Purdue University
Purdue e-Pubs

ECE Technical Reports | Electrical and Computer Engineering

10-21-1994

EXPLICIT ORTHONORMAL BASES FOR FUNCTIONS EXHIBITING THE ROTATIONAL SYMMETRIES OF A PLATONIC SOLID

Yibin Zheng
Purdue University School of Electrical Engineering

Peter C. Doerschuk
Purdue University School of Electrical Engineering

EXPLICIT ORTHONORMAL BASES FOR FUNCTIONS EXHIBITING THE ROTATIONAL SYMMETRIES OF A PLATONIC SOLID

YIBIN ZHENG
PETER C. DOERSCHUK

TR-EE 94-34
OCTOBER 1994

SCHOOL OF ELECTRICAL ENGINEERING
PURDUE UNIVERSITY
WEST LAFAYETTE, INDIANA 47907-1285

Explicit Orthonormal Bases for Functions Exhibiting the Rotational Symmetries of a Platonic Solid[1]

Yibin Zheng
Peter C. Doerschuk

School of Electrical Engineering
Purdue University

October 21, 1994

[1]Supported by U. S. National Science Foundation grant MIP-9110919, a Purdue Research Foundation Research Grant, and a Whirlpool Faculty Fellowship. Corresponding author: Peter C. Doerschuk, 1285 Electrical Engineering Building, Purdue University, West Lafayette, IN 47907-1285; (317) 494–1742, (317) 494–6440 (Fax), doerschu@ecn.purdue.edu (Internet).

Abstract

We compute explicit orthonormal bases for functions invariant under the rotational symmetries of a Platonic solid. Each function in the basis is a linear combination of spherical harmonics. For each symmetry (icosahedral, octahedral, tetrahedral) the calculation has three steps: First derive a bilinear equation for the coefficients by comparing the expansion of a symmetrized delta function in both spherical harmonics and the symmetric harmonics. The equation is parameterized by the location (θ_0, ϕ_0) of the delta function and must be satisfied for all locations. Second, express the dependence on the delta function location in a Fourier (ϕ_0) and Taylor (θ_0) series and thereby derive a new system of bilinear equations by comparing selected coefficients. Third, derive a recursive solution of the new system and explicitly solve the recursion with the aid of symbolic computation. The results for the icosahedral case are important for structural studies of small spherical viruses.

Key words:: spherical harmonics; rotational symmetries, finite; Platonic solids, icosahedron, dodecahedron, octahedron, cube, tetrahedron.

Contents

1 Introduction

Spherical harmonics are a complete orthonormal basis for smooth functions on the sphere. If, however, the function is required to have a symmetry then spherical harmonics are not convenient because the symmetry implies complicated relationships between the weights in the expansion of the function as a weighted sum of spherical harmonics. In particular, we are interested in functions that are required to exhibit the symmetries of the icosahedron. This group plays a prominent, role in at least three problems: the structure of small spherical viruses [13], fullerenes [10], and quasicrystals [3]. Therefore we would like to determine a complete orthonormal basis for smooth icosahedrally-symmetric functions on the sphere. Since this is a subspace of srnooth functions on the sphere and because so much is known about spherical harmonics, it is natural to compute each element in the desired basis as a linear combination of spherical harmonics. Though we call these functions icosahedral harmonics, this terminology is somewhat different than that used for spherical harmonics. In particular, only the lowest order spherical harmonic actually has the symmetry of the sphere (invariant under any rotation around any axis) while every icosahedral harmonic has the symmetry of the icosahedron (invariant under each of 60 different rotations described in Fact **3).**

When computing an icosahedral harmonic as a linear combination of spherical harmonics, the only task is to determine the coefficients in the linear combination. There has been extensive work on this problem [1, 2, **3**, 6, 7, 9, 12, 14, 15] [4, A. Klug cited on p. 413]. One of the more complete treatments is due to La Porte [12], who derived explicit expressions for icosahedral harmonics up to order 21. To the best of our knowledge, none of the existing literature describes a general explicit expression for icosahedral harmonics of arbitrary order. In the remainder of this paper we derive such an expression by a novel method, specifically, by equating the expansions of an icosahedrally symmetric delta function in spherical harmonics and icosahedral harmonics. Our motivation for the calculation was to derive icosahedral harmonics for use in viral structure problems. However, the same technique can be applied to determine general explicit expressions for tetrahedral harmonics and octahedral harmonics and we also describe these simpler calculations.

2 The Relationship Between Icosahedral and Spheriical Harmonics

Theorem 1 *Let $h(\theta,\phi)$ be invariant under a rotation* R. *Then the real and imaginary parts of h are separately invariant under the rotation R.*

Proof: See Appendix A □

Let $Y_{l,m}(\theta,\phi)$ be spherical harmonics (we use the conventions of Jackson [8]) indexed by l and m. It is well known [8, Eq. 3.53] that

$$Y_{l,m}(\theta,\phi) = N_{l,m} P_{l,m}(\cos\theta) e^{im\phi} \tag{1}$$

where $P_{l,m}(x)$ are the associated Legendre functions [8, Eq. 3.49] and

$$N_{l,m} = \sqrt{\frac{21+1}{4\pi}\frac{(l-m)!}{(l+m)!}}.$$

Spherical harmonics are closely related to rotations. Let R be a rotation of three-dimensional space described in terms of the Euler angles a, β, γ and having inverse R^{-1}. Let O_R be the corresponding rotation in function space: $O_R[f(\vec{x})] = f(R^{-1}(\vec{x}))$.

Theorem 2 *Any rotational operation on a spherical harmonic $Y_{l,m}(\theta,\phi)$ will yield a linear combination of spherical harmonics of only the same l, that is,*

$$O_R[Y_{l,m}(\theta,\phi)] = \sum_{m'=-l}^{+l} D_{l,m,m'}(\alpha,\beta,\gamma)Y_{l,m'}(\theta,\phi)$$

where the $D_{l,m,m'}$ coefficients are Wigner's D coefficients and have the following expressions:

$$D_{l,m,m'}(\alpha,\beta,\gamma) = e^{-im'\alpha}d_{l,m,m'}(\beta)e^{-im\gamma}$$

$$d_{l,m,m'}(\beta) = \sum_{k=0}^{l+m} \frac{(-1)^k\sqrt{(l+m-m)!(l+m')!(l-m')!}}{(l-m'-k)!(l+m-k)!(m'-m+k)!k!}(\cos\frac{\beta}{2})^{2l+m-m'-2k}(-\sin\frac{\beta}{2})^{m'-m+2k}$$

Proof: See Ref. [16]. □

Theorem 3 *Let $f(\theta,\phi)$ be invariant under N rotation operators denoted by R_i for $i = 1,\ldots,N$. Let f have spherical harmonic expansion $f(\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} b_{l,m}Y_{l,m}(\theta,\phi)$. Then, for each $l = 0,1,\ldots$, the function f_l defined by $f_l(\theta,\phi) = \sum_{m=-l}^{+l} b_{l,m}Y_{l,m}(\theta,\phi)$ is also invariant under the R_i for $i = 1,\ldots,N$.*

Proof: See Appendix A □

Our goal is to determine a set of basis functions T_α where

1. T_α are a complete orthonormal basis for smooth icosahedrally symmetric functions on the sphere.
2. T_α are real, as allowed by Theorem 1.
3. Each T_α is a linear combination of $Y_{l,m}$ for fixed l, as allowed by Theorem 3. In particular, assume that there are N_l icosahedral harmonics that are linear combinations of $Y_{l,m}$ ($m = -l,\ldots,+l$), and therefore $N_l \leq 2l+1$, and denote them as $T_{l,n}(\theta,\phi)$ with $n = 0,\ldots,N_l - 1$:

$$T_{l,n}(\theta,\phi) = \sum_{m=-l}^{+l} b_{l,n,m}Y_{l,m}(\theta,\phi) \quad (2)$$

The orthanormality condition is

$$\int T^*_{l,n}(\theta,\phi)T_{l',n'}(\theta,\phi)\mathrm{d}\Omega = \delta_{l,l'}\delta_{n,n'} \quad (3)$$

where the complex conjugation is optional since the $T_{l,n}$ are real and $\mathrm{d}\Omega = \sin\theta\mathrm{d}\theta\mathrm{d}\phi$ in spherical coordinates. The task of this paper is to find the $b_{l,n,m}$ coefficients in Eq. 2. For each $l = 0,1,\ldots$ there are N_l sets of $2l+1$ coefficients.

La Porte [12] proves the following result regarding N_l:

Theorem 4 (La Porte [12]) *For l even, the number N_l (denoted by $N_l^{(\text{even})}$) satisfies the relationship*

$$\frac{1}{(1-x^6)(1-x^{10})} = \sum_{l=0}^{\infty} N_l^{(\text{even})}x^l$$

while for l odd, the number N_l (denoted by $N_l^{(\text{odd})}$) is

$$N_l^{(\text{odd})} = \begin{cases} N_{l-15}^{(\text{even})} & l \geq 15 \\ 0, & 0 \leq l < 15 \end{cases} \quad (4)$$

The first fact about the $b_{l,n,m}$ coefficients can be determined simply from the choice that $T_{l,n}$ are real and $Y_{l,-m}(\theta,\phi) = (-1)^m Y^*_{l,m}(\theta,\phi)$ [8, **Eq.** 3.541:

Fact 1 *For* each $l = 0, 1, \ldots,$ n $= 0, \ldots, N_l,$ and m $= -l, \ldots, +l,$

$$b_{l,n,m} = (-1)^m b^*_{l,n,-m}$$

Proof: Since $T_{l,n}$ are real, it follows that

$$\begin{aligned}
0 &= T_{l,n}(\theta,\phi) - T^*_{l,n}(\theta,\phi) \\
&= \sum_{m=-l}^{+l} b_{l,n,m} Y_{l,m}(\theta,\phi) - \sum_{m=-l}^{+l} b^*_{l,n,m} Y^*_{l,m}(\theta,\phi) \\
&= \sum_{m=-l}^{+l} b_{l,n,m} Y_{l,m}(\theta,\phi) - \sum_{m=-l}^{+l} b^*_{l,n,m}(-1)^m Y_{l,-m}(\theta,\phi) \\
&= \sum_{m=-l}^{+l} b_{l,n,m} Y_{l,m}(\theta,\phi) - \sum_{m=-l}^{+l} b^*_{l,n,-m}(-1)^m Y_{l,m}(\theta,\phi) \\
&= \sum_{m=-l}^{+l} \left[b_{l,n,m} - b^*_{l,n,-m}(-1)^m\right] Y_{l,m}(\theta,\phi).
\end{aligned}$$

Multiply by $Y^*_{l',m'}(\theta,\phi)$, integrate over solid angles in θ and ϕ (do), and use the orthonormality of the spherical harmonics to obtain (after renaming the indices $l' \to l$ and $m' \to m$) the result that $0 = b_{l,n,m} - b^*_{l,n,-m}(-1)^m$ as desired. □

The second fact relates the orthonormality of the $b_{l,n,m}$ coefficients to the orthonormality of the $T_{l,n}$:

Fact 2 $T_{l,n}$ ($l = 0, 1, \ldots,$ n $= 0, \ldots, N_l - 1$) are *orthonormal* if and only *if*

$$\sum_{m=-l}^{+l} b_{l,n,m} b^*_{l,n',m} = \delta_{n,n'}.$$

Proof: First note that $T_{l,n}$ and $T_{l',n'}$ are automatically orthonormal for $l \neq l'$ because $Y_{\cdot,\cdot}$ are orthonormal and $T_{l,n}$ and $T_{l',n'}$ are constructed from $Y_{l,m}$ for m $= -l, \ldots, +l$ and $Y_{l',m}$ for m $= -l', \ldots, +l'$ respectively. So it remains only to consider orthonormality of the $T_{l,n}$ functions within a fixed l. The equivalence between orthonormality of the $T_{l,n}$ functions within a fixed l and the orthonormality of the $b_{l,n,m}$ coefficients within a fixed l follows from the following equalities:

$$\begin{aligned}
\int T^*_{l,n}(\theta,\phi) T_{l,n'}(\theta,\phi) d\Omega &= \int \left[\sum_{m=-l}^{+l} b_{l,n,m} Y_{l,m}(\theta,\phi)\right]^* \left[\sum_{m'=-l}^{+l} b_{l,n',m'} Y_{l,m'}(\theta,\phi)\right] d\Omega \\
&= \sum_{m=-l}^{+l} \sum_{m'=-l}^{+l} b^*_{l,n,m} b_{l,n',m'} \int Y^*_{l,m}(\theta,\phi) Y_{l,m'}(\theta,\phi) d\Omega \\
&= \sum_{m=-l}^{+l} \sum_{m'=-l}^{+l} b^*_{l,n,m} b_{l,n',m'} \delta_{m,m'} \\
&= \sum_{m=-l}^{+l} b^*_{l,n,m} b_{l,n',m}.
\end{aligned}$$

□

3 The Approach for Computing $b_{l,n,m}$

Many authors compute the $b_{l,n,m}$ coefficients based on Theorem 2. More specifically, Theorem 2 implies that

$$b_{l,n,m} = \sum_{m'=-l}^{+l} D_{l,m,m'}(\alpha, \beta, \gamma) b_{l,n,m'} \tag{5}$$

where D is the Wigner's matrix associated with any one of the 60 rotational symmetries of the icosahedron. Study of Eq. 5 was successful in obtaining a few low-order icosahedral harmonics. however, due to the relatively complicated expression of the Wigner coefficients;, it was not able to give a general expression for the $b_{l,n,m}$ coefficients for any given order l.

In this paper we adopt a different approach. Specifically, we express an icosahedrally symmetric function in terms of both spherical harmonics $Y_{l,m}(\theta, \phi)$ and the unknown icosahedral harmonics $T_{l,n}(\theta, \phi)$ and then, by comparing the expansion coefficients, we extract the $b_{l,n,m}$ coefficients. The natural choice for the function is the icosahedrally symmetric delta function because a delta function contains finite components at all spatial frequencies and therefore the expansion of the icosahedrally symmetric delta function will involve all of the TI,,. In more detail, the plan has the following steps:

1. Express an icosahedrally symmetric delta function in terms of $Y_{l,m}(\theta, \phi)$ and in terms of $T_{l,n}(\theta, \phi)$.
2. Equate the two expansions.
3. From the resulting equality extract a bilinear equation for the $b_{l,n,m}$ coefficients where the equation is parameterized by the location on the sphere, denoted by (θ_0, ϕ_0), of the delta function. This equation must be satisfied for any choice of (θ_0, ϕ_0).
4. Express both sides of the bilinear equation in a Fourier series in ϕ_0 and a. Taylor series in θ_0 which gives an equality between two doublely-infinite sums. Corresponding coefficients in the two sums must be equal.
5. By equating corresponding coefficients of $\theta_0^j e^{ik\phi_0}$ for certain (j,k), derive a second system of bilinear equations for the $b_{l,n,m}$ coefficients.
6. Derive a recursive solution for the second set of bilinear equations.
7. With the aid of *Mathematica*, solve the recursions to give exact values for the $b_{l,n,m}$ coefficients.

4 The Fundamental Bilinear Equation for $b_{l,n,m}$

For our concrete calculations, we choose the coordinate system (Figure 1) used by Altmann [1] and La Porte [12] in which the z axes passes through two opposite vertices and the xz plane includes one edge of the icosahedron. Let (θ_0, ϕ_0) be the (arbitrary) spherical coordinates: of a delta function within the first asymmetric unit. Let $\{(\theta_k, \phi_k) : k = 1, 2, \ldots, 59\}$ be spherical coordinates of delta. functions in the remaining 59 asymmetric units generated by applying rotations in the icosahedral group. The locations of these additional 59 delta functions are given by Fact 3:

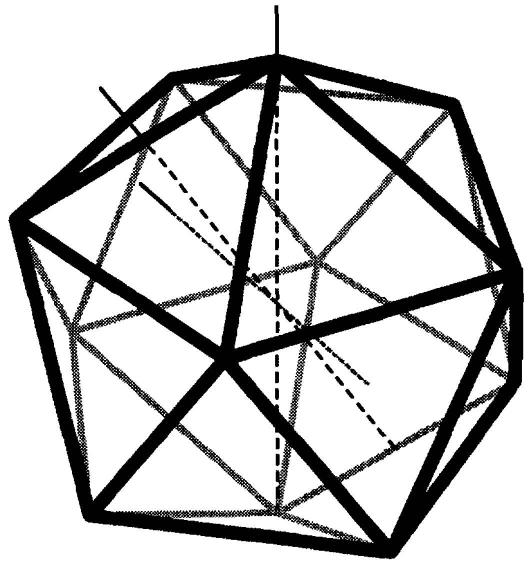

Figure 1: An icosahedron and 3 of its axes of rotational symmetry. One axis of each type of rotational symmetry—5-fold, 3-fold, and 2-fold—is shown.

Fact *3 As a function of the parameters θ_0 and ϕ_0, the 60 symmetry-related positions on the unit sphere are:*

$$\{(\theta_k,\phi_k):k=0,1,\ldots,59\}=\{(\theta_0,\phi_k):k=0,1,\ldots,4\}\bigcup(\bigcup_{n=0}^{4}\{(\gamma_n,\alpha_n+k\frac{2\pi}{5}):k=0,1,\ldots,4\})$$
$$\bigcup(\bigcup_{n=0}^{4}\{(\pi-\gamma_n,\pi-\alpha_n+k\frac{2\pi}{5}):\mathrm{k}=0,1,\ldots,4))\bigcup\{(\pi-\theta_0,\pi-\phi_k):\mathrm{k}=0,1,\ldots,4\}$$

where ϕ_k,γ_k, and α_k are related to θ_0 and ϕ_0 by

$$\begin{aligned}\phi_k &= \phi_0+k\frac{2\pi}{5}\\ \cos\gamma_k &= \cos\beta\cos\theta_0+\sin\beta\sin\theta_0\cos\phi_k\\ \sin\alpha_k &= -\frac{\sin\theta_0\sin\phi_k}{\sin\gamma_k} \qquad k=0,1,\ldots,4\end{aligned} \tag{6}$$

and $\beta=\arctan 2$.

Proof: Use the geometric relations of the icosahedron. □

Explicitly, the icosahedral delta function is

$$\Delta(\theta_0,\phi_0;\theta,\phi)=\frac{1}{60}\sum_{k=0}^{59}\delta(\cos\theta-\cos\theta_k)\delta(\phi-\phi_k)$$

where $\delta(x)$ is the usual Dirac delta function, and (θ_k,ϕ_k) are locations of the delta functions obeying icosahedral symmetry. Obviously,

$$\int\Delta(\theta_0,\phi_0;\theta,\phi)\mathrm{d}\Omega_{\theta,\phi}=1.$$

The following fact describes the relationship between **A** and the $T_{l,n}$:

Fact 4 The functions $T_{l,n}$ ($l = 0, 1, \ldots$, n = $0, \ldots, N_l$) are a complete orthonormal basis for smooth icosahedrally-symmetric functions on the sphere if and only if

$$\Delta(\theta_0, \phi_0; \theta, \phi) = \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} T_{l,n}(\theta_0, \phi_0) T_{l,n}(\theta, \phi). \tag{7}$$

Proof: First assume that $T_{l,n}$ are a complete orthonormal basis. **Eq.** 7 follours from the follo - ing calculations: Let $f(\theta, +)$ be a smooth icosahedrally-symmetric function on the sphere. By completeness it follows that

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} f_{l,n} T_{l,n}(\theta, \phi) \tag{8}$$

and by orthonormality that

$$f_{l,n} = \int T^*_{l,n}(\theta, \phi) f(\theta, \phi) \mathrm{d}\Omega. \tag{9}$$

Use **Eq.** 9 in **E**q. 8 to get

$$\begin{aligned} f(\theta, \phi) &= \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} \left[\int T^*_{l,n}(\theta', \phi') f(\theta', \phi') \mathrm{d}\Omega' \right] T_{l,n}(\theta, \phi) \\ &= \int \left[\sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} T^*_{l,n}(\theta', \phi') T_{l,n}(\theta, \phi) \right] f(\theta', \phi') \mathrm{d}\Omega' \end{aligned}$$

w

which implies that

$$\Delta(\theta', \phi'; \theta, \phi) = \sum_{l=0}^{\infty} \sum_{n=O}^{N_l-1} T^*_{l,n}(\theta', \phi') T_{l,n}(\theta, \phi)$$

from which **Eq.** 7 follows since the $T_{l,n}$ are real.

