $\mathbb{HP}(n)$. This is equivalent to showing that for any two non-equivalent points in different fibres on S^{4n+3} , there exists a function in $\tilde{\mathcal{P}}_{k,k}^Q$ which separates these points.

Let $Q, Q' \in S^{4n+3}$ be two non-equal unit length variables in $n + 1$ quaternion dimensions, and let us denote,

$$Q = (q_0, q_1, \dots, q_n)$$

$$Q' = (q'_0, q'_1, \dots, q'_n)$$

where each quaternion variable, $q_i = \rho_i g_i$ or $q'_i = \rho'_i g'_i$. ρ_i is then the real norm of q_i , and $g_i \in SP(1)$ is a unit quaternion.

There are now three cases to consider;

- 1) There exists some i such that $\rho_i \neq \rho'_i$,
- 2) $\rho_i = \rho'_i$ for all i but there exists some i such that $g_i g_0^{-1} \neq g'_i (g'_0)^{-1}$ i.e., the relative angles between the variables of Q differ from those of Q'
- 3) $\rho_i = \rho'_i$ and $g_i g_0^{-1} = g'_i (g'_0)^{-1}$ for all i .

In case (1), the polynomial $f = q_i \bar{q}_i$ separates the points Q and Q' . Clearly $f \in \oplus_k \tilde{\mathcal{P}}_{k,k}^Q$ and since $\rho_i \neq \rho'_i$, $f(Q) = |\rho_i|^2$ which is not equal to $f(Q') = |\rho'_i|^2$.

In case (2), the polynomial, $h = q_0 \bar{q}_i$ separates Q and Q' . Again, $h \in \oplus_k \tilde{\mathcal{P}}_{k,k}^Q$ and

$$h(Q) = \rho_0 g_0 \overline{(\rho_i g_i)} = \rho_0 \rho_i g_0 \bar{g}_i$$

$$h(Q') = \rho'_0 g'_0 \overline{(\rho'_i g'_i)} = \rho'_0 \rho'_i g'_0 \bar{g}'_i.$$

$\rho_0 \rho_i = \rho'_0 \rho'_i$, and $g_0 \bar{g}_i \neq g'_0 \bar{g}'_i$ thus h separates Q and Q' .

In case (3), $\rho_i = \rho'_i$ for all i and there exists some $g \in SP(1)$ such that $g'_i = g_i g$ for all i . However, this is equivalent to the statement that Q and Q' differ only by the multiplication of a unit quaternion, $Q' = Qg$, and the two points are therefore in the same fibre. As previously stated, it is not necessary to separate points in the same fibre as they are projected to the same point in $\mathbb{HP}(n)$.

Therefore, the Stone-Weierstrass conditions are satisfied and the spectrum calculated in Sec. 4.2.1 is the complete spectrum of the Laplacian on $\mathbb{HP}(n)$ ■

5.2.3 Comparison of the spectrum on $\mathbb{HP}(1)$ with that of S^4

As the spectrum of the Laplacian on $\mathbb{CP}(1)$ was compared to that on S^2 in Sec. 4.1.5, we now compare the spectrum of the Laplacian on $\mathbb{HP}(1)$ calculated in Sec. 4.2.1 to that on S^4 .

From Equation 5.23 and Equation 5.24, the spectrum of the Laplacian on a unit radius S^4 is;

$$\begin{aligned}\lambda_k(S^4) &= k(k+3), \\ m_k(S^4) &= \frac{1}{6}(2k+3)(k+2)(k+1).\end{aligned}\tag{5.42}$$

The argument in Sec. 4.1.5 may be exactly duplicated in the case of $\mathbb{H}P(1)$, to prove that the holomorphic curvature of the quaternion Projective Space is 4, and its relative radius is therefore, 2. Substituting $n = 1$ into Equation 5.2.1, the spectrum of the Laplacian on $\mathbb{H}P(1)$ is,

$$\begin{aligned}\lambda_k(\mathbb{H}P(1)) &= 4k(k+3), \\ m_k(\mathbb{H}P(1)) &= \frac{1}{6}(k+2)(k+1)(2k+3).\end{aligned}\tag{5.43}$$

Dividing these eigenvalues by 4 we get,

$$\begin{aligned}\lambda'_k(\mathbb{H}P(1)) &= k(k+3), \\ m'_k(\mathbb{H}P(1)) &= \frac{1}{6}(2k+3)(k+2)(k+1).\end{aligned}\tag{5.44}$$

which match the eigenvalues and multiplicities of the spectrum of the Laplacian on S^4 .

5.2.4 The Pullback of a connection over $\mathbb{H}P(n)$

Consider the canonical line bundle over $\mathbb{H}P(1)$ pulled back over its principal bundle:

$$\begin{array}{ccccc}\mathbb{H}^2 & & \mathbb{H}^2 & & \\ \downarrow & & \downarrow & & \\ \tilde{E} & \xrightarrow{\tilde{q}} & E & & \\ \downarrow \tilde{p} & & \downarrow p & & \\ SP(1) & \hookrightarrow S^7 & \xrightarrow{q} & \mathbb{H}P(1) & \end{array} \quad \begin{array}{l} \xi^* : \\ \\ \\ \end{array} \quad \begin{array}{l} : \xi \\ \\ \\ \end{array}$$

$\mathbb{H}P(1)$ is equal to the set of all quaternion lines through the origin in \mathbb{H}^2 (or \mathbb{R}^4). $E = \{(P, Q) \in \mathbb{H}P(1) \times \mathbb{H}^2 \mid Q \in P\}$. The projection, $p : (P, Q) \mapsto P$ and q takes a point $x \in S^7$ to

the quaternion plane containing the “great circle” (S^3) on which x lies. $\tilde{E} = \{(x, q(x), Q) \in S^7 \times \mathbb{HP}(1) \times \mathbb{H}^2 | Q \in q(x)\}$, $\tilde{p} : (x, q(x), Q) \mapsto x$, and $\tilde{q} : (x, q(x), Q) \mapsto (q(x), Q) \in E$.

As in Sec. 4.1.6 we wish to determine how a frame of orthonormal sections on ξ^* will transform under $SP(1)$ (unit quaternion) multiplication. Let us construct a frame of orthonormal sections, $\{\hat{\phi}_1, \hat{\phi}_2, \hat{\phi}_3, \hat{\phi}_4\}$ such that any section, $\hat{\sigma} = \sum_{i=1}^4 f_i \hat{\phi}_i$ where $f_i : S^7 \rightarrow \mathbb{R}$. Then let;

$$\hat{\phi}_1 : x \mapsto (x, q(x), \vec{x}),$$

$$\hat{\phi}_2 : x \mapsto (x, q(x), i\vec{x}),$$

$$\hat{\phi}_3 : x \mapsto (x, q(x), j\vec{x}),$$

$$\hat{\phi}_4 : x \mapsto (x, q(x), k\vec{x}),$$

Clearly all vectors lie in the same plane, $\vec{x}, i\vec{x}, j\vec{x}, k\vec{x} \in q(x)$ and they form an orthonormal frame of the quaternion plane, $q(x)$.

If $g \in SP(1)$, we wish to show that,

$$g\hat{\sigma}(x) = \hat{\sigma}(gx) \tag{5.45}$$

$g\hat{\phi}_1(x) = g(x, q(x), \vec{x}) = (gx, q(x), g\vec{x})$ and $\hat{\phi}_1(gx) = (gx, q(gx), g\vec{x}) = (gx, q(x), g\vec{x})$ thus Equation 5.45 holds for $\hat{\phi}_1$ and is similarly true for $\hat{\phi}_2, \hat{\phi}_3$ and $\hat{\phi}_4$.

Therefore, the sections on ξ^* undergo a rotation equal to the $SP(1)$ rotation by which they are multiplied, and thus we will construct functions on S^7 which undergo an equal but opposite rotation for every $SP(1)$ multiplication.