Seconcl, assume the A formula. Let $f(\theta, \phi)$ be a smooth icosahedrally-symmetric function on the sphere. The A formula implies completeness by the following calculation:

$$\begin{aligned} f(\theta, \phi) &= \int \Delta(\theta, \phi; \theta', \phi') f(\theta', \phi') \mathrm{d}\Omega' \\ &= \int \left[\sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} T_{l,n}(\theta, \phi) T_{l,n}(\theta', \phi') \right] f(\theta', \phi') \mathrm{d}\Omega' \\ &= \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} \left[\int T_{l,n}(\theta', \phi') f(\theta', \phi') \mathrm{d}\Omega' \right] T_{l,n}(\theta, \phi) \\ &= \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} f_{l,n} T_{l,n}(\theta, \phi). \end{aligned} \tag{10}$$

In order to prove that the $T_{l,n}$ are orthonormal, apply **Eq.** 10 to $f(\theta, \phi) = T_{l',n'}(\theta, \phi)$ to get

$$T_{l',n'}(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} \left[\int T_{l,n}(\theta', \phi') T_{l',n'}(\theta', \phi') \mathrm{d}\Omega' \right] T_{l,n}(\theta, \phi)$$

which implies that

$$0 = \sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} \left[\delta_{l,l'} \delta_{n,n'} - \int T_{l,n}(\theta', \phi') T_{l',n'}(\theta', \phi') \mathrm{d}\Omega' \right] T_{l,n}(\theta, \phi). \tag{11}$$

By construction (Eq. 2) and the orthonormality of $Y_{l,m}$, it follows that $\int T_{l,n}T_{l',n'}\mathrm{d}\Omega = \int T^*_{l,n}T_{l',n'}\mathrm{d}\Omega = \delta_{l,l'}\eta(n,n')$ for some function η. Therefore, Eq. 11 simplifies to

$$0 = \sum_{n=0}^{N'_l-1}\left[\delta_{n,n'} - \int T_{l',n}(\theta',\phi')T_{l',n'}(\theta',\phi')\mathrm{d}\Omega'\right]T_{l,n}(\theta,\phi).$$

By the linear independence of the $T_{l,n}$ for fixed l it follows that the bracket is zero for each n. Therefore, the $T_{l,n}$ are orthonormal. □

The following fact is used in the simplification of the the bilinear equation determining the $b_{l,n,m}$ coefficients.

Fact 5 For *any* θ_0 *and* ϕ_0,

$$\sum_{k=0}^{59} Y_{l,m}(\theta_k,\phi_k) = \begin{cases} 5N_{l,m}\Big[P_{l,m}(\cos\theta_0)\left(e^{im\phi_0}+(-1)^l e^{-im\phi_0}\right) \\ \quad + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)\left(e^{im\alpha_k}+(-1)^l e^{-im\alpha_k}\right)\Big], & m=5\mu \text{ with } \mu\in\mathcal{Z} \\ 0, & \text{otherwise}\end{cases}$$

where $\mathcal{Z}$ *are* the integers.

Proof:

$$\begin{aligned}
\sum_{k=0}^{59} Y_{l,m}(\theta_k,\phi_k) &= \sum_{k=0}^{59} N_{l,m}P_{l,m}(\cos\theta_k)e^{im\phi_k} \\
&= N_{l,m}\sum_{k=0}^{29}\left[P_{l,m}(\cos\theta_k)e^{im\phi_k} + P_{l,m}(\cos(\pi-\theta_k))e^{im(\pi-\phi_k)}\right] \\
&= N_{l,m}\sum_{k=0}^{29}\left[P_{l,m}(\cos\theta_k)e^{im\phi_k} + P_{l,m}(-\cos\theta_k)(-1)^m e^{-im\phi_k}\right] \\
&= N_{l,m}\sum_{k=0}^{29}\left[P_{l,m}(\cos\theta_k)e^{im\phi_k} + (-1)^{l+m}P_{l,m}(\cos\theta_k)(-1)^m e^{-im\phi_k}\right] \\
&= N_{l,m}\sum_{k=0}^{29}P_{l,m}(\cos\theta_k)\left[e^{im\phi_k}+(-1)^l e^{-im\phi_k}\right] \\
&= N_{l,m}\sum_{q=0}^{5}\sum_{p=0}^{4}P_{l,m}(\cos\theta_{5q+p})\left[e^{im\phi_{5q+p}}+(-1)^l e^{-im\phi_{5q+p}}\right] \\
&= N_{l,m}\sum_{q=0}^{5}\sum_{p=0}^{4}P_{l,m}(\cos\theta_{5q})\left[e^{im(\phi_{5q}+p\frac{2\pi}{5})}+(-1)^l e^{-im(\phi_{5q}+p\frac{2\pi}{5})}\right] \\
&= N_{l,m}\sum_{q=0}^{5}P_{l,m}(\cos\theta_{5q})\left[e^{im\phi_{5q}}\sum_{p=0}^{4}e^{imp\frac{2\pi}{5}}+(-1)^l e^{-im\phi_{5q}}\sum_{p=0}^{4}e^{-imp\frac{2\pi}{5}}\right] \\
&= \begin{cases}5N_{l,m}\sum_{q=0}^{5}P_{l,m}(\cos\theta_{5q})\left[e^{im\phi_{5q}}+(-1)^l e^{-im\phi_{5q}}\right], & m=5\mu \text{ with } \mu\in\mathcal{Z} \\ 0, & \text{otherwise}\end{cases} \qquad (12)
\end{aligned}$$

since

$$\sum_{p=0}^{4} e^{\pm imp\frac{2\pi}{5}} = \begin{cases} 5, & m=5\mu \text{ with } \mu\in\mathcal{Z} \\ 0, & \text{otherwise}\end{cases}$$

Finally, the conclusion follows from using Fact **3** in Eq. 12. □

Fact 6 is the fundamental equation for determining the $b_{l,n,m}$ coefficients:

Fact 6 The $b_{l,n,m}$ *($l = 0, 1, ..;$ $n = 0, \ldots, N_l - 1$; $m = -l, \ldots, +l$) coefficients* satisfy each of the following equivalent relationships for arbitrary θ_0 and ϕ_0:

$$\sum_{n=0}^{N_l-1} b_{l,n,m} T_{l,n}(\theta_0, \phi_0) = \frac{1}{60} \sum_{k=0}^{59} Y^*_{l,m}(\theta_k, \phi_k) \tag{13}$$

$$\sum_{n=0}^{N_l-1} b_{l,n,m} T_{l,n}(\theta_0, \phi_0) = \begin{cases} \frac{1}{12} N_{l,m} \Big[P_{l,m}(\cos\theta_0) \left(e^{im\phi_0} + (-1)^l e^{-im\phi_0}\right) \\ \quad + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k) \left(e^{im\alpha_k} + (-1)^l e^{-im\alpha_k}\right) \Big]^*, & m = 5\mu \text{ with } \mu \in \mathbb{Z} \\ 0, & \text{otherwise} \end{cases} \tag{14}$$

$$\sum_{n=0}^{N_l-1} \sum_{m'=-l}^{+l} b_{l,n,m'} b_{l,n,m} Y_{l,m'}(\theta_0, \phi_0) = \frac{1}{60} \sum_{k=0}^{59} Y_{l,m}(\theta_k, \phi_k) \tag{15}$$

for any $l = 0, 1, \ldots$ *and* $m = -l, \ldots, +l$.

Proof: Write $\Delta(\theta_0, \phi_0; \theta, \phi)$ in terms of both icosahedral harmonics and spherical harmonics and equate the two expressions:

$$\sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} T_{l,n}(\theta_0, \phi_0) T_{l,n}(\theta, \phi) = \Delta(\theta_0, \phi_0; \theta, \phi) = \frac{1}{60} \sum_{k=0}^{59} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k, \phi_k) Y_{l,m}(\theta, \phi). \tag{16}$$

Substitute Eq. 2 into Eq. 16 to obtain

$$\sum_{l=0}^{\infty} \sum_{n=0}^{N_l-1} \sum_{m=-l}^{+l} T_{l,n}(\theta_0, \phi_0) b_{l,n,m} Y_{l,m}(\theta, \phi) = \frac{1}{60} \sum_{k=0}^{59} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k, \phi_k) Y_{l,m}(\theta, \phi). \tag{17}$$

Multiply Eq. **17** by $Y^*_{l',m'}(\theta, \phi)$, integrate over solid angles in θ and ϕ ($d\Omega_{\theta,\phi}$), and use the orthonormality of the spherical harmonics to obtain (after renaming the indices $l' \rightarrow l$, $m' \rightarrow m$) Eq. **13.** Use Fact 5 in Eq. **13** to obtain Eq. **14.** Use Eq. 2 in Eq. **13** to obtain Eq. **15.** □

The purpose of Eq. **15** is to demonstrate explicitly the bilinear nature of the equations. Notice, for example, from Eq. 15, that there is no coupling between different values of l.

From Eq. **14** we immediately obtain the following properties of the $b_{l,n,m}$ coefficients:

Fact 7 *If* $m \neq 5\mu$ with $\mu \in \mathbb{Z}$ then $b_{l,n,m} = 0$.

Proof: Multiply Eq. **14** by $T^*_{l,n'}(\theta_0, \phi_0)$, integrate over solid angles in θ_0 and ϕ_0 ($d\Omega$), and use the orthonormality of $T_{l,n}$ (Eq. **3**) to find (after renaming the index $n' \rightarrow$ n) that $b_{l,n,m} = 0$ unless $m = 5\mu$ with $\mu \in \mathbb{Z}$. □

Fact 8 For l even, $b_{l,n,m}$ is real. For l odd, $b_{l,n,m}$ is imaginary.

Proof: For l even, the right hand side of Eq. 14 is

$$\frac{1}{6}N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos(m\phi_0)+\sum_{k=0}^{4}P_{l,m}(\cos\gamma_k)\cos(m\alpha_k)\right]$$

which is real while for l odd, the right hand side of Eq. 14 is

$$-i\frac{1}{6}N_{l,m}\left[P_{l,m}(\cos\theta_0)\sin(m\phi_0)+\sum_{k=0}^{4}P_{l,m}(\cos\gamma_k)\sin(m\alpha_k)\right]$$

which is imaginary. Multiply Eq. 14 by $T^{*}_{l,n'}(\theta_0,\phi_0)$ which is real, integrate over solid angles in θ_0 and ϕ_0 ($d\Omega$), and use the orthonormality of $T_{l,n}$ (Eq. 3) to find (after renaming; the index $n' \longrightarrow n$) that $b_{l,n,m} = \kappa$ where $\kappa \in$ R (R is the real numbers) when l is even and $b_{l,n,m} = i\kappa'$ where $\kappa' \in \mathcal{R}$ when l is odd. Therefore the conclusion follows. □

Fact 9 $b_{l,n,m} = b_{l,n,-m}(-1)^{l+m}$.

Proof: Facts 1 and 8 imply, for l even, that $b_{l,n,m} = (-1)^m b_{l,n,-m}$ and, for l odd, that $b_{l,n,m} = -(-1)^m b_{l,n,-m}$. By combining these two cases, the conclusion follows. □

Fact 10 *For l odd, $b_{l,n,0} = 0$.*

Proof: Take m = 0 in Fact 9. □

Fact 11

$$T_{l,n}(\theta,+) = \begin{cases} \sum_{m=0}^{+l}\frac{2}{1+\delta_{m,0}}N_{l,m}b_{l,n,m}P_{l,m}(\cos\theta)\cos m\phi & l \text{ even} \\ \\ \sum_{m=1}^{+l}2N_{l,m}ib_{l,n,m}P_{l,m}(\cos\theta)\sin m\phi & l \text{ odd} \end{cases}$$

Proof: By using Fact 9 and $Y_{l,-m}(\theta,\phi) = (-1)^m Y^{*}_{l,m}(\theta,\phi)$ [8, Eq. 3.54] to combine the complex exponential terms in Eq. 2 we get, for l even, that

$$\begin{aligned} T_{l,n}(\theta,\phi) &= b_{l,n,0}N_{l,0}P_l(\cos\theta)+\sum_{m=1}^{+l}2b_{l,n,m}N_{l,m}P_{l,m}(\cos 0)\cos m\phi \\ &= \sum_{m=0}^{+l}\frac{2}{1+\delta_{m,0}}N_{l,m}b_{l,n,m}P_{l,m}(\cos\theta)\cos m\phi. \end{aligned}$$

The same calculation for l odd, using also Fact 10, gives the result that

$$T_{l,n}(\theta,\phi) = \sum_{m=1}^{+l}2N_{l,m}ib_{l,n,m}P_{l,m}(\cos\theta)\sin m\phi.$$

□

Fix the value of l. To this point, the only restriction on $T_{l,n}$ for n $= 0,\ldots,N_l-1$ which we have employed is that the functions must be orthonormal. We now add an additional restriction in terms of the $b_{l,n,m}$. Here, and throughout the remainder of the paper, let $\lfloor x \rfloor$ denote the integer part of x.

Fact 12 *The $b_{l,n,m}$ coefficients can be chosen so that*

$$t_{l,n} = \min\{m \in \{0,\ldots,l\} : b_{l,n,m} \neq 0\}$$

satisfy

$$t_{l,0} < t_{l,1} < \ldots < t_{l,N_l-1} \tag{18}$$

where the inequalities are strict. In a basis satisfying Eq. 18, it follows that $b_{l,n,m} = 0$ for $m < 5n$.

Proof: We need only consider $m = 5\mu$ for $\mu = 0, \ldots, \lfloor l/5 \rfloor$ by Facts 7 and 9. Construct the matrix

$$\begin{bmatrix} b_{l,0,0} & b_{l,0,5} & \cdots & b_{l,0,\lfloor l/5 \rfloor 5} \\ \vdots & \vdots & & \vdots \\ b_{l,N_l-1,0} & b_{l,N_l-1,5} & \cdots & b_{l,N_l-1,\lfloor l/5 \rfloor 5} \end{bmatrix}$$

which is full rank (rank N_l) because the $b_{l,n,m}$ are orthonormal (Fact 2). Determine the transformation to an intermediate basis which satisfies Eq. 18 by applying Gaussian elimination. However, the intermediate basis need not be an orthonormal basis. Therefore, apply Gram-Schmidt orthogonalization, starting with the N_l th row, to transform to an orthonormal basis while still satisfying Eq. 18. The final claim (i.e., $b_{l,n,m} = 0$ for $m < 5n$) follows from the strict inequalities and Fact 7. □

We now modify the $b_{l,n,m}$ notation slightly to incorporate results to this point. First, Facts 9 and 11 imply that the icosahedral harmonics are completely determined by the $b_{l,n,m}$ coefficients for which $m \geq 0$. Therefore, $b^{\text{new}}_{l,n,m}$ is only defined for $m \geq 0$ and in the remainder of the paper, $m \geq 0$ and $m' \geq 0$ unless otherwise designated. Second, we absorb the "i" that occurs for l odd into the definition of $b^{\text{new}}_{l,n,m}$ so that $b^{\text{new}}_{l,n,m}$ is always real (Fact 8). In summary, the new definition, for $l = 0, 1, \ldots, n = 0, \ldots, N_l - 1$, and $m = 0, \ldots, l$, is

$$b^{\text{new}}_{l,n,m} = \begin{cases} b_{l,n,m}, & l \text{ even} \\ i b_{l,n,m}, & l \text{ odd} \end{cases}$$

For the remainder of this paper we will use only the new notation and therefore will not include the superscript "new". The l odd case will not appear until Fact 18.

The remainder of the calculation of the $b_{l,n,m}$ coefficients is the same in plan but different in details for l even versus l odd. We will show the l even case and then state the results for l odd.

Fact 13 *For l even and $m = 5\mu$ with $\mu = 0, \ldots, \lfloor l/5 \rfloor$, the $b_{l,n,m}$ coefficients satisfy the following relationship for arbitrary θ_0 and ϕ_0:*

$$\begin{aligned} &\sum_{m'=0}^{l} \sum_{n=0}^{\min(N_l-1,\lfloor m/5 \rfloor,\lfloor m'/5 \rfloor)} b_{l,n,m} \frac{2}{1+\delta_{m',0}} N_{l,m'} b_{l,n,m'} P_{l,m'}(\cos\theta_0) \cos m'\phi_0 \\ = &\ \frac{1}{6} N_{l,m} \left[P_{l,m}(\cos\theta_0) \cos m\phi_0 + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k) \cos m\alpha_k \right] \end{aligned} \tag{19}$$

Proof: The current fact is a specialization of Fact 6. Evaluate Fact 11 at $(\theta, \phi) = (\theta_0, \phi_0)$ and apply Fact 12 to get

$$T_{l,n}(\theta_0, \phi_0) = \sum_{m'=5n}^{+l} \frac{2}{1+\delta_{m',0}} N_{l,m'} b_{l,n,m'} P_{l,m'}(\cos\theta_0) \cos m'\phi_0.$$

Use this result in the left hand side of Eq. 14 and l even on the right hand side of Eq. 14 to get

$$\sum_{n=0}^{N_l-1} b_{l,n,m} \sum_{m'=5n}^{+l} \frac{2}{1+\delta_{m',0}} N_{l,m'} b_{l,n,m'} P_{l,m'}(\cos\theta_0)\cos m'\phi_0$$
$$= \frac{1}{6} N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\phi_0 + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)\cos m\alpha_k\right].$$

Rewrite the summations using the equality

$$\sum_{n=0}^{N_l-1}\sum_{m'=5n}^{+l} = \sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m'/5\rfloor)}$$

to find that

$$\sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m'/5\rfloor)} b_{l,n,m}\frac{2}{1+\delta_{m',0}} N_{l,m'} b_{l,n,m'} P_{l,m'}(\cos\theta_0)\cos m'\phi_0$$
$$= \frac{1}{6} N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\phi_0 + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)\cos m\alpha_k\right].$$

Finally, use Fact 12 applied to the $b_{l,n,m}$ factor to demonstrate the claim. □

5 Series Expansions

For each l, Eq. 19 represents a system of equations (indexed by m) for the $b_{l,\cdot,\cdot}$ coefficients which must be satisfied for any choice of θ_0 and ϕ_0. We are not able to solve these systems directly. Therefore we express the functional dependence on θ_0 and ϕ_0 of both the right and left hand sides as infinite series and equate the coefficients of corresponding terms on the right and left hand sides in order to derive new systems of equations. Possible choices include Fourier series and Taylor series and, especially for the Taylor series, possible variables include θ_0 and $\cos\theta_0$. Because of the dependence of γ_k and α_k on θ_0 and ϕ_0, the calculations are complicated and the choice we were able to pursue successfully was a Fourier series in ϕ_0 (i.e., $e^{ik\phi_0}$) and a Taylor series in θ_0 (i.e., θ_0^k). In fact, we are not able to compute all of the coefficients in the Fourier-Taylor expansion but only the coefficients of terms like $\theta_0^m e^{\pm im\phi_0}$. It turns out that equating corresponding coefficients of this type leads to systems of equations that can be solved recursively. The computation of these coefficients requires some apparatus which we now develop. Any alternative approach which computes the coefficients of the terms $\theta_0^m e^{\pm im\phi_0}$ will lead to the same results.

5.1 Definitions and Abstract Results for $\mathcal{P}$ and Q

Definition 1 *Let $S = [0,a]\times[0,2\pi)$ be the sphere and **S** be a vector space over the complex field of smooth complex-valued functzons on S.*

Definition 2 *The operator $\mathcal{Z}$ from functions f in **S** to complex-valued sequences d on $\mathcal{Z}\times(\mathcal{Z}^+\cup\{0\})$ is defined by*

$$d_{m,k} = k!\left(\frac{d^k}{d\theta^k}\frac{1}{2\pi}\int_0^{2\pi} f(\theta,\phi)e^{-im\phi}d\phi\right)\bigg|_{\theta=0} \quad \textit{for } m=\ldots,-1,0,+1,\ldots \textit{ and } k=0,1,.$$

where $\mathcal{Z}^+$ are the nonnegative integers.

These are the coefficients of the Fourier-Taylor expansion.

Definition 3 *The operator Z^{-1} from complex-valued sequences d on $2 \times (\mathcal{Z}^+ \cup \{0\})$ to functions f in S is defined by*

$$f(\theta,\phi) = \sum_{m=-\infty}^{cc} \sum_{k=|m|}^{\infty} d_{m,k}\theta^k e^{im\phi} \text{ for } (\theta,\phi) \in S.$$

Notice that $k \geq |m|$ not $k \geq 0$

Definition 4 *The function space $\mathcal{P}$ is those functions $f \in S$ such that if $d = Z[f]$ then $f = Z^{-1}[d]$.*

The name "$\mathcal{P}$" comes from "Platonic." In the following, c_1 and c_2 are complex-valued constants.