5.2.5 The Spectrum of the Laplacian on the canonical bundle

As in the complex case, the desired non-invariant functions on S^{4n+3} which make up the spectrum of the Laplacian on ξ over $\mathbb{HP}(n)$ are the invariant functions multiplied on the right by a quaternion factor.

Let us denote such harmonic functions as $\tilde{\mathcal{H}}_{k+1,k}^Q$. From Theorem 1, the eigenvalues of these

functions will be, $\hat{k}(\hat{k} + \hat{n} - 1)$ where $\hat{k} = 2k + 1$ and $\hat{n} = 4n + 3$. Thus,

$$\lambda_k = (2k + 1)(2k + 4n + 3). \quad (5.46)$$

To construct the non-invariant functions on S^{4n+3} , we take the invariant functions in $n + 1$ quaternion dimensions and multiply them on the right by a quaternion factor. For simplicity's sake, we carry out the calculation of multiplicities over $\mathbb{HP}(1)$.

When $n = 1$, the functions are in two quaternion dimensions, q_0, q_1 . From Equation 5.40 the number of invariant $2k$ quaternion dimensional polynomials is,

$$N_k = \binom{k+5}{k} - \binom{k+3}{k-2}.$$

Each of these functions ends with one of the six invariant factors listed in Sec. 4.2.1. However, when multiplying on the right by either q_0 or q_1 the following redundancies occur:

$$q_2 \bar{q}_2 \cdot q_1 = q_1 \bar{q}_2 \cdot q_2$$

$$q_2 \bar{q}_1 \cdot q_1 = q_1 \bar{q}_1 \cdot q_2.$$

Therefore, the number of non-invariant $2k + 1$ quaternion dimensional polynomials is;

$$N_{k+1,k} = 2N_k - 2N_{k-1},$$

and the number of non-invariant harmonic $2k + 1$ quaternion dimensional polynomials is therefore,

$$\dim \tilde{\mathcal{H}}_{k+1,k}^Q = N_{k+1,k} - N_{k,k-1} = 2(N_k - 2N_{k-1} + N_{k-2}) \quad (5.47)$$

Therefore, the eigenvalues and multiplicities of the Laplacian on the canonical fibre bundle over $\mathbb{HP}(1)$ are;

$$\lambda_k = (2k + 1)(2k + 7), \quad (5.48)$$

$$m_k = 2(N_k - 2N_{k-1} + N_{k-2}),$$

where $N_k = \binom{k+5}{k} - \binom{k+3}{k-2}$. It remains to be proven that these functions form the complete spectrum. This proof is carried out in Sec. 4.2.6.

5.2.6 Completeness of the spectrum over the canonical bundle

As in Sec. 4.1.8, the Stone-Weierstrass theorem is applied to the set of eigenvectors of the Laplacian on the line bundle determined in Sec. 4.2.5. This set is, $\{\tilde{\mathcal{H}}_{k,k+1}^Q\}$.

Let $Q, Q' \in S^{4n+3} \subset \mathbb{H}^{n+1}$ where,

$$Q = (q_0 \dots q_n) = (\rho_0 g_0 \dots \rho_n g_n)$$

$$Q' = (q'_0 \dots q'_n) = (\rho'_0 g'_0 \dots \rho'_n g'_n)$$

where $g_i, g'_i \in SP(1)$.

One of the following three cases will then apply;

- 1) There exists some $i \in \{0 \dots n\}$ such that $\rho_i \neq \rho'_i$. Then $f = q_i \bar{q}_i \bar{q}_i$ separates Q and Q' .
- 2) $\rho_i = \rho'_i \ \forall i \in \{0 \dots n\}$ and there exists some $j \in \{0 \dots n\}$ such that $g_j g_0^{-1} = g'_j g'_0{}^{-1}$. Then $f = q_j \bar{q}_0 \bar{q}_i$ separates Q and Q' .
- 3) $\rho_i = \rho'_i$ and $g_i g_0^{-1} = g'_i g'_0{}^{-1} \forall i \in \{0 \dots n\}$, in which case there exists some $g \in SP(1)$ such that $Q' = Qg$ and thus Q and Q' project to the same point on $\mathbb{HP}(n)$ and need not be separated.

Once again, the above calculations are not carried out in detail, as they are almost identical to those in Sec. 4.2.5.

Chapter 6

Fitting of Theory to Existing Data

In 1978, Bernstein and Webb [2] measured the $\Gamma_8 \otimes (e_g \oplus t_{2g})$ spectrum of the octahedral molecule, IrF_6 . This experiment involved measuring the low temperature, high energy absorption spectrum of IrF_6 crystals slightly doped with another transition metal hexafluoride. In analysis of their data, Bernstein and Webb attempted to identify Jahn-Teller active frequencies, ν_2 and ν_5 corresponding to $\Gamma_8 \otimes e_g$ and $\Gamma_8 \otimes t_{2g}$ respectively. They further pointed out that this method ignores the known coupling between the two modes in the $\Gamma_8 \otimes (e_g + t_{2g})$ problem which is what this work has attempted to calculate.

Bernstein and Webb were able to confidently identify values for ν_5 as well as values for non-Jahn-Teller active vibrations, ν_1, ν_3, ν_4 and ν_6 which couple with the Jahn-Teller active vibrations, however, no reasonable fit was made for the ν_2 frequency. These frequencies determined were identified as,

Constant	Value
ν_1	682cm^{-1}
ν_3	287cm^{-1}
ν_4	217cm^{-1}
ν_6	696cm^{-1}

Table 6.1: Non-Jahn-Teller active frequencies

The data collected by Bernstein and Webb shows crystal field splitting in many places which corresponds to a spacing of about $\pm 17\text{cm}^{-1}$ for most major lines.

The eigenvalues calculated in Sec. 6.2.5,

$$\lambda_k = (2k + 1)(2k + 7),$$

are theorized to be energy levels of IrF_6 with a scale factor and a zero-point energy:

$$E_k = (2k + 1)(2k + 7) \cdot A + B \quad (6.1)$$

If we equate the value for ν_5 determined by Bernstein and Webb with E_1 , then subsequent energy levels (displayed in Table 6.2) fit well with the existing data, where $\{E_i\}$ are the Jahn-Teller pseudorotational energies on which the frequencies, ν_1, ν_3, ν_4 and ν_6 will be built.

Due to the crystal field splitting we have taken the middle of the first three lines identified as ν_5 and thus designated, $E_1 = 223 \text{ cm}^{-1}$. Substituting this value of E_1 into Equation 6.1 and taking Bernstein and Webb's chosen origin line at zero energy, the scale factors are $A = 11.2 \text{ cm}^{-1}$ and $B = -78.05 \text{ cm}^{-1}$, and the first five Jahn-Teller energy levels are,

Jahn-Teller Energy	Calculated Frequency
E_0	0 cm^{-1}
E_1	223 cm^{-1}
E_2	535 cm^{-1}
E_3	936 cm^{-1}
E_4	1427 cm^{-1}

Table 6.2: The First Five Calculated Jahn-Teller Frequencies

These energy levels from Table 6.2 are coupled with the non-Jahn-Teller active frequencies, ν_1, ν_3, ν_4 and ν_6 from Table 6.1 and the resulting frequencies less than 1100 cm^{-1} are calculated;

Calculated Coupled Energy Level	Frequency (cm^{-1})
E_1	223
E_2	535
E_3	936
$E_0 + \nu_1$	682
$E_0 + \nu_3$	696
$E_0 + \nu_4$	287
$E_0 + \nu_6$	217
$E_1 + \nu_1$	905
$E_1 + \nu_3$	919
$E_1 + \nu_4$	510
$E_1 + \nu_6$	440
$E_2 + \nu_4$	822
$E_2 + \nu_6$	752
$E_0 + 2\nu_4$	574
$E_0 + 2\nu_6$	434
$E_1 + 2\nu_4$	797
$E_1 + 2\nu_6$	657
$E_2 + 2\nu_6$	969

Table 6.3: Calculated frequencies less than 1100 cm^{-1}

Table 6.4 displays the major bands identified by Bernstein and Webb as strong in intensity or as Jahn-Teller active, along with the assignment given them by Bernstein and Webb as well as the assignment given them as a result of this work. Crystal field splitting is considered to be active throughout these energies. Fitting was not attempted for those frequencies greater than 1100 cm^{-1} since almost all measured lines above this frequency were of weak intensity as well as the fact that at greater energies the approximation of a perfectly round $\text{HP}(1)$ becomes less accurate.

Freq. Assignment of Bernstein & Webb	Frequency cm^{-1}	Assignment of Calculated Freq.
$\nu_5^1(\text{a})$	202.7]
$\nu_5^2(\text{a})$	208.9	
$\nu_6(\text{a})$ [215.8] E_1
]	218.2	
$\nu_5^3(\text{a})$	241.5	$E_0 + \nu_6$]
	254.4]
[271.8]
ν_4	284.7	$E_0 + \nu_4$
]	292.9]
[416.6]
$2\nu_5$	419.1] $E_0 + 2\nu_6$
	452.3	$E_1 + \nu_6$]
]	461.4]

Freq. Assignment of Bernstein & Webb	Frequency cm^{-1}	Assignment of Calculated Freq.
$\nu_5 + \nu_4(\text{a})$	487.8	\rfloor
$\nu_4 + \nu_6(\text{a})$	494.9	$E_1 + \nu_4 \rfloor$
	521.7	$\rfloor \quad \rfloor$
$\nu_5 + \nu_4(\text{b})$	528.1	$\rfloor \quad \nu_4 + \nu_6$
	532.9	$\rfloor \quad \rfloor$
$\nu_4 + \nu_6(\text{b})$	538.1	$E_2 \quad \rfloor$
	554.3	\rfloor
$2\nu_4(\text{a})$	561.5	$\rfloor E_0 + 2\nu_4$
$2\nu_4(\text{b})$	612.2	\rfloor
$\nu_2(\text{a})$	645.9	$\rfloor E_1 + 2\nu_6$
$\nu_2(\text{b})$	665.5	\rfloor
$\nu_1(\text{a})$	682.1	\rfloor
$\nu_3(\text{a})$	696.3	$\rfloor \quad E_0 + \nu_1$
	721.0	$E_0 + \nu_3 \rfloor$
	724.2	\rfloor

Freq. Assignment of Bernstein & Webb	Frequency cm^{-1}	Assignment of Calculated Freq.
$3\nu_4(\text{a})$ $3\nu_4(\text{b})$	734.9	\uparrow
	742.5	$E_2 + \nu_6$
	764.8	$\uparrow E_1 + 2\nu_4 \downarrow$
	804.1	\downarrow
	806.5	\uparrow
	831.7	$E_2 + \nu_4$
	845.5	\downarrow
\uparrow $\nu_1 + \nu_5(\text{a})$ \downarrow	884.0	\uparrow
	890.3	$E_1 + \nu_1$
	923.2	\downarrow
\uparrow $\nu_1 + \nu_5(\text{b})$ \downarrow	927.1	$\uparrow E_1 + \nu_3$
	933.2	$\downarrow \quad \downarrow$
	964.4	$\downarrow E_3$
	965.6	$\uparrow E_2 + 2\nu_6$
	991.9	\downarrow
phonons	1024	phonons

Table 6.4: Major Energy Bands measured by Bernstein and Webb with assignments

Bernstein and Webb theorized that the strong line at 1024 cm^{-1} was due to a charge transfer origin and belonged in the Γ_{6g} or Γ_{7g} spectrum. The previous calculations agree with this assessment. Furthermore, based on our calculations we were able to successfully identify the Jahn-Teller excitations in the spectrum based on an equal coupling case of $\Gamma_8 \otimes (e_g \oplus t_{2g})$.

Chapter 7

Conclusion

The Jahn-Teller active pseudorotational energy spectrum of an octahedral molecule was successfully calculated to a two parameter fit. This calculation depends on the use of the Born-Oppenheimer approximation, which states that the pseudorotational spectrum is equivalent to the spectrum of the Laplacian on a specified fibre bundle with the addition of a zero-point energy. The completion of this work marks an important step in theoretical molecular spectra, due to the success of the assumption of equal Jahn-Teller coupling between the e_g and t_{2g} modes in the $\Gamma_8 \otimes (e_g \oplus t_{2g})$ problem, whereas in the past, calculations and experimental assignments have focused on either the $\Gamma_8 \otimes e_g$ or the $\Gamma_8 \otimes t_{2g}$ modes.

Further, the geometry of the eigenspace of this Laplacian is entirely determined by the electronic Hamiltonian of the given molecule. The group theoretic symmetry properties of an octahedral molecule cause the electronic Hamiltonian to act on a round S^4 . Thus, the required calculation is that of the spectrum of the Laplacian on the canonical line bundle over S^4 . Because S^4 is isomorphic to $\mathbb{H}P(1)$ it was found to be more convenient to find the spectrum of the Laplacian on the line bundle over $\mathbb{H}P(1)$. Since the pullback of this bundle over its principal bundle is a trivial bundle, the final calculation was made on this trivial pullback bundle which then induced the desired spectrum on the line bundle over $\mathbb{H}P(1) \simeq S^4$.

The final calculation of this spectrum produced the following eigenvalues,

$$\lambda_k = (2k + 1)(2k + 7) \cdot A + B \quad k = 0, 1 \dots \quad (7.1)$$

where A is a real constant corresponding to the radius of the S^4 sphere and B is a real constant

corresponding to the zero-point potential energy of the molecule.

These eigenvalues were then fit to data taken using IrF_6 by Bernstein and Webb [2]. Given the inherently uncertain nature of experimentalist assignments of Jahn-Teller active or inactive modes to the measured data, the fit obtained was encouraging. The constants used in Equation 7.1 were $A = 11.2 \text{ cm}^{-1}$ and $B = -78.05 \text{ cm}^{-1}$.

While Bernstein and Webb hypothesized the existence of two Jahn-Teller active modes corresponding to $\Gamma_8 \otimes e$ and $\Gamma_8 \otimes t_{2g}$ representations, they were unable to assign a clear value to one of these modes, that of $\Gamma_8 \otimes e$. The Jahn-Teller theory proven in Chapter 2 implies that there exists only one vibrational mode for the coupled modes, $\Gamma_8 \otimes (e \oplus t_{2g})$.

In this work the experimentally assigned vibrational frequency for $\Gamma_8 \otimes t_{2g}$ was used as the second ($k = 1$) energy level and further energies as well as non-Jahn-Teller active modes were then calculated and fit to the data. These assignments using equal Jahn-Teller coupling between e_g and t_{2g} modes were in reasonable agreement with the data as well as with the assignments of Bernstein and Webb.

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Appendix A

Basic Group Theory

Definition: A *Group*, G , is a set of elements with a multiplication operation which obeys the following four axioms:

- 1) G is closed under the multiplication operation. That is, for all $g, h \in G$, $gh \in G$.
- 2) G contains a two-sided unit. That is, there exists some $E \in G$, such that $Eg = gE = g$ for all $g \in G$.
- 3) The multiplication operation is associative. That is, for all $g, h, k \in G$, $(gh)k = g(hk)$.
- 4) Every element of G has a two-sided inverse. That is, for all $g \in G$, there exists some $h \in G$ such that $gh = hg = E$.