Property 1 *$\mathcal{P}$ is a subspace of S, that is, if $f_1 \in \mathcal{P}$ and $f_2 \in \mathcal{P}$ then $f = c_1 f_1 + c_2 f_2 \in \mathcal{P}$. It follows that if $N \in \mathcal{Z}^+$ is finite and $f_k \in \mathcal{P}$ for $k = 1, \ldots, N$ then $f = \sum_{k=1}^{N} c_k f_k \in$ P.*

Proof: Let $f_i \in$ P, $d_1 = Z[f_1]$, $f_2 \in \mathcal{P}$, $d_2 = Z[f_2]$, and $f = c_1 f_1 + c_2 f_2$. Then, by direct computatiori from the definition of Z (Definition 2), $d = Z[f] = c_1 d_1 + c_2 d_2$. Therefore, by direct computation from the definition of Z^{-1} (Definition 3), $Z^{-1}[d] = c_1 f_1 + c_2 f_2 = f$ so that f is in $\mathcal{P}$. □

Definition 5 *Let $f \in$ P with $d = Z[f]$. The operator Q from $\mathcal{P}$ to $\mathcal{P}$ is defined by*

$$Q[f(\theta,\phi)] = \sum_{m=-\infty}^{+\infty} d_{m,|m|}\theta^{|m|}e^{im\phi}.$$

For example, $Q[l + 8 + \theta^2 \sin 2\phi] = 1 + \theta^2 \sin 24$.

The following properties describe important abstract characteristics of functions in $\mathcal{P}$ and the result of applying Q.

Property 2 *If $f \in \mathcal{P}$ then $Q[Q[f]] = Q[f]$.*

Proof: This result follows immediately from the definition of Q. □

Property 3 *Q is linear: $Q[c_1 f_1 + c_2 f_2] = c_1 Q[f_1] + c_2 Q[f_2]$. It follows that if $N \in \mathcal{Z}^+$ is finite and $f_k \in \mathcal{P}$ for $k = 1, \ldots, N$ then $Q[\sum_{k=1}^{N} c_k f_k] = \sum_{k=1}^{N} c_k Q[f_k]$.*

Proof: Let

$$f_1(\theta,\phi) = \sum_{m=-\infty}^{\infty} \sum_{k=|m|}^{\infty} d_{m,k}^{(1)}\theta^k e^{im\phi} \tag{20}$$

$$f_2(\theta,\phi) = \sum_{m=-\infty}^{\infty} \sum_{k=|m|}^{\infty} d_{m,k}^{(2)}\theta^k e^{im\phi}. \tag{21}$$

Since P is a subspace (Property 1), $c_1 f_1 + c_2 f_2 \in \mathcal{P}$. Furthermore,

$$\begin{aligned} Q[c_1 f_1(\theta,\phi) + c_2 f_2(\theta,\phi)] &= \sum_{m=-\infty}^{\infty} \left(c_1 d_{m,|m|}^{(1)} + c_2 d_{m,|m|}^{(2)}\right)\theta^{|m|}e^{im\phi} \\ &= c_1 Q[f_1(\theta,\phi)] + c_2 Q[f_2(\theta,\phi)]. \end{aligned}$$

Property 4 *If* $f_1 \in \mathcal{P}$ *and* $f_2 \in \mathcal{P}$*, then* $f_1 f_2 \in \mathcal{P}$ *and* $Q[f_1 f_2] = Q[Q[f_1]Q[f_2]]$. *It follows that if* $N \in \mathcal{Z}^+$ *is finite and* $f_k \in \mathcal{P}$ *for* $k = 1, \ldots, N$ *then* $\prod_{k=1}^{N} f_k \in \mathcal{P}$ *and* $Q\left[\prod_{k=1}^{N} f_k\right] = Q\left[\prod_{k=1}^{N} Q[f_k]\right]$.

Proof: See Appendix *B*. □

Property 5 *If* g *is a polynomial,* $g(x) = \sum_{k=0}^{N} g_k x^k$*, and* $f \in \mathcal{P}$*, then* $g(f) \in \mathcal{P}$ *and* $Q[g(f)] = Q[g(Q[f])]$.

Proof: This result is a corollary of Properties 3 and 4. □

Conjecture 1 *If* g *is a suitable function and* $f \in \mathcal{P}$*, then* $g(f) \in \mathcal{P}$ *and* $Q[g(f)] = Q[g(Q[f])]$

If g is a polynomial then this conjecture is exactly Property 5. We have not been able to extend the result to more general functions g. Difficulties include the fact that Q, viewed as a operator from $\mathcal{P}$ to $\mathcal{P}$, is not continuous for square integrable functions on the sphere (Appendix C).

Property 6 *If* $f \in \mathcal{P}$ *and non-zero, then* $1/f \in \mathcal{P}$. *Furthermore,* $Q[1/f] = Q[1/Q[f]]$

Proof: This is a special case of Conjecture 1. □

Property 7 *If* $f_1 \in \mathcal{P}$, $f_2 \in \mathcal{P}$*, and* f_2 *is non-zero, then* $f_1/f_2 \in \mathcal{P}$. *Furthermore,* $Q[f_1/f_2] = Q[Q[f_1]/Q[f_2]]$.

Proof That $f_1/f_2 \in \mathcal{P}$ follows immediately from Properties 6 and 4. The remaining claim follows from the following equalities:

$$\begin{aligned}
Q\left[\frac{f_1}{f_2}\right] &= Q\left[Q[f_1]Q\left[\frac{1}{f_2}\right]\right] && \text{by Property 4} \\
&= Q\left[Q[f_1]Q\left[\frac{1}{Q[f_2]}\right]\right] && \text{by Property 6} \\
&= Q\left[Q[Q[f_1]]Q\left[\frac{1}{Q[f_2]}\right]\right] && \text{by Property 2} \\
&= Q\left[Q\left[Q[f_1]\frac{1}{Q[f_2]}\right]\right] && \text{by Property 4} \\
&= Q\left[\frac{Q[f_1]}{Q[f_2]}\right] && \text{by Property 2.}
\end{aligned}$$

□

Conjecture 2 *If* $f_k \in \mathcal{P}$ *for* $k = 1, 2, \ldots$*, then* $\sum_{k=0}^{\infty} f_k \in \mathcal{P}$ *and* $Q\left[\sum_{k=0}^{\infty} f_k\right] = \sum_{k=0}^{\infty} Q[f_k]$.

For finite sums this is a combination of Properties 1 and 3. A proof for infinite sums requires a more precise definition of $\mathcal{P}$ which will be chosen in a way that is convenient for the proof of Conjecture 1.

5.2 Concrete Results for $\mathcal{P}$ and Q

We now describe several concrete properties.

Property 8 The spherical harmonic $Y_{l,m}(\theta,\phi)$ is in $\mathcal{P}$ and

$$Q[Y_{l,m}(\theta,\phi)] = N_{l,m} g_{l,m} \theta^{|m|} e^{im\phi}$$

where

$$g_{l,m} = \begin{cases} (-1)^m \frac{(l+m)!}{2^m (l-m)! m!} & m \geq 0 \\ \frac{2^m}{(-m)!} & m < 0 \end{cases} .$$

Proof: Since $P_{l,m}(\cos 8)$ is finite at $\theta = 0$ (in fact $P_{l,m}(1) = \delta_{m,0}$), it follows that, the Laurent series around $\theta = 0$ of $P_{l,m}(\cos\theta)$ has no negative powers of 8:

$$P_{l,m}(\cos\theta) = \sum_{k=0}^{\infty} h_{l,m,k}\theta^k$$

We shall show that $h_{l,m,k} = 0$ for k < $|m|$ and $h_{l,m,|m|} = g_{l,m}$.

The integral representation (Laplace integral) of the associated Legendre polynomials is [5, **Eq.** 8.711-2]

$$\begin{aligned} P_{l,m}(\cos 8) &= \frac{i^m}{2} \frac{(l+m)!}{I!} \int_0^{2\pi} e^{-im\psi} [\cos\theta + i \sin\theta \cos\psi]^l d\psi \\ &= \frac{i^m}{2\pi} \frac{(l+m)!}{l!} \sum_{k=0}^{l} \binom{l}{k} \cos^{l-k}\theta i^k \sin^k\theta \int_0^{2\pi} e^{-im\psi} \cos^k\psi d\psi. \end{aligned}$$

Since

$$\int_0^{2\pi} e^{-im\psi} \cos^k \psi d\psi = 0 \quad \text{if } k < |m|$$

it follows that

$$P_{l,m}(\cos 8) = \frac{i^m}{2} \frac{(l+\mathrm{m})!}{I!} \sum_{k=|m|} \binom{l}{k} \cos^{l-k}\theta i^k \sin^k 8 \int_0^{2\pi} e^{-im\psi} \cos^k \psi d\psi. \tag{22}$$

Therefore the leading term in $P_{l,m}(\cos 8)$ is $\theta^{|m|}$, hence $Y_{l,m}(\theta,\phi)$ is in $\mathcal{P}$. Using Eq. 22 in

$$h_{l,m,|m|} = \frac{1}{|m|!} \frac{\partial^{|m|}}{\partial\theta^{|m|}} P_{l,m}(\cos\theta)\bigg|_{\theta=0}$$

we find that only the $|m|! \cos^l\theta$ subterm of the k = $|m|$ term of the summation is non zero when evaluated at $\theta = 0$ because all other terms have factors of the type $\sin^3\theta$ for $j > 0$. Therefore,

$$\begin{aligned} h_{l,m,|m|} &= \frac{i^m}{2\pi} \frac{(l+m)!}{l!} \binom{l}{|m|} i^{|m|} \int_0^{2\pi} e^{-im\psi} \cos^{|m|}\psi d\psi \\ &- \frac{i^{m+|m|}}{2\pi} \frac{(I+m)!}{(I-|m|)! 2^{|m|} |m|!} \\ &= g_{l,m}. \end{aligned}$$

Property 9 The function $P_{l,m}(\cos\theta)\cos(m\phi)$ is in $\mathcal{P}$ and

$$Q[P_{l,m}(\cos\theta)\cos(m\phi)] = g_{l,m}\theta^{|m|}\cos m\phi$$

where $g_{l,m}$ is defined in Property 8.

Proof: From Eq. 1 it follows that

$$\begin{aligned}
P_{l,m}(\cos\theta)\cos(m\phi) &= \frac{1}{N_{l,m}}\Re\{Y_{l,m}(\theta,\phi)\} \\
&= \frac{1}{2N_{l,m}}[Y_{l,m}(\theta,\phi) + Y^*_{l,m}(\theta,\phi)] \\
&= \frac{1}{2N_{l,m}}[Y_{l,m}(\theta,\phi) + (-1)^m Y_{l,-m}(\theta,\phi)]
\end{aligned}$$

and therefore $P_{l,m}(\cos\theta)\cos(m\phi) \in$ P by Properties 3 and 8. Furthermore,

$$\begin{aligned}
Q[P_{l,m}(\cos\theta)\cos(m\phi)] &= \frac{1}{2N_{l,m}}[Q[Y_{l,m}(\theta,\phi)] + (-1)^m Q[Y_{l,-m}(\theta,\phi)]] \\
&= \frac{1}{2N_{l,m}}[N_{l,m}g_{l,m}\theta^{|m|}e^{im\phi} + (-1)^m N_{l,-m}g_{l,-m}\theta^{|-m|}e^{-im\phi}] \\
&= \frac{1}{2}\theta^{|m|}[g_{l,m}e^{im\phi} + (-1)^m\frac{N_{l,-m}}{N_{l,m}}g_{l,-m}e^{-im\phi}] \\
&= g_{l,m}\theta^{|m|}\cos m\phi.
\end{aligned}$$

□

Property 10 $\sin(\phi+\Phi)$, $\cos(\phi+\Phi)$, $\theta\sin(\phi+\Phi)$, $\theta\cos(\phi+\Phi)$, and $\sin\theta\sin(+ + \Phi)$, where Φ is an *arbitrary* angle, are in $\mathcal{P}$ and

$$\begin{aligned}
Q[\sin(\phi+\Phi)] &= 0 \\
Q[\cos(\phi+\Phi)] &= 1 \\
Q[\theta\sin(\phi+\Phi)] &= \theta\sin(\phi+\Phi) \\
Q[\theta\cos(\phi+\Phi)] &= \theta\cos(\phi+\Phi) \\
Q[\sin\theta\sin(\phi+\Phi)] &= \theta\sin(\phi+\Phi) \qquad (23)
\end{aligned}$$

Proof: All claims are elementary calculations, we prove only the third. Since

$$\theta\sin(\phi+\Phi) = \left(\frac{1}{2i}e^{i\Phi}\right)\theta e^{i\phi} + \left(-\frac{1}{2i}e^{-i\Phi}\right)\theta e^{-i\phi}$$

it follows that the series has non-zero $d_{m,k}$ terms only for k = 1 and m = ±1. Since Q leaves $d_{m,k}$ terms of the form $d_{m,|m|}$, it follows that Q leaves both terms and therefore the first conclusion is verified. □

Property 11 Let m, p be *non* negative integers, m ≥ p. Let Φ be an *arbitrary* angle. *Then* $0^m\cos^{m-p}(\phi+\Phi)\sin^p(\phi+\Phi)$ is in $\mathcal{P}$ and

$$\text{QIO}^m\cos^{m-p}(\phi+\Phi)\sin^p(\phi+\Phi)] = \begin{cases} \frac{2^{1-m}(-1)^r}{1+\delta_{m,0}}\theta^m\cos m(\phi+\Phi), & p = 2r, r\in\mathcal{Z}^+ \cup \{0\} \\ 2^{1-m}(-1)^r\theta^m\sin m(+ + \Phi), & p = 2r+1, r\in\mathcal{Z}^+\cup\{0\} \end{cases}$$

Proof: The case where $m = p = 0$ is trivial. We assume $m > 0$ in the remainder of the proof.

Using the binomial theorem and the complex exponential representation of sine and cosine we obtain ($\psi \doteq \phi + \Phi$)

$$\begin{aligned}
\cos^{m-p}(\phi+\Phi)\sin^p(\phi+\Phi) &= \frac{1}{2^m i^p}(e^{i\psi}+e^{-i\psi})^{m-p}(e^{i\psi}-e^{-i\psi})^p \\
&= \frac{1}{2^m i^p}\sum_{k=0}^{m-p}\binom{m-p}{k}e^{i(m-p-2k)\psi}\sum_{k'=0}^{p}\binom{p}{k'}(-1)^{k'}e^{i(p-2k')\psi} \\
&= \frac{1}{2^m i^p}\sum_{k=0}^{m-p}\sum_{k'=0}^{p}\binom{m-p}{k}\binom{p}{k'}e^{i(m-2(k+k'))\psi}(-1)^{k'}.
\end{aligned}$$

Note that in the summands above, $0 \le k + k' \le m$. It follows that $\theta^m \cos^{m-p}(\phi+\Phi)\sin^p(\phi+\Phi)$ is in $\mathcal{P}$. Furthermore,

$$\begin{aligned}
Q[\theta^m\cos^{m-p}(\phi+\Phi)\sin^p(\phi+\Phi)] &= \frac{1}{2^m i^p}\sum_{k=0}^{m-p}\sum_{k'=0}^{p}\binom{m-p}{k}\binom{p}{k'}Q[\theta^m e^{i(m-2(k+k'))\psi}](-1)^{k'} \\
&- \frac{\theta^m}{2^m i^p}[e^{im\psi} + (- \quad] \\
&= \begin{cases} 2^{1-m}(-1)^r\theta^m\cos m(\phi+\Phi), & p=2r, r\in\mathcal{Z}, r>0 \\ 2^{1-m}(-1)^r\theta^m\sin m(\phi+\Phi), & p=2r+1, r\in\mathcal{Z}, r\ge 0 \end{cases}
\end{aligned}$$

□

Property 12 *Let m_1, m_2 be positive integers. Then the functions indicated below are in $\mathcal{P}$ and*

$$\begin{aligned}
Q[\theta^{m_1}\cos m_1(\phi+\Phi)\theta^{m_2}\cos m_2(\phi+\Phi)] &= -Q[\theta^{m_1}\sin m_1(\phi+\Phi)\theta^{m_2}\sin m_2(\phi+\Phi)] \\
&- \frac{1}{2}\theta^{m_1+m_2}\cos(m_1+m_2)(\phi+\Phi) \\
Q[\theta^{m_1}\sin m_1(\phi+\Phi)\theta^{m_2}\cos m_2(\phi+\Phi)] &= \frac{1}{2}\theta^{m_1+m_2}\sin(m_1+m_2)(\phi+\Phi).
\end{aligned}$$

Proof: All three claims are elementary calculations, we prove only the first. Since

$$\theta^{m_1}\cos m_1(\phi+\Phi)\theta^{m_2}\cos m_2(\phi+\Phi) = \theta^{m_1+m_2}\left\{\frac{1}{2}\cos[(m_1+m_2)(\phi+\Phi)] + \frac{1}{2}\cos[(m_1-m_2)(\phi+\Phi)]\right\}$$

it follows, after expanding the two cosines in terms of complex exponentials, that the functions are in $\mathcal{P}$ and

$$Q[\theta^{m_1}\cos m_1(\phi+\Phi)\theta^{m_2}\cos m_2(\phi+\Phi)] = \theta^{m_1+m_2}\frac{1}{2}\cos[(m_1+m_2)(\phi+\Phi)]$$

as claimed. □

Property 13 *The function indicated below is in $\mathcal{P}$ and*

$$Q\left[\cos(m\sin^{-1}(\frac{\theta_0\sin\phi_j}{\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}}))\right] = \sum_{p=0}^{\infty}\sum_{r=0}^{\infty}c_{p,2r}Q[\theta_0^{p+2r}\cos^p\phi_j\sin^{2r}\phi_j]$$

where $c_{p,q}$ are coefficients defined by

$$f(x,y) = \cos(m\sin^{-1}(\frac{y}{\sqrt{1-(\cos\beta+x\sin\beta)^2}})) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty}c_{p,q}x^p y^q$$

Proof: Since $\theta_0 \sin\phi_j$ and $\theta_0 \cos\phi_j$ are both in $\mathcal{P}$, the fact that the function of interest is in $\mathcal{P}$ follows from the properties in Subsection 5.1. We first note that $f(x,0)$ and $f(0,y)$ are finite, hence $f(x,y)$ can be expanded into a series of non-negative powers. Second we note that $f(x,y)$ is an even function with respect to y, i.e., $f(x,y) = f(x,-y)$, therefore $c_{p,q} = 0$ for q odd. Let $x = \theta_0 \cos\phi_j$, $y = \theta_0 \sin\phi_j$. Then

$$\begin{aligned} Q[f(x,y)] &= Q[\sum_{p=0}^{\infty}\sum_{r=0}^{\infty} c_{p,2r} x^p y^{2r}] \\ &= Q[\sum_{p=0}^{\infty}\sum_{r=0}^{\infty} c_{p,2r} (\theta_0 \cos\phi_j)^p (\theta_0 \sin\phi_j)^{2r}] \\ &= \sum_{p=0}^{\infty}\sum_{r=0}^{\infty} c_{p,2r} Q[\theta_0^{p+2r} \cos^p\phi_j \sin^{2r}\phi_j] \text{ by Conjecture 2.} \end{aligned}$$

□

5.3 Specific Results for $\mathcal{P}$ and Q

We first apply the Q operator to several expressions that occur due to the geometry of the icosahedron.

Fact 14 The functions indicated below are in $\mathcal{P}$ and

$$Q[\cos\gamma_j] = \cos\beta + \theta_0 \sin\beta\cos\phi_j \tag{24}$$

$$Q[\sin\gamma_j] = Q[\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}] \tag{25}$$

$$Q[\sin\alpha_j] = Q\left[-\frac{\theta_0\sin\phi_j}{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}\right] \tag{26}$$

$$Q[\cos m\alpha_j] = Q\left[\cos\left(m\sin^{-1}\left(\frac{\theta_0\sin\phi_j}{\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}}\right)\right)\right]. \tag{27}$$

Proof: That the functions are in $\mathcal{P}$ follows from the properties in Subsection 5.1. Eq. 24 follows by applying Properties 3 and 10 to the definition of $\cos\gamma_j$ in Fact 3. Eq. 25 is a consequence of the following calculation:

$$\begin{aligned} Q[\sin\gamma_j] &= Q[\sqrt{1-\cos^2\gamma_j}] \\ &= Q[\sqrt{1-(Q[\cos\gamma_j])^2}] \text{ by Conjecture 1} \\ &= Q[\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}] \text{ by Eq. 24.} \end{aligned}$$

Eq. 26 is a consequence of the following calculation:

$$\begin{aligned} Q[\sin\alpha_j] &= Q\left[-\frac{Q[\sin\theta_0\sin\phi_j]}{Q[\sin\gamma_j]}\right] \text{ by Property 7 applied to Eq. 6} \\ &= Q\left[-\frac{\theta_0\sin\phi_j}{Q[\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}]}\right] \text{ by Eqs. 23 and 25} \end{aligned}$$

$$= Q\left[-\frac{Q[\theta_0 \sin\phi_j]}{Q[\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}]}\right]$$

$$= Q\left[-\frac{\theta_0 \sin\phi_j}{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}\right] \text{ by Property 7}$$

Finally, Eq. 27 is a consequence of the following calculation:

$$\begin{aligned} Q[\cos m\alpha_j] &= Q[\cos m \sin^{-1} \sin\alpha_j] \\ &= Q[\cos m \sin^{-1} Q[\sin\alpha_j]] \text{ by Conjecture 1} \\ &= Q\left[\cos\left(m\sin^{-1}\left(Q\left[-\frac{\theta_0\sin\phi_j}{\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}}\right]\right)\right)\right] \text{ by Eq. 26} \\ &= Q\left[\cos\left(m\sin^{-1}\left(\frac{\theta_0\sin\phi_j}{\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}}\right)\right)\right] \text{ by Conjecture 1} \end{aligned}$$

□

Being equipped with the above tools, we return to Eq. 19.

Fact 15 *The left hand side of Eq. 19 is in $\mathcal{P}$. A follows that the right hand side of Eq. 19 is also in $\mathcal{P}$.*

Proof: By Properties 3 and 9 it follows that the left hand side of Eq. 19 is in $\mathcal{P}$ as a function of (θ_0, ϕ_0). □

The key result is the following fact:

Fact 16 *For $l = 0, 2, 4, \ldots$ and $m = 5\mu$ $(0 \le m \le +l)$,*

$$\sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} \frac{2}{1+\delta_{m',0}} b_{l,n,m'} b_{l,n,m} N_{l,m'} g_{l,m'} \theta_0^{m'} \cos m'\phi_0$$

$$= \frac{1}{6} N_{l,m}\left[g_{l,m}\theta_0^m \cos m\phi_0 + \sum_{\substack{\mu'=0\\ m'=5\mu'}}^{\infty} \theta_0^{m'} 5\cos m'\phi_0 \frac{2^{1-m'}}{1+\delta_{0,m'}} \sum_{k=0}^{m'} \frac{1}{k!} P_{l,m}^{(k)}(\cos\beta)\sin^k\beta \sum_{r=0}^{\lfloor \frac{m'-k}{2}\rfloor} c_{m'-k-2r,2r}(-1)^r\right]$$

where

$$P_{l,m}^{(k)}(x) = \frac{\mathrm{d}^k P_{l,m}}{\mathrm{d}\theta^k}(x).$$

Proof: Apply the Q operator to the left and right hand sides of Eq. 19. For the left hand side we find:

$$Q\left[\sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} b_{l,n,m}\frac{2}{1+\delta_{m',0}} N_{l,m'} b_{l,n,m'} P_{l,m'}(\cos\theta_0)\cos m'\phi_0\right]$$

$$= \sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} b_{l,n,m}\frac{2}{1+\delta_{m',0}} N_{l,m'} b_{l,n,m'} Q[P_{l,m'}(\cos\theta_0)\cos m'\phi_0] \text{ by Property 3}$$

$$= \sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} \frac{2}{1+\delta_{m',0}} b_{l,n,m'} b_{l,n,m} N_{l,m'} g_{l,m'} \theta_0^{m'} \cos m'\phi_0 \text{ by Property 9}$$

For the right hand side we find:

$$
\begin{aligned}
& Q[\frac{1}{6}N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\phi_0 + \sum_{j=0}^{4} P_{l,m}(\cos\gamma_j)\cos m\alpha_j\right]] \\
= & \frac{1}{6}N_{l,m}\left[Q[P_{l,m}(\cos\theta_0)\cos m\phi_0] + \sum_{j=0}^{4} Q[P_{l,m}(\cos\gamma_j)\cos m\alpha_j]\right] \text{ by Property 3} \\
= & \frac{1}{6}N_{l,m}\left[Q[P_{l,m}(\cos\theta_0)\cos m\phi_0] + \sum_{j=0}^{4} Q[Q[P_{l,m}(\cos\gamma_j)]Q[\cos m\alpha_j]]\right] \text{ by Property 4} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{j=0}^{4} Q[Q[P_{l,m}(\cos\gamma_j)]Q[\cos m\alpha_j]]\right] \text{ by Property 9} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{j=0}^{4} Q[Q[P_{l,m}(Q[\cos\gamma_j])]Q[\cos m\alpha_j]]\right] \text{ by Conjecture 1} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{j=0}^{4} Q\left[Q\left[\sum_{k=0}^{\infty}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)(Q[\cos\gamma_j]-\cos\beta)^k\right]Q[\cos m\alpha_j]\right]\right] \\
& \text{by the Taylor series expansion of } P_{l,m} \text{ around } \cos\beta \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{j=0}^{4} Q\left[Q\left[\sum_{k=0}^{\infty}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)(\theta_0\sin\beta\cos\phi_j)^k\right]Q[\cos m\alpha_j]\right]\right] \text{ by Eq. 24} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{j=0}^{4} Q\left[\sum_{k=0}^{\infty}Q\left[\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)(\theta_0\sin\beta\cos\phi_j)^k\right]Q[\cos m\alpha_j]\right]\right] \text{ by Conjecture 2} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0\right. \\
& \left.+\sum_{j=0}^{4} Q\left[\sum_{k=0}^{\infty}Q\left[\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)(\theta_0\sin\beta\cos\phi_j)^k\right]Q\left[\cos(m\sin^{-1}\left(\frac{\theta_0\sin\phi_j}{\sqrt{1-(\cos\beta+\theta_0\sin\beta\cos\phi_j)^2}}\right))\right]\right]\right] \\
& \text{by Eq. 27} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0\right. \\
& \left.+\sum_{j=0}^{4} Q\left[\sum_{k=0}^{\infty}Q\left[\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)(\theta_0\sin\beta\cos\phi_j)^k\right]\sum_{p=0}^{\infty}\sum_{r=0}^{\infty}c_{p,2r}Q[\theta_0^{p+2r}\cos^p\phi_j\sin^{2r}\phi_j]\right]\right] \\
& \text{by Property 13} \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0\right. \\
& \left.+\sum_{j=0}^{4} Q\left[\sum_{k=0}^{\infty}\sum_{p=0}^{\infty}\sum_{r=0}^{\infty}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta c_{p,2r}Q\left[(\theta_0\cos\phi_j)^k\right]Q[\theta_0^{p+2r}\cos^p\phi_j\sin^{2r}\phi_j]\right]\right] \\
= & \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0\right. \\
& \left.+\sum_{j=0}^{4}\sum_{k=0}^{\infty}\sum_{p=0}^{\infty}\sum_{r=0}^{\infty}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta c_{p,2r}Q\left[Q\left[(\theta_0\cos\phi_j)^k\right]Q[\theta_0^{p+2r}\cos^p\phi_j\sin^{2r}\phi_j]\right]\right] \\
& \text{by Conjecture 2}
\end{aligned}
$$

$$= \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{j=0}^{4}\sum_{k=0}^{\infty}\sum_{p=0}^{\infty}\sum_{r=0}^{\infty}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta c_{p,2r}Q\left[\theta_0^{k+p+2r}\cos^{k+p}\phi_j\sin^{2r}\phi_j\right]\right]$$

by Property 4

$$= \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0\right.$$
$$\left.+\sum_{j=0}^{4}\sum_{k=0}^{\infty}\sum_{p=0}^{\infty}\sum_{r=0}^{\infty}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta c_{p,2r}\frac{2^{1-(k+p+2r)}(-1)^r}{1+\delta_{k+p+2r,0}}\theta_0^{k+p+2r}\cos(k+p+2r)\phi_j\right]$$

by Property 11

$$= \frac{1}{6}N_{l,m}\left[\qquad \cos m\phi_0\right.$$
$$\left.+\sum_{m'=0}^{\infty}\theta_0^{m'}(\sum_{j=0}^{4}\cos m'\phi_j)\frac{2^{1-m'}}{1+\delta_{0,m'}}\sum_{k=0}^{m'}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta\sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor}c_{m'-k-2r,2r}(-1)^r\right]$$

by changing the summation index (from p to $m' = k + p + 2r$) and regrouping the summands

$$= \frac{1}{6}N_{l,m}\left[g_{l,m}\theta_0^{|m|}\cos m\phi_0 + \sum_{\substack{\mu'=0\\ m'=5\mu'}}^{\infty}\theta_0^{m'}5\cos m'\phi_0\frac{2^{1-m'}}{1+\delta_{0,m'}}\sum_{k=0}^{m'}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta\sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor}c_{m'-k-2r,2r}(-1)^r\right]$$

by $\sum_{j=0}^{4}\cos m'\phi_j = \begin{cases} 5\cos m'\phi_0 & \text{if } m' = 5\mu' \\ 0 & \text{otherwise} \end{cases}$.

Equating the results for the left and right hand sides and using m ≥ 0 verifies the claim. □

For $m' = 5\mu'$ $(0 \leq m' \leq +l)$, equate the coefficient of $\theta_0^{m'}$ on both sides of Fact 16 to get

$$\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)}\frac{2}{1+\delta_{m',0}}b_{l,n,m'}b_{l,n,m}N_{l,m'}g_{l,m'}\cos m'\phi_0$$
$$= \frac{1}{6}N_{l,m}\left[\delta_{m,m'}g_{l,m}\cos m\phi_0 + 5\cos m'\phi_0\frac{2^{1-m'}}{1+\delta_{0,m'}}\sum_{k=0}^{m'}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta\sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor}c_{m'-k-2r,2r}(-1)^r\right]$$

which must hold for I $= 0, 2, 4, \ldots$, m $= 5\mu$ $(0 \leq$ m $\leq +l)$, and $m' = 5\mu'$ $(0 \leq m' \leq +$I). Division of both sides by $\frac{2}{1+\delta_{m',0}}N_{l,m'}g_{l,m'}\cos m'\phi_0$ results in

Fact 17 For I even, m $= 5\mu$ *$(0 \leq$ m $\leq +l)$,* and $m' = 5\mu'$ *$(0 \leq m' \leq +l)$,*

$$\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} b_{l,n,m'}b_{l,n,m} = C_{l,m,m'} \tag{28}$$

where

$$C_{l,m,m'} = \frac{N_{l,m}}{12N_{l,m'}}\left[\delta_{m,m'}(1+\delta_{m',0}) + \frac{5\times 2^{1-m'}}{g_{l,m'}}\sum_{k=0}^{m'}\frac{1}{k!}P_{l,m}^{(k)}(\cos\beta)\sin^k\beta\sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor}c_{m'-k-2r,2r}(-1)^r\right].$$

5.4 The Case of l Odd

The derivation of coefficients for the odd harmonics is similar to that for the even harmonics. The final expression for determining the $b_{l,n,m}$ coefficients is:

		0	5	10	15	20	25	30
	0	*	*	*	*	*	*	*
	1	0	*	*	*	*	*	*
n	2	0	0	*	*	*	*	*
	3	0	0	0	*	*	*	*
	4	0	0	0	0	*	*	*

(columns: m)

Figure 2: The $b_{l,n,m}$ Array For Fixed l. "0" indicates a guaranteed 0 element while "*" indicates a possibly nonzero element.

Fact 18 *For l odd, $m = 5\mu$ $(0 \leq m \leq +l)$, and $m' = 5\mu'$ $(0 \leq m' \leq +l)$,*

$$\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} b_{l,n,m'} b_{l,n,m} = C_{l,m,m'} \tag{29}$$

where

$$C_{l,m,m'} = \frac{N_{l,m}}{12 N_{l,m'}} \left[\delta_{m,m'} + \frac{5 \times 2^{1-m'}}{g_{l,m'}} \sum_{k=0}^{m'} \frac{1}{k!} P_{l,m}^{(k)}(\cos\beta) \sin^k\beta \sum_{r=0}^{\lfloor \frac{m'-k-1}{2} \rfloor} s_{m'-k-2r-1,2r+1} (-1)^r \right]$$

and where the $s_{p,q}$ coefficients are defined by

$$-\sin(m \sin^{-1}(\frac{y}{\sqrt{1-(\cos\beta + x\sin\beta)^2}})) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} s_{p,q} x^p y^q.$$

Note that $C_{l,m,m'}$ is defined differently for l even and l odd.

6 Recursive Solution

Eqs. 28 and 29 enable us to obtain the $b_{l,n,m}$ coefficients sequentially in n for l even and odd respectively. The symmetry of the left hand side of Eqs. 28 and 29 in m' and m implies that $C_{l,m,m'} = C_{l,m',m}$ and that we need only consider $m \geq m'$ so Eqs. 28 and 29 simplify to

$$\sum_{n=0}^{\min(N_l-1,\lfloor m'/5\rfloor)} b_{l,n,m'} b_{l,n,m} \quad = \quad C_{l,m,m'} \quad 0 \leq m' \leq l, m' \leq m \leq l. \tag{30}$$

In addition, $C_{l,m,m'}$ vanishes for $m > l$ due to the $P_{l,m}^{(k)}$ term so the same symmetry implies that $C_{l,m,m'}$ vanishes for $m' > 1$.

We now describe an algorithm for solving Eq. 30. Based on Fact 7, we are only concerned with $m = 5\mu$ and $m' = 5\mu'$. Fix the value of l. As observed following Fact 6, there is no coupling between different values of l. Construct a $N_l \times (\lfloor l/5 \rfloor + 1)$ array of the $b_{l,n,m}$ coefficients where the (i,j) th element is $b_{l,i-1,5(j-1)}$. Because of Fact 12, this array has the form shown in Figure 2. Eq. 30 describes a sum over elements in one (if $m = m'$) or two (if $m \neq$ m') columns. Suppose

```
for( μ = 0 ; μ < N_l ; μ++ ){
    for( m = 0 ; m < 5μ ; m+ = 5 ){
        b_{l,μ,m} = 0
    }
}
for( μ' = 0 ; μ' < N_l ; μ' + + ){
    b_{l,μ',5μ'} = (C_{l,5μ',5μ'} - Σ_{n=0}^{μ'-1} b²_{l,n,5μ'})^{1/2}  (Eq. 30 for m' = m = 5μ')
    for( μ = μ' + 1 ; μ <= 11/51 ; μ ++ ){
        b_{l,μ',5μ} = (C_{l,5μ',5μ} - Σ_{n=0}^{μ'-1} b_{l,n,5μ'} b_{l,n,5μ}) / b_{l,μ',5μ'}  (Eq. 30 for m' = 5μ' and m = 5μ)
    }
}
```

Figure 3: An Algorithm for the Solution of Eq. 30. The control structures are written in the C programming language.

that the values of $b_{l,n,m}$ in rows $n = 0$ and $n = 1$ are known. Then the values in row n = 2 can be determined in two steps: First, set m = $m' = 10$ for which Eq. 30 becomes

$$b_{l,0,10}^2 + b_{l,1,10}^2 + b_{l,2,10}^2 = C_{l,10,10}. \tag{31}$$

Since $b_{l,0,10}$ and $b_{l,1,10}$ are known, Eq. 31 can be solved for $b_{l,2,10}$:

$$b_{l,2,10} = \sqrt{C_{l,10,10} - b_{l,0,10}^2 - b_{l,1,10}^2}.$$

Now that $b_{l,2,10}$ is known, the remainder of the n = 2 row can be determined by evaluating Eq. 30 for $m' = 10$ and $m = 15, 20, 25, 30$. The key is that the upper limit of Eq. 30, which is determined by m', does not change as m moves across the row. Specifically, Eq. 30 becomes

$$b_{l,0,10}b_{l,0,m} + b_{l,1,10}b_{l,1,m} + b_{l,2,10}b_{l,2,m} = C_{l,10,m} \tag{32}$$

and $b_{l,0,10}$, $b_{l,0,m}$, $b_{l,1,10}$, $b_{l,1,m}$, and $b_{l,2,10}$ are known so Eq. 32 can be solved for $b_{l,2,m}$:

$$b_{l,2,m} = \left(C_{l,10,m} - b_{l,0,10}b_{l,0,m} - b_{l,1,10}b_{l,1,m}\right)/b_{l,2,10}$$

Generalization of this approach leads to the algorithm shown in Figure 3.

The algorithm of Figure 3 will fail if $b_{l,\mu',5\mu'} = 0$ for any μ' in $0, \ldots N_l - 1$. The simplest example of this problem is $l = 15$ for which $N_{15} = 1$, $C_{15,0,0} = 0$, and $C_{15,5,5}$ # 0. The complete set of equations implied by Eq. 30 is shown in Table 1. The algorithm of Figure 3 would use the (m, m') pairs marked by "†" in Table 1 which are indeterminate since $b_{15,0,0} = 0$. However, by using the (m, m') pairs marked by "§", the four $b_{15,0,m}$ can be determined by a very similar algorithm:

$$b_{15,0,0} = \sqrt{C_{15,0,0}} = \sqrt{0} = 0$$

		m			
		0	5	10	15
m'	0	$b^2_{15,0,0} = C_{15,0,0} = 0$†§	$\overbrace{b_{15,0,0}}^{=0} b_{15,0,5} = C_{15,0,5}$†	$\overbrace{b_{15,0,0}}^{=0} b_{15,0,10} = C_{15,0,10}$†	$\overbrace{b_{15,0,0}}^{=0} b_{15,0,15} = C_{15,0,15}$†
	5		$b^2_{15,0,5} = C_{15,5,5}$§	$b_{15,0,5} b_{15,0,10} = C_{15,5,10}$§	$b_{15,0,5} b_{15,0,15} = C_{15,5,15}$§
	10			$b^2_{15,0,10} = C_{15,10,10}$	$b_{15,0,10} b_{15,0,15} = C_{15,10,15}$
	15				$b^2_{15,0,15} = C_{15,15,15}$

Table 1: **Eq.** 30 for $l = 15$.

$$\begin{aligned} b_{15,0,5} &= \sqrt{C_{15,5,5}} \\ b_{15,0,10} &= C_{15,5,10}/b_{15,0,5} \\ b_{15,0,15} &= C_{15,5,15}/b_{15,0,5}. \end{aligned}$$

The algorithm of the previous paragraph can be generalized to cases where $N_l > 1$ and there are multiple zero diagonal elements by taking advantage of Fact 12. Specifically, if the algorithm determines that $b_{l,n,m} = 0$ for m $\leq t_{l,n}$ then, for any $\eta \geq 0$, it follows that $b_{l,n+\eta,m} = 0$ for $m \leq t_{l,n} + 5\eta$. The resulting algorithm is shown in Figure 4. Note two aspects of the algorithm of Figure 4: First, when a new zero is found by the "while" statement, the diagonal containing: that zero is immediately set to zero for rows beneath the current row (i.e., for $n' >$ n:). Second! because of the zeros, the upper limit on the summations $\sum_{n'} b^2_{l,n',m'}$ and $\sum_{n'} b_{l,n',m'} b_{l,n',m}$ is n $-$ 1 rather than $\min(N_l - 1, \lfloor m'/5 \rfloor)$.

In order to execute the algorithm of Figure 4 in exact arithmetic, we have used the *Mathematica* symbolic computation system. The program for performing these calculations is listed in Appendix **E.** The key fact is that $C_{l,m,m'}$ can be evaluated for arbitrary l, m, and m' through elementary calculations. In order to evaluate $P^{(k)}_{l,m}(\cos\beta) = P^{(k)}_{l,m}(\frac{1}{\sqrt{5}})$, the following fact is useful.

Fact 19 $P^{(k)}_{l,m}(x)$, where $|x| < 1$, can be expressed in the following *form*

$$P^{(k)}_{l,m}(x) = A_k(x) P_{l-1,m}(x) + B_k(x) P_{l,m}(x)$$

where $A_k(x)$ and $B_k(x)$ satisfy the following recursive relations:

$$\begin{aligned} A_{k+1}(x) &= A'_k(x) + \frac{lxA_k(x) + (l+m)B_k(x)}{1-x^2} \\ B_{k+1}(x) &= B'_k(x) + \frac{lxB_k(x) + (l-m)A_k(x)}{-1+x^2} \end{aligned}$$

with the *initialization* $A_0(x) = 0, B_0(x) = 1$.