For a finite group, the group's *order* is equal to the number of elements belonging to the group. The distinction between groups is determined solely on the basis of their *multiplication tables*.

Example: There is only one group of order 3, and its multiplication table is:

	e	b	c
e	e	b	c
b	b	c	e
c	c	e	b

Table A.1: A 3 Element Multiplication Table.

Appendix A. Basic Group Theory

which means that $bc = e$, $b^2 = c$ and so on.

Definition: If two elements of a group, $A, B \in G$ are related as, $A = X^{-1}BX$ for some $X \in G$ then they are said to be *conjugate* to each other. A complete set of all elements in a group which are conjugate to each other is called a *class*.

The elements of a group may be represented by matrices which multiply and commute in the same way that the group elements do. This set of matrices is not necessarily unique.

Definition: A *representation* of a group is a set of matrices corresponding to the set of elements such that if $M(g)$ is the matrix corresponding to the element, g , then

$$M(g)M(h) = M(gh) \text{ for all } g, h \in G.$$

This set of matrices will obey the four axioms of a group.

In order that they are able to be multiplied in arbitrary order, the matrices of a representation must be square and of the same size, $n \times n$. The *dimension* of a representation is defined as the dimension of the matrices, n . Two representations, $\{M\}$ and $\{M'\}$ of G are *equivalent* if one is obtained by a similarity transform of the other;

$$M'(g) = SM(g)S^{-1} \text{ for all } g \in G$$

for some $n \times n$ invertible matrix, S . It is easy to show that the $\{M'\}$ representation will follow the same multiplication rules and be of the same dimension as $\{M\}$.

A representation is *reducible* if there exists some similarity transform which, when applied, turns each matrix of the representation into a block diagonal matrix. For example,

$$SM(g)S^{-1} = \begin{bmatrix} M_1(g) & 0 \\ 0 & M_2(g) \end{bmatrix} \text{ for all } g \in G$$

where $M_1(g)$ is an $m \times m$ matrix for all $g \in G$ and $M_2(g)$ is an $l \times l$ matrix for all $g \in G$. If this is the case then we write,

$$M(g) = M_1(g) \oplus M_2(g)$$

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and the n -dimensional representation, M , is reduced to two m and l dimensional representations, M_1 and M_2 , where $m + l = n$.

An *irreducible representation* is one for which no such similarity transformation exists. The totally symmetric representation is a one-dimensional irreducible representation which consists entirely of one-dimensional unit matrices. Each group contains this representation.

Rather than write out a set of matrices for each representation, all the necessary information is contained in the set of *characters* (or traces) of these matrices. It is easily shown that the character of a matrix of a representation is unchanged by a similarity transformation, and thus the characters of conjugate elements are equal.

Symmetry operations on molecules form a natural group. A symmetry operation on a molecule can be a rotation, reflection or an inversion of that molecule, which leaves every atom of the molecule spatially unchanged. The set of all symmetry operations on a given molecular shape forms its *molecular symmetry group*.

All possible symmetry operations are now listed with their Schonflies notation:

E : identity element.

C_n^m : rotation around an axis by $m \cdot \frac{2\pi}{n}$ radians, $n = 2, 3, 4, 6$ and $m = 1, 2, \dots, n - 1$.

σ : reflection in a plane.

σ_h : reflection in a horizontal plane (referring to a plane through the origin perpendicular to the axis of highest symmetry).

σ_v : reflection in a vertical plane (containing the axis of highest symmetry).

σ_d : reflection in a plane diagonal to the horizontal and vertical planes.

S_n^m : rotation around an axis by $m \cdot \frac{2\pi}{n}$ and reflection in a plane perpendicular to that axis.

i : complete inversion through the origin.

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Clearly, some of these operations may be constructed from others. For example,

$$S_n^m = C_n \text{ when } m \text{ is even,}$$

$$S_2 = i.$$

In general symmetry operations do not commute (just as group operations do not necessarily commute). However, the following types of symmetry operations do commute:

- 1) rotations about the same axis
- 2) reflections through planes perpendicular to each other
- 3) inversion and any reflection or rotation
- 4) C_2 rotations about perpendicular axes
- 5) rotation and reflection in a plane perpendicular to the rotation axis.

A group is often described by a character table instead of a multiplication table. For example, the group, C_{3v} which contains an identity, two C_3 rotation axes in one class and three σ_v reflection planes in another class, has the following character table;

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Table A.2: The C_{3v} character table

The numbers in the character table are the characters (or Traces) of the matrix belonging to the row's representation and corresponding to a group element in the column's class. In general, A_1 will refer to the total symmetry representation and further, A_i 's will refer to other 1-dimensional representations. E 's will refer to 2-dimensional representations, and T 's will refer to 3-dimensional representations. The character of the identity in a given representation will

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be the dimension of that representation, since any matrix corresponding to the identity element must be the $n \times n$ identity matrix.

Many important theorems and rules concerning the construction of a character table are derived from the following theorem. The proof is not included but may be found in [9, p.371].

Theorem:

$$\sum_R [\Gamma_i(R)_{mn}] [\Gamma_j(R)_{m'n'}]^* = \frac{h}{\sqrt{l_i l_j}} \delta_{ij} \delta_{mm'} \delta_{nn'} \quad (\text{A.1})$$

where h is the order of the group, $\Gamma_i(R)_{mn}$ is the element in the m^{th} row and the n^{th} column of the matrix in the i^{th} irreducible representation corresponding to the group operation, R . l_i is the dimension of the i^{th} irreducible representation and $*$ is complex conjugation.

This theorem essentially states that any set of corresponding matrix elements of two matrices in an irreducible representation behave as orthogonal vectors in h -dimensional space.

One important result of Equation A.1 which is not proven here is that the sum of the squares of the irreducible representations' dimensions is equal to the order of the group:

$$\sum_i l_i^2 = h.$$

Substitute $m = n$ and $m' = n'$ into Equation A.1;

$$\sum_R \Gamma_i(R)_{mm} \Gamma_i(R)_{m'm'}^* = \frac{h}{l_i} \delta_{mm'}.$$

Then, summing over m and m' ,

$$\text{LHS} = \sum_m \sum_{m'} \sum_R \Gamma_i(R)_{mm} \Gamma_i(R)_{m'm'}^* = \sum_R \left(\sum_m \Gamma_i(R)_{mm} \right) \left(\sum_{m'} \Gamma_i(R)_{m'm'}^* \right) = \sum_R [\chi_i(R)]^2$$

$$\text{RHS} = \frac{h}{l_i} \sum_m \sum_{m'} \delta_{mm'} = \frac{h}{l_i} l_i = h$$

and therefore,

$$\sum_R [\chi_i(R)]^2 = h. \quad (\text{A.2})$$

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Suppose that $i \neq j$ in Equation A.1. Then we have,

$$\sum_R \Gamma_i(R)_{mn} \Gamma_j(R)_{mn} = 0 \quad i \neq j.$$

Now let $m = n$,

$$\sum_R \Gamma_i(R)_{mm} \Gamma_j(R)_{mm} = 0 \quad i \neq j.$$

Summing over m ,

$$\sum_R \chi_i(R) \chi_j(R) = \sum_m \left(\sum_R \Gamma_i(R)_{mm} \Gamma_j(R)_{mm} \right) = 0$$

and therefore,

$$\sum_R \chi_i(R) \chi_j(R) = 0 \quad i \neq j. \quad (\text{A.3})$$

Combining Equations A.2 and A.3 we have,

$$\sum_R \chi_i(R) \chi_j(R) = h \delta_{ij}. \quad (\text{A.4})$$

Reducible representations are composed of a certain number of irreducible representations. Suppose that a_j is the number of times that the block consisting of the j^{th} irreducible representation appears in a given reducible representation. If $\chi(R)$ is the matrix corresponding to the operation, R in the reducible representation then,

$$\chi(R) = \sum_j a_j \chi_j(R). \quad (\text{A.5})$$

Let us multiply Equation A.5 by the character from the i^{th} irreducible representation and sum over all operations;

$$\begin{aligned} \sum_R \chi(R) \chi_i(R) &= \sum_R \sum_j a_j \chi_j(R) \chi_i(R) \\ &= \sum_j a_j \sum_R \chi_i(R) \chi_j(R) \\ &= \sum_j a_j h \delta_{ij} = a_i h \end{aligned}$$

using Equation A.4

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Therefore, the number of times a given irreducible representation appears in the reduction of a reducible representation is,

$$a_i = \frac{1}{h} \sum_R \chi(R) \chi_i(R). \quad (\text{A.6})$$

If there exist two irreducible representations, X and Y , with basis functions, $X_1 \dots X_m$ and $Y_1 \dots Y_n$ respectively (these may be eigenfunctions of the wave equation) then we construct the *direct product representation* which has the basis functions, $X_i Y_j$.