Proof: Note that for $|x| < 1$ ([5, **Eq.** 8.733-1,2])

$$\begin{aligned} \frac{d}{dx} P_{l,m}(x) &= \frac{(l+m)P_{l-1,m}(x) - lxP_{l,m}(x)}{1-x^2} \\ \frac{d}{dx} P_{l-1,m}(x) &= \frac{lxP_{l-1,m}(x) - (l-m)P_{l,m}(x)}{1-x^2} \end{aligned} \tag{33}$$

```
for( n = 0 ; n < N_l ; n++ ){
    for( m = 0 ; m < 5n ; m+ = 5 ){
        b_{l,n,m} = 0
    }


m' = 0
for( n = 0 ; n < N_l ; n++ ){
    while( (b_{l,n,m'} = (C_{l,m',m'} - \sum_{n'=0}^{n-1} b^2_{l,n',m'})^{1/2})==0 ){
        for( n' = n + 1, m = m' + 5 ; n' < N_l ; n'++, m+ = 5 ){
            b_{l,n',m} = 0
        }
        m'+ = 5
    }
    for( m = m' + 5 ; m <= l ; m+ = 5 ){
        b_{l,n,m} = (C_{l,m',m} - \sum_{n'=0}^{n-1} b_{l,n',m'} b_{l,n',m}) / b_{l,n,m'}
    }
    m'+ = 5
```

Figure 4: An Algorithm for the Solution of Eq. 30 in the General Case. The control structures are written in the C programming language.

Now prove by induction. The claim is obviously true for $k = 0$. Suppose it is true for k, then

$$\begin{aligned} P_{l,m}^{(k+1)}(x) &= \frac{d}{dx}[A_k(x)P_{l-1,m}(x) + B_k(x)P_{l,m}(x)] \\ &= A'_k(x)P_{l-1,m}(x) + A_k(x)P'_{l-1,m}(x) + B'_k(x)P_{l,m}(x) + B_k(x)P'_{l,m}(x) \end{aligned}$$

Substitute **Eq.** 33 and collect terms. That the claim is true for $k + 1$ follows immediately. □

7 Derivation Of Explicit Forms Of Icosahedral Harmonics

To substantiate the derivations in the previous sections, in this section we derive explicit expressions for those icosahedral harmonics that can be determined from **Eq.** 30 for $m' = 0$ (the so-called "first set") or $m' = 5$ (the so-called "second set"). (Recall that $m \geq m'$ always). Notice that the first and second sets do not correspond to $n = 0$ and $n = 1$. For instance, $N_{15} = 1$ so there is only a $n = 0$ icosahedral harmonic for $l = 15$ but, because $b_{15,0,0} = 0$, it is necessary to consider $m' = 5$ in **Eq.** 30 so the single icosahedral harmonic belongs to the second set.

In Appendix D we list the coefficients for all icosahedral harmonics in the range $0 \leq 1 < 45$. Though our theory and *Mathematica* software can compute the coefficients exactly, we only tabulate results to 16 decimal digits of precision in order to save space. Please contact P.C.D. for machine-readable tables of coefficients and software.

7.1 The First Set Of Icosahedral Harmonics

The first set of icosahedral harmonics is the collection of $T_{l,n}(\theta,\phi)$ for which $b_{l,n,0} \neq 0$. Specifically, the first set is those icosahedral harmonics that are computed by the $b_{l,n,m} = (C_{l,m',m} - \sum_{n'=0}^{n-1} b_{l,n',m'} b_{l,n',m})/b_{l,n,m'}$ statement in the algorithm of Figure 4 with $n = m' = 0$. From Fact 10 we know that $b_{l,n,0} = 0$ for l odd. Therefore, there are no I-odd icosahedral harmonics in the first set.

Set $m' = 0$ in Eq. 28 to get

$$b_{l,0,0} b_{l,0,m} = \frac{N_{l,m}}{12 N_{l,0}} [2\delta_{m,0} + \frac{10}{g_{l,0}} P_{l,m}(\cos\beta) c_{0,0}].$$

Noting $g_{l,0} = 1, c_{0,0} = 1$, we obtain

$$b_{l,0,0} b_{l,0,m} = \frac{1}{6}\sqrt{\frac{(l-m)!}{(1+m)!}}[\delta_{m,0} + 5P_{l,m}(\sqrt{.5})] \tag{34}$$

Evaluate Eq. 34 at $m = 0$ to get

$$b_{l,0,0}^2 = \frac{1}{6}[1 + 5P_{l,1}(\frac{1}{\sqrt{5}})]. \tag{35}$$

Evaluation of Eq. 35 shows that $b_{l,0,0} = 0$ for $l = 2,4,8,14$. Therefore, icosahedral harmonics of order $l = 2,4,8,14$, if they exist, are not members of the first set and, in fact, Eq. 4 shows that they do not exist at all. (We have verified that icosahedral harmonics of order $l = 2,4,8,14$ do not exist in the first or second set but in order to demonstrate that a harmonic of order l does not exist at all it is necessary to check through the $(l+1)$ st set). The first four unnormalized 1-even icosahedral harmonics, obtained by exact numerical calculations from Eq. 34, are

$$\begin{aligned}
T_{0,0}(\theta,\phi) &= 1 \\
T_{6,0}(\theta,\phi) &= 3960 P_{6,0}(\cos 8) - P_{6,5}(\cos 6)\cos 54 \\
T_{10,0}(\theta,\phi) &= 896313600 P_{10,0}(\cos\theta) + 27360 P_{10,5}(\cos 8)\cos 54 + P_{10,10}(\cos\theta)\cos 10\phi \\
T_{12,0}(\theta,\phi) &= 14250297600 P_{12,0}(\cos\theta) - 55440 P_{12,5}(\cos 8)\cos 54 + P_{12,10}(\cos 8)\cos 10\phi.
\end{aligned}$$

(Division of the stated formula by $\sqrt{4\pi}$, $3600\sqrt{\frac{11\pi}{13}}$, $25920000\sqrt{1729\,\pi}$, or $399168000\sqrt{595\,\pi}$ will normalize $T_{0,0}$, $T_{6,0}$, $T_{10,0}$, or $T_{12,0}$ respectively). In Figure 5 we show spherical plots of these harmonica. The icosahedral symmetry is apparent.

7.2 The Second Set Of Icosahedral Harmonics

The second set of icosahedral harmonics is the collection of $T_{l,n}(\theta,\phi)$ for which $b_{l,n,0} = 0$, and $b_{l,n,5} \neq 0$. Specifically, the second set is those icosahedral harmonics that are computed by the $b_{l,n,m} = \left(C_{l,m',m} - \sum_{n'=0}^{n-1} b_{l,n',m'} b_{l,n',m}\right)/b_{l,n,m'}$ statement in the algorithmof Figure 4 with $n = 0,1$

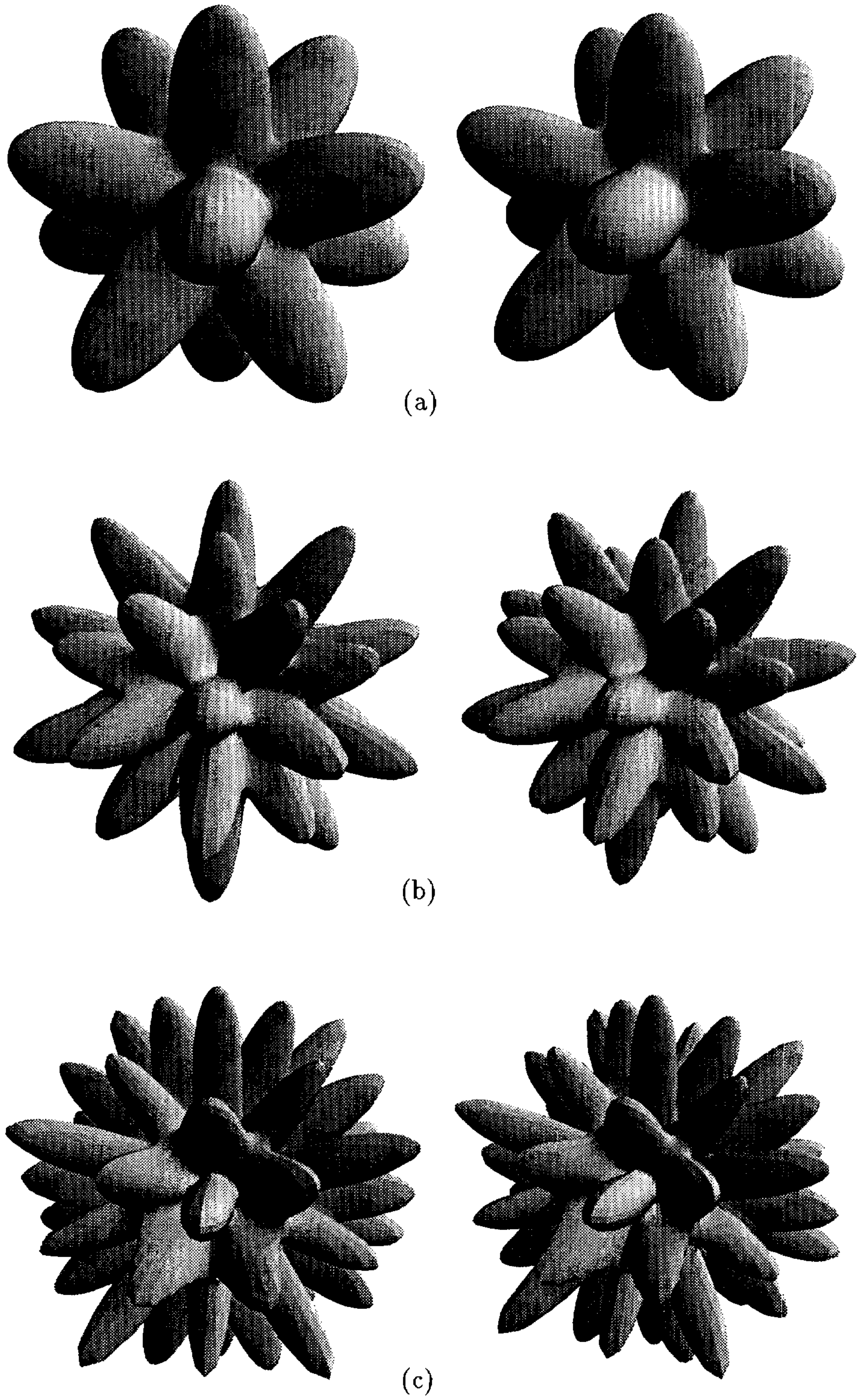

Figure 5: Icosahedral harmonics. Each stereo pair of plots shows a surface whose distance from the origin at particular θ and ϕ values is the value of $c_{l,n} + T_{l,n}(\theta, \phi)$ where $c_{l,n} = 2\max_{\theta,\phi}(|T_{l,n}(\theta, \phi)|)$. (a) $T_{6,0}$, (b) $T_{10,0}$, and (c) $T_{12,0}$. $T_{0,0}(\theta, \phi)$ takes value $1/\sqrt{4\pi}$ independent of the values of θ and ϕ so a plot of this type for $T_{0,0}$ shows a sphere.

and $m' = 5$. We now determine the $b_{l,n,m}$ coefficients. First consider the 1-even icosahedral harmonics;. Setting $m' = 5$ in Eq. 28, we obtain

$$b_{l,0,5}b_{l,0,m} + b_{l,1,5}b_{l,1,m} = \frac{N_{l,m}}{12N_{l,5}}(\delta_{|m|,5}\frac{g_{l,m}}{g_{l,5}} + \frac{5}{16g_{l,5}}\sum_{k=0}^{5}\frac{1}{k!}P_{l,m}^{(k)}(\frac{1}{\sqrt{5}})(\frac{2}{\sqrt{5}})^k \sum_{r=0}^{\lfloor(5-k)/2\rfloor} c_{5-k-2r,2r}(-1)^r \tag{36}$$

where, by applying Eq. 34 three times to achieve the second equality,

$$b_{l,0,5}b_{l,0,m} = \frac{(b_{l,0,0}b_{l,0,5})(b_{l,0,0}b_{l,0,m})}{b_{l,0,0}^2} = \sqrt{\frac{(l-5)!(l-m)!}{(l+5)!(l+m)!}}\frac{25P_{l,m}(\frac{1}{\sqrt{5}})P_{l,5}(\frac{1}{\sqrt{5}})}{6(1+5P_l(\frac{1}{\sqrt{5}}))}. \tag{37}$$

Using Eq. 37 in Eq. 36, the expression for the 1-even second-set icosahedral harmonics was worked out with the aid of *Mathematica* and is

$$b_{l,1,5}b_{l,1,m} = \frac{1}{12}\sqrt{\frac{(l-m)!(l+5)!}{(l+m)!(l-5)!}}\{\delta_{m,5} - \frac{(l-5)!}{(l+5)!}[2^5 5! u_{l,m} + \frac{50P_{l,m}(\frac{1}{\sqrt{5}})P_{l,5}(\frac{1}{\sqrt{5}})}{1+5P_l(\frac{1}{\sqrt{5}})}]\} \tag{38}$$

where

$$\begin{aligned} u_{l,m} &= \frac{1}{768}[(120 - 56l - 195l^2 - 5l^3 + 15l^4 + l^5 + 925m^2 + 95lm^2 - 195l^2m^2 - 15l^3m^2 + 275m^4 \\ &+ 25lm^4)P_{l,m}(\frac{1}{\sqrt{5}}) + \sqrt{5}(-120 - 88l + 63l^2 + 29l^3 - 3l^4 - l^5 + 120m - 32lm - 31l^2m \\ &+ 2l^3m + l^4m - 275m^2 - 260lm^2 + 30l^2m^2 + 15l^3m^2 + 275m^3 - 15lm^3 - 15l^2m^3 \\ &- 25m^4 - 25lm^4 + 25m^5)P_{l+1,m}(\frac{1}{\sqrt{5}})]. \end{aligned}$$

Evaluate Eq. 38 at $m = 5$ to get an expression for $b_{l,1,5}^2$. Evaluation of this expression using exact arithmetic shows that the smallest even l such that $b_{l,1,5}$ # 0 is $l = 30$, i.e., the lowest order second-set I-even icosahedral harmonic is $T_{30,1}(\theta, +)$. By further calculations with *Mathematica* we find that an unnormalized expression for $T_{30,1}$ is

$$\begin{aligned} T_{30,1}(\theta,\phi) &= 2157573782684478368223777575936000000P_{30,5}(\cos 8)\cos 54 \\ &+ 2404901042680144820126515200000\,P_{30,10}(\cos\theta)\cos 10\phi \\ &+ 1959363005732768563200000P_{30,15}(\cos 8)\cos 15\phi \\ &+ 7601550560755200P_{30,20}(\cos 8)\cos 204 \\ &+ \frac{7075752000}{11}P_{30,25}(\cos\theta)\cos 25\phi + 12251P_{30,30}(\cos\theta)\cos 30\phi. \end{aligned}$$

(Division of the stated formula by 115874256845437009920000000000000 $\sqrt{\frac{28072776427766064319187390671\pi}{61}}$ will normalize $T_{30,1}$). A spherical plot of $T_{30,1}(\theta,\phi)$ is shown in Figure 6. For comparison, an unnormalized expression for $T_{30,0}(\theta,\phi)$, a member of the first set, is

$$\begin{aligned} T_{30,0}(\theta,\phi) &= 8132790382558892160533487863621222400000000P_{30,0}(\cos\theta) \\ &- 47353003689115160214196322304000000P_{30,5}(\cos\theta)\cos 54 \\ &+ 16454397372215805370368000000P_{30,10}(\cos\theta)\cos 10\phi \\ &- 5570861497673472000P_{30,15}(\cos 8)\cos 15\phi + 9702264499200P_{30,20}(\cos 8)\cos 204 \\ &- 5407920P_{30,25}(\cos\theta)\cos 25\phi + P_{30,30}(\cos 8)\cos 30\phi. \end{aligned}$$

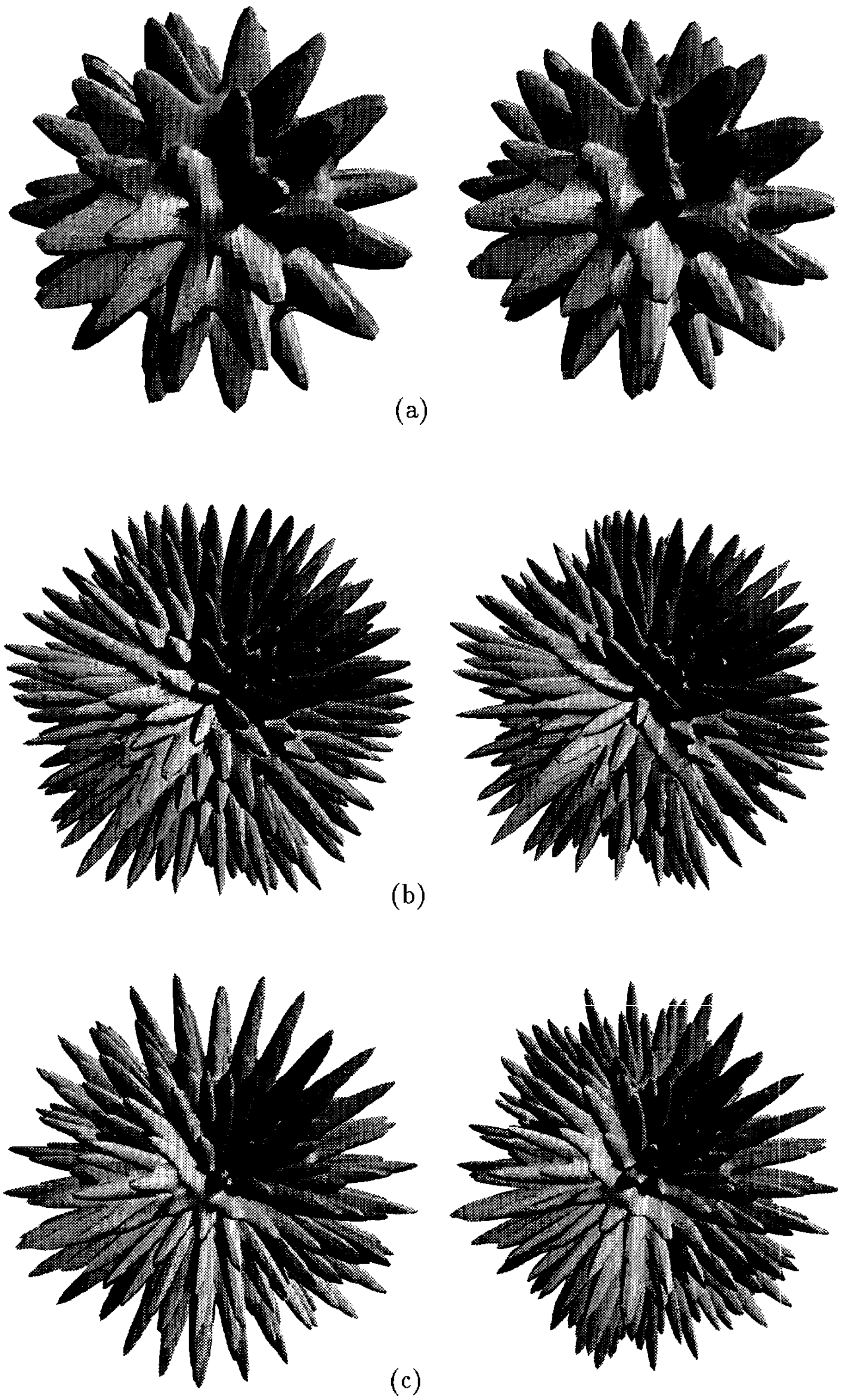

Figure 6: Icosahedral harmonics. Each stereo pair of plots shows a surface whose distance from the origin at particular θ and ϕ values is the value of $c_{l,n} + T_{l,n}(\theta, \phi)$ where $c_{l,n} = 2\max_{\theta,\phi}(|T_{l,n}(\theta, \phi)|)$. (a) $T_{15,0}$, (b) $T_{30,0}$, and (c) $T_{30,1}$.

(Division of the stated formula by 414457593456548529119232000000000000000 $\sqrt{\frac{9198155739\pi}{61}}$ will normalize $T_{30,0}$). **A** spherical plot of $T_{30,0}(\theta,\phi)$ is also shown in Figure 6.

Now let us consider the second-set 1-odd icosahedral harmonics. By setting $m' = 5$ and noting that $b_{l,n',m} = 0$ for $n' = 1,\ldots,N_l - 1$ and $m = 10, 15, \ldots, \lfloor l/5 \rfloor 5$ in **Eq.** 29 we get

$$b_{l,0,5}b_{l,0,m} = \frac{1}{12}\sqrt{\frac{(l-m)!(l+5)!}{(l+m)!(l-5)!}}\{\delta_{m,5} - 3840\frac{(l-5)!}{(l+5)!}v_{l,m}\} \tag{39}$$

where

$$\begin{aligned} v_{l,m} &= \frac{5\sqrt{5}m}{768}[\sqrt{5}(l+m)(26-3l-3l^2+10m^2)P_{l-1,m}(\frac{1}{\sqrt{5}}) \\ &+ (24-50l-20l^2+5l^3+l^4+55m^2-15lm^2-5l^2m^2+5m^4)P_{l,m}(\frac{1}{\sqrt{5}})]. \end{aligned}$$

As before, by setting $m = 5$ in **Eq.** 39 we derive an expression for $b_{l,0,5}^2$. The smallest odd l for which this. expression is nonzero is $l = 15$. Therefore, the lowest order I-odd second-set icosahedral harmonic is $T_{15,0}(\theta,\phi)$, which has the unnormalized expression

$$T_{15,0}(\theta,\phi) = -36306144000P_{15,5}(\cos 8)\sin 5\phi - 62640P_{15,10}(\cos\theta)\sin 10\phi + P_{15,15}(\cos 8)\sin 15\phi.$$

(Division of the stated formula by 3919104000000 $\sqrt{\frac{2156556441\pi}{31}}$ will normalize $T_{15,0}$). **A** spherical plot of $T_{15,0}(\theta,\phi)$ is shown in Figure 6. The nodal lines at $\phi = k\frac{2\pi}{5}$, which are due to the $\sin 5m\phi$ factors ($m = 1,2,3$), are clear. $T_{15,0}$ is, by Eq. 4, the lowest order 1-odd icosahedral harmonic among any set.

7.3 Symbolic Verification of the Icosahedral Harmonics

Because of technical difficulties in the mathematics, we were unable to prove Conjectures 1 and 2 in the der:vation of a general formulae for icosahedral harmonics. However, we believe that our use of them is reasonable and the results derived from them are correct.. We have verified explicit. instances of our calculation in two ways: First, our exact results reproduce the 6-significant)-digit results for $0 \le l \le 30$ in Ref. [7]. (For $l = 30$ Ref. [7] lists only one icosahedral harmonic, which is our $T_{30,0}$, in spite of the fact that $N_{30} = 2$). Second, for a significant subset of the icosahedral harmonics we have verified symbolically that the icosahedral harmonic is invariant under each of the 60 :symmetries in the icosahedral group. Ill particular, we have verified $T_{0,0}$, $T_{6,0}$, $T_{10,0}$, $T_{12,0}$, and $T_{15,0}$, which are all of the icosahedral harmonics with $l \le 15$, and we have verified $T_{30,0}$ and $T_{30,1}$, which are the lowest-order icosahedral harmonics for which $N_l > 1$. Such symbolic verification can be performed for any particular icosahedral harmonic by widely-available symbolic computation software. In the remainder of this subsection we describe the method and procedures to use *Mathematica* to verify the symmetries of icosahedral harmonics.

A sphe:ical harmonic $Y_{l,m}$, when expressed in terms of Cartesian coordinates, is a polynomial in x, y, z of order l. Therefore, an icosahedral harmonic is also since an icosahedral harmonic is a linear combination of spherical harmonics of the same order. **A** rotation of the harmonic is simply a linear transformation of the coordinates. The transformation will yield a (generally different) homogeneous polynomial of the same order in the transformed coordinates. The invariance under icosahedral symmetry is verified if, for the 60 transformations in the icosahedral group, the polynomials before and after the transformation are the same.

There are 2 reasons for using Cartesian rather than spherical coordinates for the verification:

R_0	R_1	R_2	R_3	R_4	R_5	R_6	R_7	R_8	R_9
1	S	S^2	S^3	S^4	ST	TR_5	TR_6	$T^{-1}R_5$	$T^{-1}R_8$
R_{10}	R_{11}	R_{12}	R_{13}	R_{14}	R_{15}	R_{16}	R_{17}	R_{18}	R_{19}
SR_5	SR_6	SR_7	SR_8	SR_9	SR_{10}	SR_{11}	SR_{12}	SR_{13}	SR_{14}
R_{20}	R_{21}	R_{22}	R_{23}	R_{24}	R_{25}	R_{26}	R_{27}	R_{28}	R_{29}
$S^{-1}R_5$	$S^{-1}R_6$	$S^{-1}R_7$	$S^{-1}R_8$	$S^{-1}R_9$	$S^{-1}R_{20}$	$S^{-1}R_{21}$	$S^{-1}R_{22}$	$S^{-1}R_{23}$	$S^{-1}R_{24}$

Table 2: The First 30 Icosahedral Rotations in Terms of S and T.

1. The rotational operation is more easily expressed in Cartesian coordinates than spherical coordinates (a linear transformation versus complicated angular relations).

2. Most symbolic computation software handles polynomials much better than trigonometric functions, specifically, the manipulation of polynomials (collecting terms, expansion and factorization, etc.) is fairly mechanical and the behavior of the output is predictable, while the manipulation of trigonometric functions requires the use of possibly many trigonometric identities and the sequence of their application may greatly change the appearance of the output, so without the intelligent interference of the user, the symbolic computation software rarely arrives at the simplest form of a trigonometric expression.

It is not necessary to separately verify the invariance of the icosahedral harmonic under each of the 60 rotations of the icosahedral group. If a function is invariant under the unitary operations S, U and P, which are defined below, then it is invariant under all 60 rotations of the icosahedral group, because any rotation in the icosahedral group is a product of S, U, P and their inverses.

The operation S is a rotation about the z axis (a five-fold axis), USU^{-1} is a rotation about a different five-fold axis, and P is a quasi spatial reflection operation. In the coordinate system used in this paper (Figure 1), S, U, and P have the following matrix representations:

$$\begin{aligned} S &= \begin{bmatrix} \cos\frac{2\pi}{5} & -\sin\frac{2\pi}{5} & 0 \\ \sin\frac{2\pi}{5} & \cos\frac{2\pi}{5} & 0 \\ 0 & 0 & 1 \end{bmatrix} \\ U &= \begin{bmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{bmatrix} \\ P &= \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \end{aligned}$$

Table 2 tabulates the first 30 rotations of the icosahedral group in terms of S and T $= USU^{-1}$. The second 30 rotations are related to the first 30 rotations by

$$R_{i+30} = PR_i, \quad i = 0, 1, \ldots, 29.$$

In Appendix F, we give a concrete illustration of the needed computations by verifying that $T_{6,0}$ is invariant under the operation U. The necessary *Mathematica* programs are contained in Appendix G.

8 Other Polyhedral Harmonics

Using the same idea and techniques, we can derive the complete orthonormal sets of harmonics with octebedral and tetrahedral symmetries. Since the cube is dual to the octahedron and the dodecahedron is dual to the icosahedron, it is not necessary to compute cubic and dodecahedral harmonics. Below we only outline the calculations and have suppressed the details. Please contact P.C.D. for machine-readable tables of coefficients and software.

8.1 Octahedral Harmonics

Choose appropriate coordinates such that the spherical coordinates of the vertices of the underlying octahedrcn are:

$$\{(0,0),(\frac{\pi}{2},0),(\frac{\pi}{2},\frac{\pi}{2}),(\frac{\pi}{2},\pi),(\frac{\pi}{2},\frac{3\pi}{2}),(\pi,0)\}$$

Express the octahedrally symmetric delta function in terms of both spherical harmonics and the unknown octahedral harmonics. After simplification this gives

- l is even

$$\begin{aligned}&\sum_{m'\geq 0}\sum_{4n<m'} b_{l,n,m}\frac{2}{1+\delta_{m',0}}N_{l,m'}b_{l,n,m'}P_{l,m'}(\cos\theta_0)\cos m'\phi_0\\ =\ &\frac{1}{3}N_{l,m}[P_{l,m}(\cos\theta_0)\cos m\phi_0+\frac{1}{2}\sum_{k=0}^{3}P_{l,m}(\cos\gamma_k)\cos m\alpha_k] \qquad m=4\mu\end{aligned}$$

- l is odd

$$\begin{aligned}&\sum_{m'>0}\sum_{4n<m'} b_{l,n,m}N_{l,m'}b_{l,n,m'}P_{l,m'}(\cos\theta_0)\sin m'\phi_0\\ =\ &\frac{1}{3}N_{l,m}[P_{l,m}(\cos\theta_0)\sin m\phi_0+\frac{1}{2}\sum_{k=0}^{3}P_{l,m}(\cos\gamma_k)\sin m\alpha_k] \qquad m=4\mu\end{aligned}$$

where α_k,γ_k have the same definitions as in the icosahedral case with $\beta=\pi/2$ and $\phi_k=\phi_0+k\frac{\pi}{2}$. Using the series expansion techniques, we obtain expressions for determining tht: coefficients $b_{l,n,m}$:

- l is even

$$\sum_{4n\leq m'} b_{l,n,m'}b_{l,n,m}=\frac{N_{l,m}}{6N_{l,m'}}[\delta_{m,m'}(1+\delta_{m',0})+\frac{2^{2-m'}}{g_{l,m'}}\sum_{k=0}^{m'}\frac{1}{k!}P_{l,m}^{(k)}(0)\sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor}c_{m'-k-2r,2r}(-1)^r]$$

- l is odd

$$\sum_{4n\leq m'} b_{l,n,m'}b_{l,n,m}=\frac{N_{l,m}}{6N_{l,m'}}[\delta_{m,m'}+\frac{2^{2-m'}}{g_{l,m'}}\sum_{k=0}^{m'}\frac{1}{k!}P_{l,m}^{(k)}(0)\sum_{r=0}^{\lfloor\frac{m'-k-1}{2}\rfloor}s_{m'-k-2r-1,2r+1}(-1)^r]$$

where $c_{p,q}$ and $s_{p,q}$ are defined by

$$\begin{aligned}\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}c_{p,q}x^py^q &= \cos(m\arcsin(\frac{y}{\sqrt{1-x^2}}))\\ \sum_{p=0}^{\infty}\sum_{q=0}^{\infty}s_{p,q}x^py^q &= -\sin(m\arcsin(\frac{y}{\sqrt{1-x^2}})).\end{aligned}$$

8.2 Tetrahedral Harmonics

The spherical coordinates of the vertices of the underlying tetrahedron are

$$\{(0,0),(\beta,0),(\beta,\frac{2\pi}{3}),(\beta,\frac{4\pi}{3})\}$$

where $\beta = \pi - \arccos\frac{1}{3}$. Because the vertices of the tetrahedron do not have spatial reflection $(\mathbf{x} \rightarrow -\mathbf{x})$ symmetries, the coefficients $b_{l,n,m}$ for tetrahedral harmonics may be complex. It is more convenient to introduce the dual tetrahedron which has vertex coordinates that are spatial reflection!; of those of the primal tetrahedron, specifically,

$$\{(\pi,0),(\pi-\beta,\pi),(\pi-\beta,\frac{5\pi}{3}),(\beta,\frac{\pi}{3})\},$$

so that the coefficients $b_{l,n,m}$ can be chosen real (or pure imaginary) as in the icosahedral case. Let, $\delta^{(p)}(\theta_0,\phi_C;\theta,\phi)$ be the delta function associated with the primal tetrahedron and let $\delta^{(d)}(\theta_0,\phi_0;\theta,\phi)$ be the delta function associated with the dual tetrahedron. Further, let

$$\begin{aligned}\delta^{(+)}(\theta_0,\phi_0;\theta,\phi) &= \delta^{(p)}(\theta_0,\phi_0;\theta,\phi)+\delta^{(d)}(\theta_0,\phi_0;\theta,\phi)\\ \delta^{(-)}(\theta_0,\phi_0;\theta,\phi) &= \delta^{(p)}(\theta_0,\phi_0;\theta,\phi)-\delta^{(d)}(\theta_0,\phi_0;\theta,\phi)\end{aligned}$$

Instead of expanding $\delta^{(p)}(\theta_0,\phi_0;6,\phi)$, we expand $\delta^{(\pm)}(\theta_0,\phi_0;\theta,\phi)$ in terms of both spherical harmonics and the unknown tetrahedral harmonics. This will give us two independent sets of tetrahedral harmonics. The master equations for determining the coefficients are:

- l is even

$$\begin{aligned}&\sum_{m'\geq 0}\sum_{3n<m'} b^{(+)}_{l,n,m}\frac{2}{1+\delta_{m',0}}N_{l,m'}b^{(+)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\cos m'\phi_0\\ =\ &\frac{1}{4}N_{l,m}[P_{l,m}(\cos\theta_0)\cos m\phi_0+\sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\cos m\alpha_k]\\ &\sum_{m'\geq 0}\sum_{3n<m'} b^{(-)}_{l,n,m}\frac{2}{1+\delta_{m',0}}N_{l,m'}b^{(-)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\sin m'\phi_0\\ =\ &\frac{1}{4}N_{l,m}[P_{l,m}(\cos\theta_0)\sin m\phi_0+\sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\sin m\alpha_k] \qquad m=3\mu\end{aligned}$$

- I is odd

$$\begin{aligned}&\sum_{m'\geq 0}\sum_{3n<m'} b^{(+)}_{l,n,m}N_{l,m'}b^{(+)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\sin m'\phi_0\\ =\ &\frac{1}{4}N_{l,m}[P_{l,m}(\cos\theta_0)\sin m\phi_0+N\sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\sin m\alpha_k]\\ &\sum_{m'\geq 0}\sum_{3n<m'} b^{(-)}_{l,n,m}N_{l,m'}b^{(-)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\cos m'\phi_0\\ =\ &\frac{1}{4}N_{l,m}[P_{l,m}(\cos\theta_0)\cos m\phi_0+\sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\cos m\alpha_k] \qquad m=3\mu\end{aligned}$$

where α_k γ_k are defined as before (with the new value of β and $\phi_k = \phi_0 + k\frac{2\pi}{3}$). The final expressions for determining $b_{l,n,m}$ coefficients are

- l is even

$$\sum_{3n\leq m'} b^{(+)}_{l,n,m'} b^{(+)}_{l,n,m} = \frac{N_{l,m}}{8N_{l,m'}}[\delta_{m,m'}(1+\delta_{m',0}) + \frac{3\times 2^{1-m'}}{g_{l,m'}} \sum_{k=0}^{m'} \frac{1}{k!} P^{(k)}_{l,m}(\cos\beta)\sin^k\beta \sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor} c_{m'-k-2r,2r}(-1)^r]$$

$$\sum_{3n\leq m'} b^{(-)}_{l,n,m'} b^{(-)}_{l,n,m} = \frac{N_{l,m}}{8N_{l,m'}}[\delta_{m,m'}(1+\delta_{m',0}) + \frac{3\times 2^{1-m'}}{g_{l,m'}} \sum_{k=0}^{m'} \frac{1}{k!} P^{(k)}_{l,m}(\cos\beta)\sin^k\beta \times \times \sum_{r=0}^{\lfloor\frac{m'-k-1}{2}\rfloor} s_{m'-k-2r-1,2r+1}(-1)^r]$$

- l is odd

$$\sum_{4n\leq m'} b^{(+)}_{l,n,m'} b^{(+)}_{l,n,m} = \frac{N_{l,m}}{8N_{l,m'}}[\delta_{m,m'} + \frac{3\times 2^{1-m'}}{g_{l,m'}} \sum_{k=0}^{m'} \frac{1}{k!} P^{(k)}_{l,m}(\cos\beta)\sin^k\beta \sum_{r=0}^{\lfloor\frac{m'-k-1}{2}\rfloor} s_{m'-k-2r-1,2r+1}(-1)^r]$$

$$\sum_{3n\leq m'} b^{(-)}_{l,n,m'} b^{(-)}_{l,n,m} = \frac{N_{l,m}}{8N_{l,m'}}[\delta_{m,m'} + \frac{3\times 2^{1-m'}}{g_{l,m'}} \sum_{k=0}^{m'} \frac{1}{k!} P^{(k)}_{l,m}(\cos\beta)\sin^k\beta \sum_{r=0}^{\lfloor\frac{m'-k}{2}\rfloor} c_{m'-k-2r,2r}(-1)^r]$$

where $c_{p,q}$ and $s_{p,q}$ are defined the same as in the icosahedral case with the new value of β.

9 Acltnowledgements

We would like to thank Professor John E. Johnson (Department of Biological Sciences, Purdue University) for drawing our attention to this problem and for his enthusiastic interest in the results.

Appendix

A Proofs of Theorems 1 and 3

Proof of Theorem 1: Let $f(\theta,\phi) \doteq \Re h(\theta,\phi)$ and $g(\theta,\phi) = \Im h(\theta,\phi)$. Applying the rotation R gives

$$f(\theta,\phi) + ig(\theta,\phi) = h(\theta,\phi) = R[h(\theta,\phi)] = R[f(\theta,\phi) + ig(\theta,\phi)] = R[f(\theta,\phi)] + iR[g(\theta,\phi)]. \quad (40)$$

Since a rotation of a real function is a real function, it follows that taking the real and imaginary parts of Eq. 40 gives the desired result that f and g are separately invariant: $R(f(\theta,\phi)) = f(\theta,\phi)$ and $R(g(\theta,\phi)) = g(\theta,\phi)$. □

Proof of Theorem 3: Applying R_i gives

$$\begin{aligned}
\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} b_{l,m}Y_{l,m}(\theta,\phi) &= f(\theta,\phi) \\
&= R_i f(\theta,\phi) \\
&= R_i \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} b_{l,m}Y_{l,m}(\theta,\phi) \\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} b_{l,m} \sum_{m'=-l}^{+l} D_{l,m,m'}(R_i)Y_{l,m'}(\theta,\phi) \quad \text{by Theorem 2} \\
&= \sum_{l=0}^{\infty}\sum_{m'=-l}^{+l} \left(\sum_{m=-l}^{+l} b_{l,m}D_{l,m,m'}(R_i)\right) Y_{l,m'}(\theta,\phi).
\end{aligned}$$

Multiply by $Y^*_{l',m''}(\theta,\phi)$, integrate over solid angles $d\Omega$, and use the orthonormality of the spherical harmonics to get (after renaming the indices $l' \to l$ and $m'' \to m'$)

$$b_{l,m'} = \sum_{m=-l}^{+l} b_{l,m}D_{l,m,m'}(R_i). \quad (41)$$

Now consider the f_l. Apply R_i to get

$$\begin{aligned}
R_i f_l(\theta,\phi) &= R_i \sum_{m=-l}^{+l} b_{l,m}Y_{l,m}(\theta,\phi) \\
&= \sum_{m=-l}^{+l} b_{l,m} \sum_{m'=-l}^{+l} D_{l,m,m'}(R_i)Y_{l,m'}(\theta,\phi) \\
&= \sum_{m'=-l}^{+l} \left(\sum_{m=-l}^{+l} \quad m \quad m \quad m \quad i\right) Y_{l,m'}(\theta,\phi) \\
&= \sum_{m'=-l}^{+l} b_{l,m'}Y_{l,m'}(\theta,\phi) \quad \text{by Eq. 41} \\
&= f_l(\theta,\phi).
\end{aligned}$$

B Proof of Property 4

Let f_1 and f_2 be defined as in Eqs. 20 and 21. Set $d^{(1)}_{m,k} = d^{(2)}_{m,k} = 0$ for $k < |m|$ so that Eqs. 20 and 21 can be rewritten in the form

$$\begin{aligned} f_1(\theta,\phi) &= \sum_{m=-\infty}^{+\infty} \sum_{k=-\infty}^{+\infty} d^{(1)}_{m,k} \theta^k e^{im\phi} \\ f_2(\theta,\phi) &= \sum_{m=-\infty}^{+\infty} \sum_{k=-\infty}^{+\infty} d^{(2)}_{m,k} \theta^k e^{im\phi}. \end{aligned}$$

Then

$$f_1(\theta,\phi) f_2(\theta,\phi) = \sum_{m=-\infty}^{+\infty} \sum_{m'=-\infty}^{+\infty} \sum_{k=-\infty}^{+\infty} \sum_{k'=-\infty}^{+\infty} d^{(1)}_{m,k} d^{(2)}_{m',k'} \theta^{k+k'} e^{i(m+m')\phi}.$$

Change vsriables from m and m' to n and n' using the transformation

$$\begin{aligned} \begin{pmatrix} n \\ n' \end{pmatrix} &= \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} m \\ m' \end{pmatrix} \\ \begin{pmatrix} m \\ m' \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} n \\ n' \end{pmatrix} \end{aligned}$$

and change variables from k and k' and l and l using the same transformation to get

$$\begin{aligned} f_1(\theta,\phi) f_2(\theta,\phi) &= \sum_{n=-\infty}^{+\infty} \sum_{l=-\infty}^{+\infty} \left(\sum_{n'=-\infty}^{+\infty} \sum_{l'=-\infty}^{+\infty} d^{(1)}_{n',l'} d^{(2)}_{n-n',l-l'} \right) \theta^l e^{in\phi} \\ &= \sum_{n=-\infty}^{+\infty} \sum_{l=-\infty}^{+\infty} \tilde{d}_{n,l} \theta^l e^{in\phi} \end{aligned} \quad (42)$$

where

$$\begin{aligned} \tilde{d}_{n,l} &= \sum_{n'=-\infty}^{+\infty} \sum_{l'=-\infty}^{+\infty} d^{(1)}_{n',l'} d^{(2)}_{n-n',l-l'} \\ &= \sum_{n'=-\infty}^{+\infty} \sum_{l'=|n'|}^{+\infty} d^{(1)}_{n',l'} d^{(2)}_{n-n',l-l'} \end{aligned}$$

since $d^{(1)}_{n',l'} = 0$ for $l < |n'|$.