Let R be a symmetry operation, then define x_{ij} and y_{ij} as;

$$RX_i = \sum_{j=1}^m x_{ji} X_j$$

$$RY_k = \sum_{l=1}^n y_{lk} Y_l.$$

Then,

$$RX_i Y_k = \sum_{j=1}^m \sum_{l=1}^n x_{ji} y_{lk} X_j Y_l = \sum_{j,l} z_{jl,ik} X_j Y_l.$$

If we denote the direct product group with the index, z , then,

$$\chi_z(R) = \sum_{j,l} z_{jl,ij} = \sum_{j=1}^m \sum_{l=1}^n x_{ji} y_{li} = \chi_X(R) \chi_Y(R).$$

Therefore,

$$\chi_{12}(R) = \chi_1(R) \chi_2(R). \quad (\text{A.7})$$

Finally, the characters of a symmetric product of a representation with itself are defined;

$$[\chi(R)^2] = \frac{1}{2} [\chi(R)^2 + \chi(R^2)] \quad (\text{A.8})$$

and the characters of an antisymmetric product are;

$$\{\chi(R)^2\} = \frac{1}{2} [\chi(R)^2 - \chi(R^2)]. \quad (\text{A.9})$$

Appendix B

Fibre Bundles

The following is a brief summary of Fibre Bundles and their Characteristic Classes. Those familiar with these concepts may skip this appendix. Alternatively for a more thorough coverage the reader is directed to [18] or [25] for bundles and to [24, 21] for Topological material.

B.1 Basic Definitions

Definition: A *manifold* is an n -dimensional space which is locally homeomorphic to \mathbb{R}^n . That is, a manifold, M , is covered by a (not necessarily finite) union of subspaces, $\{U_\alpha\}$, such that for each U_α there exists a homomorphism, $h_\alpha : V_\alpha \rightarrow U_\alpha$, where V_α is an open subset of \mathbb{R}^n . Furthermore, for any two subspaces where $U_\alpha \cap U_\beta \neq \emptyset$ there exists a set of continuous change-of-basis functions from U_α to U_β .

Example: The simplest example of a smooth manifold is \mathbb{R}^n , which is covered by itself and is homomorphic to \mathbb{R}^n by the identity map.

Example: The two dimensional sphere, S^2 , embedded in \mathbb{R}^3 is a two dimensional manifold which can be broken into the top half plus a small strip (defined by the azimuthal angle; $0 \leq \psi \leq \frac{\pi}{2} + \epsilon, \epsilon > 0$) and the bottom half plus a strip; $(\frac{\pi}{2} - \epsilon \leq \psi \leq \pi)$. Each “half” is homomorphic to the plane, \mathbb{R}^2 .

Definition: A *tangent vector* to a manifold, M , at the point $x \in M$ is a vector in \mathbb{R}^n which can be expressed as the instantaneous velocity vector of some path through x in M . In this way the path defines the vector. The vector space consisting of all vectors tangent to M at x is called

the tangent space of M at x , denoted $T_x(M)$.

Definition: The *normal space* of M is the space of all vectors normal to $T_x(M)$ for all $x \in M$, where normal to M implies, if $M \subset \mathbb{R}^m$ for some $m \in \mathbb{Z}$ then $T_x M \subset T_x \mathbb{R}^m$, $x \in M \subset \mathbb{R}^m$.

Definition: A real *vector bundle*, ξ , consists of a *total space*, E , a projection map, $\pi : E \rightarrow B$, as well as a vector space structure on the subset $\pi^{-1}(b) \subset E$ for all $b \in B$. B is called the *base space* and E is called the *total space* of the bundle. The set $\pi^{-1}(b) = F_b$ is called the *fibre* over b . The vector bundle, ξ is displayed below,

$$\xi : \quad \begin{array}{ccc} F & \hookrightarrow & E \\ & & \downarrow \pi \\ & & B \end{array}$$

where the space F is homomorphic to F_b for all $b \in B$. If the dimension of F_b is n , for all $b \in B$ then the fibre bundle is said to be n dimensional.

Every vector bundle satisfies the following *local triviality* condition; for every $b \in B$, there is a neighborhood, $U \subset B$, and a bundle isomorphism, h , such that the following square commutes:

$$\begin{array}{ccc} U \times \mathbb{R}^k & \xrightarrow{h} & p^{-1}(U) \\ \downarrow p' & \circlearrowleft & \downarrow p \\ U & \xrightarrow{\text{Identity}} & U \end{array}$$

The restriction of h to each fibre; $h : b \times \mathbb{R}^k \rightarrow p^{-1}(b)$ is a vector space isomorphism for all $b \in U$.

If a fibre bundle consists of $p : E \rightarrow B$ and B is covered by open spaces, $\{V_i\}$ then we denote the local trivialization maps as $\{\phi_i\}$;

$$\begin{aligned} \phi_i : V_i \times \mathbb{R}^n &\rightarrow p^{-1}(V_i) \\ \phi_i : V_i &\mapsto E \times \mathbb{R}^n \end{aligned}$$

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The *transition functions* in the base space from V_i to V_j are denoted $\{g_{ji}\}$;

$$g_{ij} : V_i \cap V_j \times \mathbb{R}^n \rightarrow V_i \cap V_j \times \mathbb{R}^n$$

$$g_{ij} : (b, x) \mapsto (b, y)$$

such that,

$$g_{ij} = \phi_j^{-1} \circ \phi_i.$$

Definition: A *cross-section* of a bundle is a continuous function, $\sigma : B \rightarrow E$ taking each $b \in B$ to a vector in F_b .

Example: An infinitely tall cylinder is a fibre bundle over a circle:

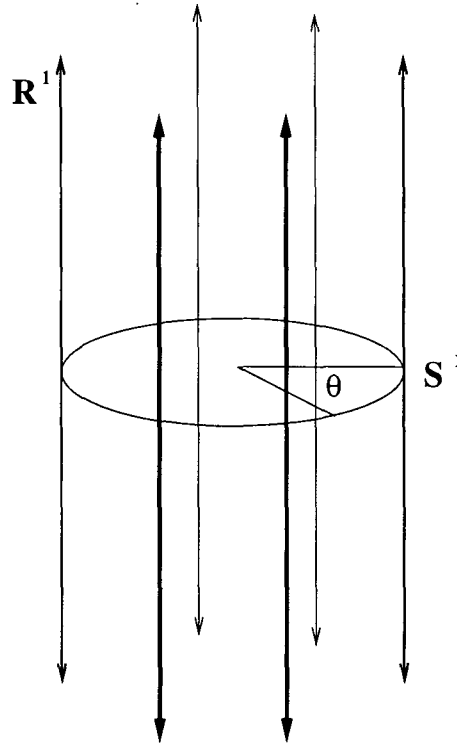


Figure B.1: A real line bundle over S^1

where S^1 , the horizontal circle, is the base space and each fibre over a given θ , ($0 \leq \theta \leq 2\pi$) is simply the line passing vertically through the circle at θ . A point in the total space, (θ, x) , is a point on the cylinder, defined by both a point on the circle at angle, θ , and the distance, x ,

along the line running through that point. This bundle is trivial. The fibres are lines, each homeomorphic to \mathbb{R}^1 and sections are just curves around the cylinder. In other words, a section, $\sigma : S^1 \rightarrow S^1 \times \mathbb{R}^1$ takes a point, θ , on S^1 to a point on the cylinder directly “above” θ , and thus σ traces out a path around the cylinder which is periodic, with period 2π .

Example: The Möbius band is a non-trivial bundle over S^1 . That is, the total space, $E \neq S^1 \times \mathbb{R}^1$. The fibres are each homomorphic to \mathbb{R}^1 but each section, $\sigma : S^1 \rightarrow E$ must be an anti-periodic function. In other words, once we go around the S^1 by 2π , the space has undergone a twist and the function $\sigma(2\pi) = -\sigma(0)$.

Definition: If ξ and η are fibre bundles over the same base space, B , they are *isomorphic* if and only if there exists a homomorphism,

$$h : E(\xi) \rightarrow E(\eta)$$

which takes $F_b(\xi)$ isomorphically to $F_b(\eta)$ for each $b \in B$.

Definition: We define the *Tangent Bundle* of a manifold M , denoted τ_M , as the bundle over M with fibres,

$$F_b(\tau_M) = T_b(M). \quad (\text{B.1})$$

B.2 Constructing new vector bundles

1) Let ξ be the bundle, $\pi : E \rightarrow B$ and let $B' \subset B$. The *restriction* of ξ to the new base, B' , is $\pi' : E' \rightarrow B'$ where $E' = \pi^{-1}(B')$ and $\pi' = \pi|_{E'}$. This *restricted bundle* is written, $\xi|_{B'}$. It should also be noted that the restricted bundle is simply a special case of the pullback bundle, (defined below).

2) Let B_2 be an arbitrary topological space and ξ be the bundle, $\pi : E \rightarrow B$. If $f : B_2 \rightarrow B$,

then the *pullback bundle*, $f^*\xi$, over B_2 is :

$$\begin{array}{ccc} f^*\xi : & E_2 & \xrightarrow{\quad} E & : \xi \\ & \downarrow & & \downarrow \pi \\ & B_2 & \xrightarrow{\quad f \quad} & B \end{array}$$

where $E_2 = \{(b, e) | b \in B_2, e \in E, f(b) = \pi(e)\}$ and $\pi_2(b, e) = b$. Thus, the following diagram commutes;

$$\begin{array}{ccc} E_2 & \xrightarrow{\hat{f}} & E \\ \pi_2 \downarrow & \circlearrowleft & \downarrow \pi \\ B_2 & \xrightarrow{\quad f \quad} & B \end{array}$$

where $\hat{f}(b, e) = e$.

3) The *Cartesian Product* of two bundles, ξ_1 and ξ_2 , is $\xi_1 \times \xi_2$ and corresponds to;

$$\begin{array}{ccc} \xi_1 \times \xi_2 : F_1 \times F_2 & \hookrightarrow & E_1 \times E_2 \\ & & \downarrow \\ & & B_1 \times B_2 \end{array}$$

where $(\pi_1 \times \pi_2)^{-1}(b_1, b_2) = F_{b_1}(\xi_1) \times F_{b_2}(\xi_2)$.

5) The *Whitney Sum* of two bundles, ξ_1 and ξ_2 , both over the same base space is $\xi_1 \oplus \xi_2 = d^*(\xi_1 \times \xi_2)$, where $d : B \rightarrow B \times B$ takes $b \mapsto (b, b)$. Each fibre, $F_b(\xi_1 \oplus \xi_2) \simeq F_b(\xi_1) \oplus F_b(\xi_2)$.

Definition: If ξ and η are bundles over the same base space and $E(\xi) \subset E(\eta)$ then ξ is a *sub-bundle* of η and we write $\xi \subset \eta$.

6) If $\xi \subset \eta$ and η (and thus $E(\eta)$) has a Euclidean metric, then ξ^\perp is the *orthogonal compliment* of F , where $F_b(\xi^\perp) = \{v \in F_b(\eta) | v \cdot w = 0 \text{ for all } w \in F_b(\xi)\}$ and $E(\xi^\perp) = \bigcup_b \{F_b(\xi^\perp)\}$.

7) Following from the definition of the Tangent Bundle is the *Normal Bundle*, ν . If the base

space, $B' \hookrightarrow B$ for some B and TB' is a sub-bundle of TB , then the normal bundle over B' is the orthogonal complement of TB' in TB .

7) If η is a bundle with projection map, $p : E \rightarrow B$ and ξ is a bundle with projection map, $q : X \rightarrow B$ with the same base space, then the *pullback bundle*, η^* , of η over ξ is defined by the following commutative square:

$$\begin{array}{ccc} & F & F \\ \eta^* : \downarrow & \downarrow & \downarrow \\ & \tilde{E} & \xrightarrow{\tilde{q}} E \\ & \downarrow \tilde{p} & \downarrow p \\ \xi : \hookrightarrow X & \xrightarrow{q} & B \end{array} \quad \begin{array}{c} \\ \\ \\ \circlearrowleft \\ \end{array} \quad \begin{array}{c} \\ \\ \\ \end{array} : \eta$$

where the total space of η^* is $\tilde{E} = \{(x, y) \in X \times E \mid p(y) = q(x)\}$ and the projections $\tilde{q} : (x, y) \mapsto y$ and $\tilde{p} : (x, y) \mapsto x$. η^* is simply the induced bundle of η over another Fibre bundle.

8) The following is a definition of an *associated principal bundle*.

Let ξ be a k -dimensional fibre bundle,

$$\begin{array}{ccc} \xi : & F & \hookrightarrow E \\ & & \downarrow \pi \\ & & B \end{array}$$

with transition functions, $g_{ij} : U_i \cap U_j \times \mathbb{R}^k \rightarrow U_i \cap U_j \times \mathbb{R}^k$ for subspaces $U_i, U_j \in B$. Now restrict the transition functions to each fibre, $\pi^{-1}(b)$, for every $b \in B$.

$$g_{ij}^{(b)} : b \times \mathbb{R}^k \rightarrow b \times \mathbb{R}^k.$$

$g_{ij}^{(b)}$ is now an isometry of \mathbb{R}^k and is therefore an element of $O(k)$. We may now define a

continuous map,

$$g_{ij} : U_i \cap U_j \rightarrow G = O(k)$$

$$b \mapsto g_{ij}^{(b)} \in O(k).$$

G is denoted as the *structure map* of the bundle.

We now define $\tilde{\xi}$, as the *associated principal bundle* of ξ . $\tilde{\xi}$ has the same base space, B , with fibres, G equal to the structure group of ξ . $\tilde{\xi}$ also has the same trivialization neighborhoods, with transition functions,

$$\tilde{g}_{ij} : U_i \cap U_j \times G \rightarrow U_i \cap U_j \times G$$

$$(b, g) \mapsto (b, g_{ij}^{(b)} \cdot g)$$

The total space of $\tilde{\xi}$ will be denoted, \tilde{E} . Let Z be the union of the locally trivial fibres, $Z = \bigcup_i \{U_i \times G\}$ and let q_i be the inclusion map,

$$q_i : U_i \times G \hookrightarrow Z.$$

Two point in Z are equivalent, $(b_1, g_1) \sim (b_2, g_2)$ if and only if $b_1 = b_2 \in U_i \cap U_j$ and $g_2 = g_{ij}^{(b)} g_1$. The total space of the associated principal bundle is then the quotient space, $\tilde{E} = Z / \sim$. where $q : Z \rightarrow E$. Finally, the projection map of $\tilde{\xi}$ is simply, $p : (b, g) \mapsto b$, which is well defined, since if $(b_1, g_1) \sim (b_2, g_2)$ then $b_1 = b_2$.