Based on Eq. 42, $f_1 f_2$ is in $\mathcal{P}$ if and only if $\tilde{d}_{n,l} = 0$ for $l < |n|$. It would be sufficient to show that $l < |n|$ and $l \geq |n'|$ implies that $d^{(2)}_{n-n',l-l'} = 0$. For this it would bt: sufficient to show that $l < |n|$ and $l \geq |n'|$ implies that $l - l' < |n - n'|$. But $l < |n|$ and $-l' \leq -|n'|$ implies $l - l < |n - |n'|| \leq |n - n'|$ where the final inequality is the standard complex variables result that $|z_1| - |z_2| \leq |z_1 + z_2| \leq |z_1| + |z_2|$. Therefore, $f_1 f_2$ is in $\mathcal{P}$ and it follows that any finite product of functions in **P** is in **P**.

Now prove $Q[f_1 f_2] = Q[Q[f_1]Q[f_2]]$. First compute $Q[f_1 f_2]$. The variables $\tilde{d}_{n,l}$ are defined by

$$\tilde{d}_{n,l} = \sum_{n'=-\infty}^{+\infty} \sum_{l'=-\infty}^{+\infty} d^{(1)}_{n',l'} d^{(2)}_{n-n',l-l'}$$

$$= \sum_{n'=-\infty}^{+\infty} \sum_{l'=|n'|}^{+\infty} d^{(1)}_{n',l'} d^{(2)}_{n-n',l-l'}$$

since $d^{(1)}_{n',l'} = 0$ for $l' < |n'|$

$$= \sum_{n'=-\infty}^{+\infty} \sum_{l'=|n'|}^{l-|n-n'|} d^{(1)}_{n',l'} d^{(2)}_{n-n',l-l'}$$

since $d^{(2)}_{n-n',l-l'} = 0$ for $l - l' < |n - n'|$

Therefore,

$$\tilde{d}_{n,|n|} = \sum_{n'=-\infty}^{+\infty} \sum_{l'=|n'|}^{|n|-|n-n'|} d^{(1)}_{n',l'} d^{(2)}_{n-n',|n|-l'}$$

Consider cases:

1. Assume $n \geq 0$:

   (a) Assume $n' > n \geq 0$:

   $$\sum_{l'=|n'|}^{|n|-|n-n'|} = \sum_{l'=n'}^{n+n-n'} = \sum_{l'=n'}^{2n-n'}$$

   This requires $2n - n' \geq n' \Leftrightarrow 2n \geq 2n' \Leftrightarrow n' \leq n \Leftrightarrow$ contradiction.

   (b) Assume $0 \leq n' \leq n$:

   $$\sum_{l'=|n'|}^{|n|-|n-n'|} = \sum_{l'=n'}^{n-n+n'} = \sum_{l'=n'}^{n'}$$

   (c) Assume $n' < 0$:

   $$\sum_{l'=|n'|}^{|n|-|n-n'|} = \sum_{l'=-n'}^{n-n+n'} = \sum_{l'=-n'}^{n'}$$

   This requires $n' \geq -n' \Leftrightarrow$ contradiction.

   Therefore

   $$\begin{aligned} \tilde{d}_{n,|n|} &= \sum_{n'=-\infty}^{+\infty} \sum_{l'=|n'|}^{|n|-|n-n'|} d^{(1)}_{n',l'} d^{(2)}_{n-n',|n|-l'} \\ &= \sum_{n'=0}^{n} d^{(1)}_{n',n'} d^{(2)}_{n-n',n-n'} \\ &= \sum_{n'=0}^{n} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|}. \end{aligned}$$

2. Assume $n < 0$:

   (a) Assume $n' > 0$:

   $$\sum_{l'=|n'|}^{|n|-|n-n'|} = \sum_{l'=n'}^{-n+n-n'} = \sum_{l'=n'}^{-n'}$$

   This requires $-n' \geq n' \Leftrightarrow$ contradiction.

(b) Assume $n \leq n' \leq 0$:

$$\sum_{l'=|n'|}^{|n|-|n-n'|} = \sum_{l'=-n'}^{-n+n-n'} = \sum_{l'=-n'}^{-n'}$$

(c) Assume $n' < n < 0$:

$$\sum_{l'=|n'|}^{|n|-|n-n'|} = \sum_{l'=-n'}^{-n-n+n'} = \sum_{l'=-n'}^{-2n+n'}$$

This requires $-2n + n' \geq -n' \Leftrightarrow -2n \geq -2n' \Leftrightarrow n \leq n' \Leftrightarrow$ contradiction.

Therefore

$$\begin{aligned}
\tilde{d}_{n,|n|} &= \sum_{n'=-\infty}^{+\infty} \sum_{l'=|n'|}^{|n|-|n-n'|} d^{(1)}_{n',l'} d^{(2)}_{n-n',|n|-l'} \\
&= \sum_{n'=n}^{0} d^{(1)}_{n',-n'} d^{(2)}_{n-n',-n+n'} \\
&= \sum_{n'=n}^{0} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|}.
\end{aligned}$$

So, by combining the cases $n \geq 0$ and $n < 0$, we get

$$\tilde{d}_{n,|n|} = \sum_{n'=\min(0,n)}^{\max(0,n)} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|}.$$

Now compute $Q[f_1]$, $Q[f_2]$, and finally $Q[Q[f_1]Q[f_2]]$ and compare with the result for $Q[f_1 f_2]$.

$$\begin{aligned}
Q[f_1] &= \sum_{m=-\infty}^{+\infty} d^{(1)}_{m,|m|} \theta^{|m|} e^{im\phi} \\
Q[f_2] &= \sum_{m=-\infty}^{+\infty} d^{(2)}_{m,|m|} \theta^{|m|} e^{im\phi} \\
Q[f_1]Q[f_2] &= \sum_{m=-\infty}^{+\infty} d^{(1)}_{m,|m|} \theta^{|m|} e^{im\phi} \sum_{m'=-\infty}^{+\infty} d^{(2)}_{m',|m'|} \theta^{|m'|} e^{im'\phi} \\
&= \sum_{m=-\infty}^{+\infty} \sum_{m'=-\infty}^{+\infty} d^{(1)}_{m,|m|} d^{(2)}_{m',|m'|} \theta^{|m|+|m'|} e^{i(m+m')\phi}
\end{aligned}$$

Change variables from m, m' to n, n' as before to get

$$Q[f_1]Q[f_2] = \sum_{n=-\infty}^{+\infty} \sum_{n'=-\infty}^{+\infty} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|} \theta^{|n'|+|n-n'|} e^{in\phi}.$$

This is a function in $\mathcal{P}$ because $Q[f_1]$ and $Q[f_2]$ are functions in $\mathcal{P}$ and products of functions in $\mathcal{P}$ are in $\mathbf{P}$. Therefore

$$Q[Q[f_1]Q[f_2]] = \sum_{n=-\infty}^{+\infty} \sum_{\{n':|n'|+|n-n'|=|n|\}} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|} \theta^{|n|} e^{in\phi} \tag{43}$$

Consider cases:

1. Assume $n \geq 0$:

   (a) Assume $n' > n \geq 0$: $\{n' : |n'| + |n - n'| = |n|\} \Leftrightarrow \{n' : n' - n + n' = n\} \Leftrightarrow \{n' : 2n' = 2n\} \Leftrightarrow \{n' : n' = n\} \Leftrightarrow$ contradiction.

   (b) Assume $0 \leq n' \leq n$: $\{n' : |n'| + |n - n'| = |n|\} \Leftrightarrow \{n' : n' + n - n' = n\} \Leftrightarrow 0 = 0 \Leftrightarrow$ no further restriction on n'.

   (c) Assume $n' < 0$: $\{n' : |n'| + |n - n'| = |n|\} \Leftrightarrow \{n' : -n' + n - n' = n\} \Leftrightarrow \{n' : -2n' = 0\} \Leftrightarrow \{n' : n' = 0\} \Leftrightarrow$ contradiction.

   Therefore

$$\sum_{n=0}^{\infty} \sum_{\{n':|n'|+|n-n'|=|n|\}} = \sum_{n=0}^{\infty} \sum_{n'=0}^{n}.$$

2. Assume $n < 0$:

   (a) Assume $n' > 0$: $\{n' : |n'| + |n - n'| = |n|\} \Leftrightarrow \{n' : n' - n + n' = -n\} \Leftrightarrow \{n' : 2n' = 0\} \Leftrightarrow \{n' : n' = 0\} \Leftrightarrow$ contradiction.

   (b) Assume $n \leq n' \leq 0$: $\{n' : |n'| + |n - n'| = |n|\} \Leftrightarrow \{n' : -n' - n + n' = -n\} \Leftrightarrow \{n' : 0 = 0\} \Leftrightarrow$ no further restriction on n'.

   (c) Assume $n' < n < 0$: $\{n' : |n'| + |n - n'| = |n|\} \Leftrightarrow \{n' : -n' + n - n' = -n\} \Leftrightarrow \{n' : -2n' = -2n\} \Leftrightarrow \{n' : n' = n\} \Leftrightarrow$ contradiction.

   Therefore

$$\sum_{n=-\infty}^{-1} \sum_{\{n':|n'|+|n-n'|=|n|\}} = \sum_{n=-\infty}^{-1} \sum_{n'=n}^{0}.$$

So, by combining the cases $n \geq 0$ and $n < 0$, we get

$$\sum_{n=-\infty}^{+\infty} \sum_{\{n':|n'|+|n-n'|=|n|\}} = \sum_{n=-\infty}^{+\infty} \sum_{n'=\min(0,n)}^{\max(0,n)} \tag{44}$$

Apply **Eq.** 44 to **Eq.** 43 to get

$$\begin{aligned} Q[Q[f_1]Q[f_2]] &= \sum_{n=-\infty}^{+\infty} \sum_{n'=\min(0,n)}^{\max(0,n)} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|} \theta^{|n|} e^{in\phi} \\ &= \sum_{n=-\infty}^{+\infty} \left(\sum_{n'=\min(0,n)}^{\max(0,n)} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|} \right) \theta^{|n|} e^{in\phi} \\ &= \sum_{n=-\infty}^{+\infty} d'_{n,|n|} \theta^{|n|} e^{in\phi} \end{aligned}$$

where $d'_{n,|n|}$ is defined to be

$$d'_{n,|n|} = \sum_{n'=\min(0,n)}^{\max(0,n)} d^{(1)}_{n',|n'|} d^{(2)}_{n-n',|n-n'|}.$$

Since $d'_{n,|n|} = \tilde{d}_{n,|n|}$ it follows that $Q[f_1 f_2] = Q[Q[f_1]Q[f_2]]$ is verified.

The general case is proved by induction:

$$\begin{aligned} Q[\prod_{j=0}^{N} f_j] &= Q[Q[\prod_{j=0}^{N-1} f_j]Q[f_N]] \\ &= Q[Q[\prod_{j=0}^{N-1} Q[f_j]]Q[Q[f_N]]] \\ &= Q[\prod_{j=0}^{N} Q[f_j]]. \end{aligned}$$

C Q Is Not Continuous

Define

$$\begin{aligned} S &= \text{unit sphere in } R^3 \\ \|f\|_{L_p(S)} &= \left(\int |f(\omega)|^p \mathrm{d}\Omega\right)^{1/p} \\ L_p(S) &= \left\{f : S \to C : \|f\|_{L_p(S)} < \infty\right\} \\ T &= \text{unit circle in C} \\ \|f\|_{L_p(T)} &= \left(\frac{1}{2\pi}\int_{-\pi}^{+\pi} |f(t)|^p \mathrm{d}t\right)^{1/p} \\ L_p(T) &= \left\{f : T \to C : \|f\|_{L_p(T)} < \infty\right\} \end{aligned}$$

The spaces $L_p(S)$ and $L_p(T)$ have the topology induced by the norms $\|\cdot\|_{L_p(S)}$ and $\|\cdot\|_{L_p(T)}$ respectively.

Lemma 1 $Q : L_p(S) \to L_p(S)$ is not bounded for $p = 2$.

Proof: Counter example to the assertion that Q is bounded. Define

$$\begin{aligned} p(\theta) &= \begin{cases} 1, & 0 \le \theta < \pi \\ -1, & \pi \le \theta < 2\pi \\ 0, & \text{otherwise} \end{cases} \\ x(\theta) &= \sum_{n=-\infty}^{+\infty} p(\theta - n2\pi). \end{aligned}$$

The Fourier series coefficients of x are

$$a_k = \frac{1}{2\pi}\int_0^{2\pi} x(\theta)e^{-jk\theta}\mathrm{d}\theta = j\frac{1}{k\pi}\left((-1)^k - 1\right)$$

and the partial sums are

$$x_n(\theta) = \sum_{k=-n}^{+n} a_k e^{jk\theta} = \frac{2}{\pi}\sum_{k=1}^{n} \frac{2}{2k+1}\sin(2k+1)\theta.$$

The key theoretical result is [17, Section 4.26 Eq. 7]

$$\lim_{n\to\infty} ||x(\theta) - x_n(\theta)||_{L_2(T)} = 0.$$

Define

$$f_n(\theta,\phi) = 1 - x_n(\theta)$$

(i.e., independent of ϕ). Note that

$$\begin{aligned} ||f_n||_{L_p(S)} &= \left(\int |f_n(\omega)|^p \mathrm{d}\Omega\right)^{1/p} \\ &= \left(\int_0^{2\pi}\int_0^{\pi} (1 - x_n(\theta)|^p \sin\theta \mathrm{d}\theta \mathrm{d}\phi\right)^{1/p} \\ &= \left(2\pi\int_0^{\pi} |1 - x_n(\theta)|^p \sin\theta \mathrm{d}\theta\right)^{1/p} \end{aligned}$$

which is obviously finite for $1 \leq p \leq \infty$ so $f_n \in L_p(S)$ for $1 \leq p \leq \infty$. Furthermore,

$$\begin{aligned} \lim_{n\to\infty} ||f_n||_{L_p(S)} &= \lim_{n\to\infty}\left(2\pi\int_0^{\pi} |1 - x_n(\theta)|^p \sin\theta \mathrm{d}\theta\right)^{1/p} \\ &\leq \lim_{n\to\infty}\left(2\pi\int_0^{\pi} |1 - x_n(\theta)|^p \,\mathrm{d}\theta\right)^{1/p} \\ &= \lim_{n\to\infty}\left(2\pi\int_0^{\pi} |x(\theta) - x_n(\theta)|^p \,\mathrm{d}\theta\right)^{1/p} \\ &\leq \lim_{n\to\infty}\left(2\pi\int_{-\pi}^{+\pi} |x(\theta) - x_n(\theta)|^p \,\mathrm{d}\theta\right)^{1/p} \\ &\leq (4\pi^2)^{1/p} \lim_{n\to\infty}\left(\frac{1}{2\pi}\int_{-\pi}^{+\pi} |x(\theta) - x_n(\theta)|^p \,\mathrm{d}\theta\right)^{1/p} \\ &\leq (4\pi^2)^{1/p} \lim_{n\to\infty} ||x(\theta) - x_n(\theta)||_{L_p(T)} \\ &= 0 \end{aligned}$$

for $p = 2$.

Expand f_n as a Taylor series in θ to find that

$$f_n(\theta,\phi) = 1 + \sum_{k=1}^{\infty} d_{0,k}^{(n)}\theta^k$$

Therefore

$$\begin{aligned} Q[f_n] &= 1 \\ ||Q[f_n]||_{L_p(S)} &= 4\pi. \end{aligned}$$

Boundedness of Q requires the existence of c independent of n such that

$$||Q[f_n]||_{L_p(S)} \leq c||f_n||_{L_p(S)}.$$

But this is impossible because the left hand side has value 4π independent of n while the right hand side goes to 0 as n goes to ∞. □

Since Q is not bounded it is not continuous [11, Thm. 2.7-9 p. 97].

D Table of Icosahedral Harmonics

	1 = 0	6	10
$m = 0$	$2.820947917738781 \times 10^{-1}$	$6.746726148605862 \times 10^{-1}$	$4.691941147166168 \times 10^{-1}$
5		$-1.703718724395419 \times 10^{-4}$	$1.43221646738894 \times 10^{-5}$
10			5.23470931063209 x 10^{-10}

	$l = 12$	15	16
$m = 0$	$8.257237892937810 \times 10^{-1}$		$7.266060945668594 \times 10^{-1}$
5	$-3.21243304269289 \times 10^{-6}$	$-1.981609297252692 \times 10^{-6}$	$9.4847286780344 \times 10^{-7}$
10	$5.794431895189197 \times 10^{-11}$	$-3.418925633631284 \times 10^{-12}$	$-1.84241038811857 \times 10^{-12}$
15		$5.458054970675743 \times 10^{-17}$	$-1.17921811835546 \times 10^{-17}$

	I = 18	20	21
	9.002655639988 x 10^{-1}	1.974780890363718 x 10^{-1}	
	-4.983700158317558 x	3.407144393312143 x	$4.092807665027534 \times 10^{-7}$
10	2.95803665617139 x 10^{-13}	$2.227863454007644 \times 10^{-13}$	$-3.010993744539446 \times 10^{-14}$
15	$-1.333890988533275 \times 10^{-18}$	$6.341985647126132 \times 10^{-20}$	$-6.788856747248027 \times 10^{-20}$
20		$1.15898860510346 \times 10^{-24}$	$1.769037092778827 \times 10^{-25}$

	$l = 22$	24	25
$m = 0$	$9.37575294971949 \times 10^{-1}$	$9.21002314556901 \times 10^{-1}$	
5	$1.384569813591985 \times 10^{-7}$	$-1.421035598340473 \times 10^{-7}$	$-7.836655445742523 \times 10^{-8}$
10	$-5.112584978701351 \times 10^{-14}$	$1.41618895252736 \times 10^{-14}$	$-2.212844336129518 \times 10^{-14}$
15	$2.516822842735015 \times 10^{-20}$	$-3.592455208180777 \times 10^{-21}$	$-3.108175909252568 \times 10^{-21}$
20	$4.848248656832747 \times 10^{-26}$	$5.399914634711366 \times 10^{-27}$	$-2.351130649241877 \times 10^{-28}$
25			$6.664202520526863 \times 10^{-33}$

	$l = 26$	27	28
$m = 0$	$3.860047773473439 \times 10^{-1}$		1.109757377696939
5	$1.172309989757126 \times 10^{-7}$	$-1.212289006689981 \times 10^{-7}$	$2.466285348255486 \times 10^{-8}$
10	$7.210763030113126 \times 10^{-15}$	$5.001166305854851 \times 10^{-15}$	$-3.796785188178502 \times 10^{-15}$
15	$-1.841009178201948 \times 10^{-21}$	$6.81115797800298 \times 10^{-23}$	$3.831523631119293 \times 10^{-22}$
20	$-3.081476412319671 \times 10^{-28}$	$-2.439701260119987 \times 10^{-28}$	$-7.253047020276402 \times 10^{-29}$
25	$-9.61759179875053 \times 10^{-34}$	$1.77966069978407 \times 10^{-34}$	$-5.53498704233547 \times 10^{-35}$

	$l = 30$	31	32
$m = 0$	$9.01569227139824 \times 10^{-1}$		$5.912043206775618 \times 10^{-1}$
5	$-5.249368166465911 \times 10^{-8}$	$4.066423227257543 \times 10^{-8}$	$4.516106993595139 \times 10^{-8}$
10	$1.824069922388993 \times 10^{-15}$	$2.147891855582007 \times 10^{-15}$	$2.856322894969714 \times 10^{-16}$
15	$-6.175638444747661 \times 10^{-23}$	$-4.260982316778084 \times 10^{-23}$	$-5.312331540457917 \times 10^{-23}$
20	$1.075554968785223 \times 10^{-29}$	$-9.05248128889912 \times 10^{-30}$	$3.475695412280682 \times 10^{-30}$
25	$-5.995007894572019 \times 10^{-36}$	$-3.974788085024645 \times 10^{-37}$	$3.686048735186758 \times 10^{-37}$
30	$1.108560758031187 \times 10^{-42}$	$1.810012789173336 \times 10^{-42}$	$3.370317401055845 \times 10^{-43}$