B.3 Characteristic Classes

Fibre bundles over a given base space are characterized by naming them according to their characteristic classes. Every real vector bundle, ξ , of dimension, n , has $n + 1$ Stiefel-Whitney classes which are cohomology classes of the base space,

$$w_i(\xi) \in H^i(B(\xi); \mathbb{Z}_2).$$

Following are the seven defining properties of Stiefel-Whitney classes. $H^i(B(\xi); \mathbb{Z}_2)$ is the cohomology group of the base space, $B(\xi)$, with coefficients in the group, \mathbb{Z}_2 . A good background on the subject of homology and cohomology theory is given in [24, 21].

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1) The first Stiefel-Whitney class of any bundle is always 1; $w_0 = 1 \in H^0(B(\xi); \mathbb{Z}_2)$

2) All Stiefel-Whitney classes of index greater than the bundle's dimension are zero;

$$w_j = 0 \text{ for all } j > n.$$

3) If two bundles have the same base space; $B(\xi) = B(\eta)$ then the direct sum of these bundles have Stiefel-Whitney classes,

$$w_k(\xi \oplus \eta) = \sum_{j=0}^k w_j(\xi) w_{k-j}(\eta). \quad (\text{B.2})$$

4) If f maps the base space of one bundle to another, $f : B(\xi) \rightarrow B(\eta)$ then

$$w_i(\xi) = f^* w_i(\eta) \quad (\text{B.3})$$

where f^* is the pullback of f .

5) If two bundles are isomorphic, $\xi \simeq \eta$, then their Stiefel-Whitney classes are identical.

$$w_i(\xi) = w_i(\eta). \quad (\text{B.4})$$

Similarly, it is important to note that if two bundles are not isomorphic then their Stiefel-Whitney classes cannot all be equal. However, identical Stiefel-Whitney classes does not imply isomorphic vector bundles, with the exception of line bundles (one dimensional vector bundles).

6) If ξ is a trivial bundle then all Stiefel-Whitney classes are zero.

$$w_i(\xi) = 0 \text{ for all } i > 0. \quad (\text{B.5})$$

7) If ξ is a trivial bundle then

$$w_i(\xi \oplus \eta) = w_i(\eta) \text{ for all } i. \quad (\text{B.6})$$

Definition: The *total Stiefel-Whitney class* of ξ is defined as,

$$w(\xi) = \sum_{i=0}^n w_i(\xi). \quad (\text{B.7})$$

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Beyond simple real vector spaces are oriented spaces:

Definition: A vector space, V , has two distinct *orientations*, each an equivalence class on the bases of V . Suppose $\{v_1, \dots, v_n\}$ and $\{w_1, \dots, w_n\}$ are two ordered bases for V . These bases are related by;

$$w_i = \sum_{j=1}^n a_{ij} v_j \quad (\text{B.8})$$

and are considered equivalent if and only if $\det[a_{ij}] > 0$.

It is important to note that the choice of an orientation for V is equivalent to the choice of a preferred generator for the singular homology group, $H_n(V, V_0; \mathbb{Z})$ and thus a preferred generator, u_V , for $H^n(V, V_0; \mathbb{Z})$. V_0 is simply the set of non-zero vectors in V .

Definition: An *orientation of a fibre bundle*, ξ , is defined by a function which assigns an orientation to each fibre, F_b , in ξ . This orientation must be preserved by the local triviality homomorphism between $N \times \mathbb{R}^n$ and $\pi^{-1}(N)$ for all neighborhoods, $N \subset B(\xi)$, determined by $b \in N$.

An alternate definition of an orientable vector bundle is one which has a trivialization atlas (the spanning set of open spaces and transition functions) such that all transition functions are elements of the group, $SO(N)$.

For an n -dimensional oriented fibre bundle, ξ , with projection map, $\pi : E \rightarrow B$, $H^i(E, E_0; \mathbb{Z}) = 0$ for all $i < n$ and there exists only one class in $H^n(E, E_0; \mathbb{Z})$ which is u , such that;

$$u|_{(F_b, F_b^0)} = u_{F_b} \in H^n(F_b, F_b^0; \mathbb{Z}) \text{ for all } b \in B. \quad (\text{B.9})$$

Definition: The *Euler Class* of an n -dimensional oriented fibre bundle, ξ , is defined by;

$$e(\xi) = (\pi^*)^{-1} j^*(u) \in H^n(B; \mathbb{Z}) \quad (\text{B.10})$$

where $j^* : H^n(E, E_0) \rightarrow H^n(E)$ in the cohomology exact sequence, and $\pi^* : H^n(B) \rightarrow H^n(E)$. π^* is the pullback of the projection map, $\pi : E \rightarrow B$ and is an isomorphism since E is continuously deformable into B .

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The Euler class of a fibre bundle has the following properties:

- 1) The Euler class of a bundle changes sign if the orientation of the bundle is reversed.
- 2) If ξ is an n -dimensional, oriented bundle and n is odd then,

$$e(\xi) + e(\xi) = 0.$$

- 3) If $f : B \rightarrow B'$ is covered by an orientation preserving bundle map, $F : \xi \rightarrow \xi'$ then

$$e(\xi) = f^*e(\xi').$$

- 4) The homomorphism, $h : H^n(B; \mathbb{Z}) \rightarrow H^n(B; \mathbb{Z}/2)$ takes $e(\xi) \mapsto w_n(\xi)$ which implies the following property;

- 5) $e(\xi \oplus \eta) = e(\xi)e(\eta)$ and $e(\xi \times \eta) = e(\xi) \times e(\eta)$.

We may also begin with a real n -dimensional fibre bundle, ξ , and *complexify* it, creating $\xi' = \xi \otimes \mathbb{C}$, a complex n -dimensional bundle. Each fibre, F_b , of ξ is a real n -dimensional vector space. The corresponding fibre, F'_b of ξ' is a complex n -dimensional vector space such that,

$$F'_b = F_b \times \mathbb{C} = F_b \oplus iF_b. \quad (\text{B.11})$$

Of course, for any complex n -dimensional bundle, η , there is a canonical underlying real $2n$ -dimensional bundle, η_R , arrived at by simply ignoring the complex structure on the fibres of η .

With a complex n -dimensional bundle, η , we can construct the following new bundles:

- 1) The *conjugate bundle*, $\bar{\eta}$, to η is the complex n -dimensional bundle such that,

$$\eta_R = \bar{\eta}_R.$$

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$\bar{\eta}_R$ has the opposite complex structure to η so that the map, $f : E(\eta) \rightarrow E(\bar{\eta}_R)$ is defined by $f : \lambda e \mapsto \bar{\lambda} f(e)$ for all $\lambda \in \mathbb{C}$. In this case, f is fibrewise complex conjugation, the equivalent of multiplying by i .

2) The *dual bundle*, $\text{Hom}_{\mathbb{C}}(\eta, \mathbb{C})$, of η is the bundle over the same base space, $B(\eta)$, whose fibre corresponding to $F_b(\eta)$ is $\text{Hom}_{\mathbb{C}}(F_b, \mathbb{C})$.

Now we may introduce a new kind of characteristic class for complex fibre bundles.

Definition: The *Chern classes* of the complex n -dimensional bundle, η , are;

$$c_i(\eta) \in H^{2i}(B; \mathbb{Z}) \quad (\text{B.12})$$

where $c_n(\eta) = e_n(\eta_R)$, the top Euler class of the underlying real bundle.

$$c_i(\eta) = 0 \text{ for all } i > n, \quad c_0(\eta) = 1 \text{ and} \quad (\text{B.13})$$

$$c_i(\eta) = \pi_0^{*-1} c_i(\eta_0). \quad (\text{B.14})$$

where π_0^* is the isomorphism, $\pi_0^* : H^{2i}(B) \rightarrow H^{2i}(E_0)$. η_0 is the $(n-1)$ -dimensional fibre bundle whose *base space* is E_0 , the set of non-zero vectors in $E(\eta)$. (v, F) specifies a point in E_0 and thus the fibre of η_0 over a vector, v , is the orthogonal complement to v in the fibre, F , and is an n -dimensional vector space, as shown in the following diagram,

$$\begin{array}{ccc} \eta_0 : & \mathbb{C}^{n-1} & \hookrightarrow E(\eta) \\ & & \downarrow \\ \eta : & S^{2n-1} = \mathbb{C}^n & \hookrightarrow E_0 \\ & & \downarrow \pi_0 \\ & & B \end{array}$$

π_0^* is an isomorphism for $i < n$ due to the homotopy type of the fibres of η which are that of S^{2n-1} . Thus, $c_{n-1}(\eta_0) = e_n(\eta_{0R})$ since $c_{n-1}(\eta_0)$ is the top Chern class of η_0 and $c_{n-1}(\eta)$

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is well defined as $\pi_0^{*-1}c_{n-1}(\eta_0) = \pi_0^{*-1}e_{n-1}(\eta_{0R}) \cdot c_{n-2}(\eta_0)$ and therefore $c_{n-2}(\eta)$ can be found inductively just as $c_{n-1}(\eta)$ was. This process may be repeated until we find $c_i(\eta) = 0$ for all $i < 0$.

Alternatively, the Chern classes of a complex n -dimensional bundle, η , may be defined in terms of the Chern classes of the universal bundle, γ^n , over $G_n(\mathbb{C}^\infty)$.

The Infinite Grassmanian manifold, $G_n(\mathbb{C}^\infty)$, is the union of all finite Grassmanian manifolds,

$$G_n(\mathbb{C}^\infty) = \bigcup_{k \geq n} G_n(\mathbb{C}^k),$$

where $G_n(\mathbb{C}^k)$ is the set of all complex n -planes through the origin in \mathbb{C}^{n+k} . The topology on $G_n(\mathbb{C}^\infty)$ is the inductive topology, which means that a subset, $U \subset G_n(\mathbb{C}^\infty)$ is open if and only if $U \cap G_n(\mathbb{C}^k)$ is open for each $k \in \mathbb{Z}$, $k \geq n$.

The universal bundle, γ^n , has total space,

$$E(\gamma^n) = G_n \times \mathbb{C}^\infty \tag{B.15}$$

where G_n refers to $G_n(\mathbb{C}^\infty)$ and $\pi : E(\gamma^n) \rightarrow G_n$ takes (n -plane \mathcal{X} , vector $x \in \mathcal{X}$) \mapsto n -plane $\mathcal{X} \in G_n$.

The universal bundle over $G_n(\mathbb{R}^\infty)$ is defined identically using real n -plane bundles.

Theorem B.1: $H^*(G_n(\mathbb{C}^\infty); \mathbb{Z})$ is the cohomology ring over \mathbb{Z} freely generated by the Chern classes $c_1(\gamma^n), \dots, c_n(\gamma^n)$.

Furthermore,

Theorem B.2: For any complex n -dimensional fibre bundle, η , there exists a function, $f : \eta \rightarrow \gamma^n$ such that the Chern classes of η are determined by $c_i(\eta) = f^*c_i(\gamma^n)$.

Definition: The *total Chern class* of the fibre bundle, η , is defined;

$$c(\eta) = \sum_{i=1}^n c_i(\eta).$$

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Just as for the Stiefel-Whitney classes or the Euler classes, the Chern classes obey the following properties:

- 1) For any two complex n -dimensional fibre bundles, ξ and η ,

$$c(\xi \oplus \eta) = c(\xi)c(\eta). \quad (\text{B.16})$$

- 2) For any complex n -dimensional bundle, ξ ,

$$c_i(\bar{\xi}) = (-1)^i c_i(\xi) \quad (\text{B.17})$$

where $\bar{\xi}$ is the dual bundle to ξ .

Definition: For a real n -plane bundle, ξ , the *Pontrjagin Classes*,

$$p_i(\xi) \in H^{4i}(B; \mathbb{Z}) \quad (\text{B.18})$$

are defined as,

$$p_i(\xi) = (-1)^i c_{2i}(\xi \otimes \mathbb{C}). \quad (\text{B.19})$$

$p_0(\xi) = 1, p_i(\xi) = 0$ for all $i > n/2$ and the total Pontrjagin class is defined as

$$p(\xi) = \sum_{i=1}^{[n/2]} p_i(\xi)$$

where $[n/2]$ is the largest integer less than or equal to $n/2$.

The following properties are true for Pontrjagin classes:

- 1) If f is a bundle map, $f : \xi \rightarrow \eta$ then,

$$p_i(\xi) = f^* p_i(\eta). \quad (\text{B.20})$$

- 2) If ϵ is a trivial n -plane bundle then,

$$p(\xi \oplus \epsilon) = p(\xi) \text{ for all bundles, } \xi. \quad (\text{B.21})$$

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3) For any two bundles, ξ and η ,

$$p(\xi \oplus \eta) = p(\xi)p(\eta) \text{ Mod } 2. \quad (\text{B.22})$$

By Theorems B.1 and B.2 it is easily shown that the Pontrjagin classes are defined by the Chern classes and are equal to:

$$p_k(\eta_R) = c_k(\eta)^2 - 2c_{k-1}(\eta)c_{k+1}(\eta) + \dots \pm 2c_1(\eta)c_{2k-1}(\eta) \mp 2c_{2k}(\eta). \quad (\text{B.23})$$

Appendix C

The quaternion Numbers

The following conventions and theorems may be found in [23].

The set of quaternion numbers, denoted \mathbb{H} to honor William Hamilton, is a non-commutative field over the real numbers, generated by four elements, $1, i, j$ and k , such that;

$$i^2 = j^2 = k^2 = -1 \quad (\text{C.1})$$

and

$$ij = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j. \quad (\text{C.2})$$

For a given element of the quaternions, $x = x_0 + x_1i + x_2j + x_3k \in \mathbb{H}, x_i \in \mathbb{R}$, the conjugate of x is $\bar{x} = x_0 - x_1i - x_2j - x_3k$ and the norm of x is $|x|^2 = x\bar{x}$.

The following convention of multiplication on the right is used to define multiplication in a quaternion vector field. Let v and w be elements in a quaternion vector space, V , and $x, y \in \mathbb{H}$ be quaternion numbers. Then,

$$(v + w)x = vx + wx, \quad v(x + y) = vx + vy, \quad v(xy) = (vx)y. \quad (\text{C.3})$$

Another way to look at a quaternion vector space is as a complex vector space with an operator, Θ , called the *quaternion structure map*. Θ is anti-linear and $\Theta^2 = -1$. A complex n -dimensional

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vector space, W , is then transformed into a quaternion n -dimensional space by the following conventions;

$$vi = w, \quad vj = \Theta v, \quad vk = (vi)j = \Theta(w) = -i\Theta v \quad (\text{C.4})$$

where $v \in W$. Multiplication on the right refers to multiplication by a unit quaternion and multiplication on the left is just by the complex number i or by the structure map, Θ .

We can now view W as a quaternion space and give it a basis, $\{e_i, \Theta e_i\}$ over \mathbb{C} , where $i = 1 \dots n$ and n is the quaternion dimension of W .