	$l = 33$	34	35
$m = 0$		1.242957162616307	
5	$4.486285313525142 \times 10^{-8}$	$2.380278380794479 \times 10^{-9}$	$-6.032316664388148 \times 10^{-9}$
10	$-8.52285852319967 \times 10^{-16}$	$-4.725495304789349 \times 10^{-16}$	$-4.525952834415354 \times 10^{-16}$
15	$1.008085340956216 \times 10^{-23}$	$1.584241562420297 \times 10^{-23}$	$-1.974304602544374 \times 10^{-23}$
20	$5.272366428771854 \times 10^{-31}$	$-7.281659645442291 \times 10^{-31}$	$-5.245009573501727 \times 10^{-31}$
25	$-2.499264840327398 \times 10^{-37}$	$6.326030738966593 \times 10^{-38}$	$-8.87544935404272 \times 10^{-39}$
30	$6.70116055428839 \times 10^{-44}$	$2.273849328188475 \times 10^{-44}$	$-9.93054644122186 \times 10^{-47}$
35			$1.253856873891649 \times 10^{-50}$

	$l = 36$	37	38
$m = 0$	$8.56692849713775 \times 10^{-1}$		$8.02920876707103 \times 10^{-1}$
5	$-2.152533913520913 \times 10^{-8}$	$-2.122177182350715 \times 10^{-8}$	$1.911274555252725 \times 10^{-8}$
10	$3.804515951584917 \times 10^{-16}$	$-2.743111103464194 \times 10^{-16}$	$-2.434891556327175 \times 10^{-17}$
15	$-3.749484450202822 \times 10^{-24}$	$5.092490758073693 \times 10^{-24}$	$-2.598492653811124 \times 10^{-24}$
20	$6.58716976948225 \times 10^{-32}$	$1.142912702558767 \times 10^{-32}$	$7.806577174288525 \times 10^{-32}$
25	$-1.080807166661601 \times 10^{-38}$	$-7.406812860704781 \times 10^{-39}$	$-2.136777280783503 \times 10^{-39}$
30	$2.345992971190676 \times 10^{-45}$	$-2.019602205408182 \times 10^{-46}$	$-1.528700910628074 \times 10^{-46}$
35	$-2.867106842446356 \times 10^{-52}$	$2.536169134780216 \times 10^{-52}$	$-5.377901999001163 \times 10^{-53}$

	$l = 39$	40	41
$m = 0$		1.33588637256797	
5	$-1.921472637729343 \times 10^{-8}$	$-2.222877700343102 \times 10^{-9}$	$5.106552332260171 \times 10^{-9}$
10	$1.844404284013966 \times 10^{-16}$	$-7.781110244333583 \times 10^{-17}$	$1.237898502324493 \times 10^{-16}$
15	$-1.282826197584042 \times 10^{-24}$	$1.23300080075066 \times 10^{-24}$	$1.198805920770535 \times 10^{-24}$
20	$3.242397542911047 \times 10^{-33}$	$-1.826761158766107 \times 10^{-32}$	$-9.291183030874 09 \times 10^{-33}$
25	$5.469150678188241 \times 10^{-40}$	$4.798290114278227 \times 10^{-40}$	$-3.847457531098831 \times 10^{-40}$
30	$-9.41556094573599 \times 10^{-47}$	$-2.083888698912835 \times 10^{-47}$	$-4.780007598610431 \times 10^{-48}$
35	$1.100216050831976 \times 10^{-53}$	$-3.99452386976723 \times 10^{-54}$	$-3.416126089592718 \times 10^{-56}$
40		$1.033497023010075 \times 10^{-61}$	$6.161843595946462 \times 10^{-61}$

	$l = 42$	43	44
$m = 0$	$8.06071321824356 \times 10^{-1}$		1.011111294485445
5	$-8.63760995566038 \times 10^{-9}$	$1.164911977536833 \times 10^{-8}$	$8.56099642897334 \times 10^{-9}$
10	$1.017062390750238 \times 10^{-16}$	$4.068515022247794 \times 10^{-17}$	$-1.8708832046258 \times 10^{-17}$
15	$-4.810395831967041 \times 10^{-25}$	$-5.586860979470261 \times 10^{-25}$	$-1.785868201272553 \times 10^{-25}$
20	$9.94869187201453 \times 10^{-34}$	$2.646041577375465 \times 10^{-33}$	$2.896782107262829 \times 10^{-33}$
25	$-2.161763116615656 \times 10^{-41}$	$3.161354500569589 \times 10^{-41}$	$-3.871580673004682 \times 10^{-41}$
30	$4.327504389994189 \times 10^{-48}$	$-2.283643210069411 \times 10^{-48}$	$5.236495191096205 \times 10^{-49}$
35	$-3.748264428640973 \times 10^{-55}$	$-4.081559696939951 \times 10^{-56}$	$2.670334941512591 \times 10^{-56}$
40	$3.419400195443956 \times 10^{-62}$	$1.857415764225622 \times 10^{-62}$	$4.286637228246185 \times 10^{-63}$

Table **3:** Table of $b_{l,n,m}$ coefficients for $T_{l,n}$ for n $= 0$ and $l \in \{0, 1, \ldots, 44\}$

	$l = 30$	36	40
$m = 5$	$2.448476817539395 \times 10^{-8}$	$1.803441604722151 \times 10^{-8}$	$1.932825739861001 \times 10^{-9}$
10	$2.729150909570428 \times 10^{-15}$	$4.48552570399961 \times 10^{-16}$	$8.46281746373447 \times 10^{-17}$
15	$2.223541523901881 \times 10^{-22}$	$4.42763367294824 \times 10^{-24}$	$2.185857402650686 \times 10^{-24}$
20	$8.62645832774495 \times 10^{-30}$	$-3.304529063250246 \times 10^{-31}$	$3.772670014340045 \times 10^{-32}$
25	$7.299788172714104 \times 10^{-37}$	$-9.17215096845515 \times 10^{-39}$	$4.09207555121917 \times 10^{-40}$
30	$1.390278734957254 \times 10^{-41}$	$-6.356669301255897 \times 10^{-46}$	$3.586951882500613 \times 10^{-48}$
35		$-1.482301423807387 \times 10^{-51}$	$9.24608924171111 \times 10^{-56}$
40			$5.478206798694867 \times 10^{-60}$
	$l = 42$		
$m = 5$	$1.225965666804088 \times 10^{-8}$		
10	$7.336055391266129 \times 10^{-17}$		
15	$-2.057018909283102 \times 10^{-27}$		
20	$-9.56403128492941 \times 10^{-33}$		
25	$1.547346440349331 \times 10^{-40}$		
30	$2.864253792321392 \times 10^{-48}$		
35	$1.869449403196465 \times 10^{-55}$		
40	$9.13353520771848 \times 10^{-62}$		

Table 4: Table of $b_{l,n,m}$ coefficients for $T_{l,n}$ for n = 1 and $l \in \{0, 1, \ldots, 44\}$.

E *Mathematica* Programs for Computing Icosahedral Harmonics

```
(* Mathematica Program for generating icosahedral harmonics. *)

BeginPackage["IcosahedralT`"]

(* Warning: Computation of higher order icosahedral harmonics may
            take a lot of time. It is advisable to save the icosahedral
            harmonics once they are formed by the program. *)

IcosahedralT::usage =
             "IcosahedralT[l,n] gives the n-th set of the l-th order
             normalized icosahedral harmonics in terms of the regular
             spherical harmonics Y. "

(* Y appears to substitute for SphericalHarmonicY used in Mathematica *)



Begin["`Private`"]

(* The simplest icosahedral harmonic is a constant. The normalization
   of the icosahedral harmonics are such that
   Integrate[T[l,n,theta,phi]*Sin[theta],{theta,0,Pi}, {phi,0,2*Pi}]=60 *)

IcosahedralT[0,0] := Sqrt[15/Pi]
```

```
xp=1/Sqrt[5]

(* Number of icosahedral harmonics of order l. *)

Nl[l_] := Nl[l] = If[EvenQ[l],Neven[l],Nodd[l]]

Nodd[l_] := Nodd[l] = If[l>=15,Neven[l-15],0]

Neven[l_] := Neven[l] = Coefficient[Normal[Series [sel[x],{x,0,l}]], x^l]

sel[x_] := 1/((1 - x^6)*(1 - x^10))

delta[n_] := If[n==0,1,0]

NP[l_,m_] := Sqrt[(2*l+1)*(l-m)!/(4*Pi*(l+m)!)]

g[l_,m_] := (-1)^m*(l+m)!/(l-m)!/(2*m)!!

(* Compute the c or s coefficients. *)

fc[m_] := Cos[m*ArcSin[(5^(1/2)*y)/(2*(1 - x - x^2)^(1/2))]]

fs[m_] := -Sin[m*ArcSin[(5^(1/2)*y)/(2*(1 - x - x^2)^(1/2))]]

c[p_,q_,m_] := c[p,q,m] = Coefficient[cie[m],x^p*y^q]/.{x->0,y->0}
s[p_,q_,m_] := s[p,q,m] = coefficient[sie[m],x^p*y^q]/.{x->0,y->0}

(* Compute the k-th derivative of the associated Legendre functions. *)

P[l_, m_, k_, x_] :=
  Simplify[LegendreP[l - 1, m, x]*A[l,m,k, x]+LegendreP[l, m, x]*B[l,m,k, x]]

A[l_,m_,0, x_] = 0

A[l_,m_,k_, x_] := A[l,m,k, x] =
   Simplify[(D[A[l,m,k - 1, y], y]/.y->x) + (l*x*A[l,m,k - 1, x] +
   (l + m)*B[l,m,k - 1, x])/(1 - x^2)]

B[l_,m_,0, x_] = 1

B[l_,m_,k_, x_] := B[l,m,k, x] =
   Simplify[(D[B[l,m,k - 1, y], y]/.y->x) - (l*x*B[l,m,k - 1, x] +
   (l - m)*A[l,m,k - 1, x])/(1 - x^2)]

IcosahedralT[l_,n_] := Module[{},

(* Check validity of l and n. *)
```

```
 If[!IntegerQ[l] || !IntegerQ[n] || l<0 || n<0 ||
    If[EvenQ[l],n>=Nl[l],n>Nl[l]] || n == 0], 0,

(* Deal with even and odd icosahedral harmonics separately *)

   If[EvenQ[l],

(* Compute the right hand side of Eq. (59), (60) *)

rhs[m_,mp_] := rhs[m,mp] =
      5*Sqrt[(l-m)!*(l+mp)!/(l+m)!/(l-mp)!]*
      Simplify[delta[m-mp]*(1+delta[mp])+
      5*2^(l-mp)/g[l,mp]*Sum[P[l,m,k,xp]*(2*xp)^k/k!*
      Sum[c[mp-k-2*r,2*r,m]*(-1)^r,{r,0,(mp-k)/2}],{k,0,mp}]];

(* Compute b[l,n,5*n]*b[l,n,m]=bp[n,m] recursively. *)

bp[n1_,m_] := bp[n1,m] =
       rhs[m,5*n1]-Sum[bp[np,5*n1]*bp[np,m]/bp[np,5*np],{np,0,n1-1}];

bp[0,m_] := bp[0,m] = rhs[m,0];

cie[m_] = Expand[Simplify[Normal[Series[fc[m],{x,0,5*n},{y,0,5*n}]]]],

rhs[m_,mp_] := rhs[m,mp] =
      5*Sqrt[(l-m)!*(l+mp)!/(l+m)!/(l-mp)!]*
      Simplify[delta[m-mp] +
      5*2^(l-mp)/g[l,mp]*Sum[P[l,m,k,xp]*(2*xp)^k/k!*
      Sum[s[mp-k-2*r-1,2*r+1,m]*(-1)^r,{r,0,(mp-k-1)/2}],{k,0,mp}]];

bp[n1_,m_] := bp[n1,m] =
       rhs[m,5*n1]-Sum[bp[np,5*n1]*bp[np,m]/bp[np,5*np],{np,1,n1-1}];

bp[1,m_] := bp[1,m] = rhs[m,5];

sie[m_] = Expand[Simplify[Normal[Series[fs[m],{x,0,5*n},{y,0,5*n}]]]]

  ];

b[5*n]=Sqrt[bp[n,5*n]];

For[m=5*n,m<=l,m+=5,b[m]=bp[n,m]/b[5*n];
    b[-m]=(-1)^(l+m)*b[m]];

Simplify[Sum[b[m]*Y[l,m],{m,-5*n,-1,-5}] + Sum[b[m]*Y[l,m],{m,5*n,l,5}]]

 ]
```

```
End[]

EndPackage[]
```

F Verification of the Symmetry of $T_{6,0}$ Under Operation U

In this appendix we illustrate the verification procedure by demonstrating that $T_{6,0}(\theta,\phi)$ is invariant under the operation U. The procedure to perform the symbolic verification is the following:

1. Express $T_{6,0}$ as a homogeneous polynomial in x, y, z. To do this:

   - Expand $P_{6,0}(\cos 8)$ and $P_{6,5}(\cos 8)$ into polynomials in $\sin\theta$ and $\cos\theta$:

$$P_{6,0}(\cos 8) = \frac{1}{16}(-5 + 105\cos^2\theta - 315\cos^4\theta + 231\cos^6 8)$$
$$P_{6,5}(\cos\theta) = -10395\cos\theta\sin^5\theta.$$

   - Write $\cos 5\phi$ (or $\sin m\phi$, m $= 5\mu$, if l is odd) as sums of products of trigonometric functions of the single angle ϕ:

$$\cos 5\phi = 5\cos\phi - 20\cos^3\phi + 16\cos^5\phi.$$

   - Expand $T_{6,0}(\theta,\phi)$ into sums of products of $\sin\theta, \cos\theta, \sin\phi, \cos\phi$:

$$\begin{aligned} T_{6,0}(\theta,\phi) &= -\frac{2475}{2} + \frac{51975\cos(\theta)^2}{2} - \frac{155925\cos(\theta)^4}{2} + \frac{114345\cos(\theta)^6}{2} \\ &+ 51975\cos(\phi)\cos(\theta)\sin(\theta)^5 - 207900\cos(\phi)^3\cos(\theta)\sin(\theta)^5 \\ &+ 166320\cos(\phi)^5\cos(\theta)\sin(\theta)^5. \end{aligned}$$

   - Apply the following transformation rules sequentially:

$$\begin{aligned} \sin^n\theta\cos^m\phi &\rightarrow x^m\sin^{n-m}8; \quad n > m > 0 \\ \sin^n\theta\sin^m\phi &\rightarrow y^m\sin^{n-m}\theta; \quad n > m > 0 \\ \cos\theta &\rightarrow z; \\ \sin^n 8 &\rightarrow (1-z^2)^{n/2}; \quad n > 0,\ n \text{ even}. \end{aligned}$$

   The result is that

$$\begin{aligned} T_{6,0}(x,y,z) &= -\frac{2475}{2} + 51975\,x\,z - 207900\,x^3 z + 166320\,x^5 z + \frac{51975\,z^2}{2} - 103950\,x\,z^3 \\ &+ 207900\,x^3 z^3 - \frac{155925\,z^4}{2} + 51975\,x\,z^5 + \frac{114345\,z^6}{2}. \end{aligned} \tag{45}$$

2. **Apply** the rotation (linear transformation) to $T_{6,0}(x, y, z)$ by making the following substitutions:

$$\begin{aligned} x &\rightarrow \frac{1}{\sqrt{5}}(-x+2z) \\ y &\rightarrow -y \\ z &\rightarrow \frac{1}{\sqrt{5}}(2x+z). \end{aligned}$$

The result is that

$$\begin{aligned} T'_{6,0}(x,y,z) &= -\frac{2475}{2} + \frac{10395\,(2\,x+z)^2}{2} - \frac{6237\,(2\,x+z)^4}{2} + \frac{22869\,(2\,x+z)^6}{50} \\ &+ 10395\,(2\,x+z)\,(-x+2\,z) - 4158\,(2\,x+z)^3\,(-x+2\,z) \\ &+ \frac{2079\,(2\,x+z)^5\,(-x+2\,z)}{5} - 8316\,(2\,x+z)\,(-x+2\,z)^3 \\ &+ \frac{8316\,(2\,x+z)^3\,(-x+2\,z)^3}{5} + \frac{33264\,(2\,x+z)\,(-x+2\,z)^5}{25} \end{aligned} \quad (46)$$

3. Expand the polynomial obtained in the Step 2 (Eq. 46) and collect terms.

4. If the polynomial obtained in Step **3** is equal to that obtained in Step 1 (Eq. 45), then the symmetry is verified. In comparing the polynomials, it may be necessary to use the collstra.int that x, y, and z lie on the surface of the unit sphere, i.e.,

$$x^2 + y^2 + z^2 = 1.$$

   That is, if the difference of the polynomials is zero or if it contains a factor of $x^2 + y^2 + z^2 - 1$, then the two polynomials are equal on the surface of the unit sphere.

   In the case of $T_{6,0}$, Eq. 46, after expansion, is exactly the same as Eq. 45.

A set of transformation rules written in *Mathematica*, which perform Steps 1–4, is listed in Appendix G.

G *Mathematica* Programs for Verifying Icosahedral :Harmonics

```
(*
   Verify the icosahedral symmetry of polynomials of
   spherical harmonics T[theta, phi].  The coordinate system
   is that defined in the text.
*)

<<Algebra'Trigonometry'

(* step 1: Transform the harmonics into polynomials of
          {Sin[phi], Cos[phi], Sin[theta], Cos[theta] };
          Note ComplexToTrig or rule0 may not be necessary,
          depending on how you write the spherical harmonics.
          Command:
```

```
            Expand[TrigReduce[ComplexToTrig[Simplify[T[theta, phi]]/.rule0]]].
*)

rule0 = {(Sin[theta]^a_)^b_->Sin[theta]^(a*b)};

(* step 2: Transform the expression obtained above into polynomials
           of Cartesian coordinates {x,y,z};
           Command:
           Expand[((%/.rule1)/.rule2)/.rule3].
*)

rule1 = {Cos[phi] *Sin[theta]->x,
         Cos[phi]*Sin[theta]^(n_)->x*Sin[theta]^(n - 1),
         Cos[phi]^(m_)*Sin[theta]^(n_)->x^m*Sin[theta]^(n - m)};

rule2 = {Sin[phi]*Sin[theta]->y,
         Sin[phi]*Sin[theta]^(n_)->y*Sin[theta]^(n - 1),
         Sin[phi]^(m_)*Sin[theta]^(n_)->y^m*Sin[theta]^(n - m)};

rule3 = {Cos[theta]->z, Sin[theta]^n_->(1-z^2)^(n/2)};

(* step 3: Now the icosahedral symmetric rotation;
           To verify symmetry under U, use rule4a;
           To verify symmetry under S, use rule4b;
           To verify symmetry under P, use rule4c;
           Command:
           Expand[%/.rule4a].
*)

rule4a = {x->(2*z - x)/Sqrt[5], y->-y, z->(z + 2*x)/Sqrt[5]};
rule4b = {x->(x*(Sqrt[5]-1)/4-y*Sqrt[5+Sqrt[5]]/(2*Sqrt[2])),
          y->(x*Sqrt[5+Sqrt[5]]/(2*Sqrt[2])+y*(Sqrt[5]-1)/4)};
rule4c = {x->-x, z->-z};

(* step 4: If the polynomial obtained in step 3 is identical to
           that in step 2, the symmetry is verified. The constraint
           x^2+y^2+z^2 = 1 may be used.
           Command:
           Factor[%-%%]/.rule5 .
*)

rule5={y^n_?EvenQ->(1-x^2-z^2)^(n/2)};
```

References

[1] S. L. Altmann. On the symmetries of spherical harmonics. Proc. Camb. Phil. *Soc.*, 53:343–367, 1957.

[2] N. V. Cohan. The spherical harmonics with the symmetry of the icosahedral group. Proc. Camb. Phil. *Soc.*, 54:28–38, 1958.

[3] L. Elcoro, J. M. Perez-Mato, and G. Madariaga. Determination of quasicrystalline structures: a refinement program using symmetry-adapted parameters. *Acta Cryst.*, A50:182–193, 1994.

[4] J. T. Finch and K. C. Holmes. Structural Studies of Viruses, volume III of *Methods* in Virology, chapter 9. Academic Press, New York and London, 1967.

[5] I. S. Gradshteyn and I. M. Ryzhik. Table of Integrals, Series, and *Products*. Academic Press, New York, fourth edition, 1980.

[6] E. Heuser-Hofmann and W. Weyrich. Three-dimensional reciprocal form factors arid momentum densities of electrons from Compton experiments: I. Symmetry-adapted series expansion of the electron inomentum density. *Z. Naturforsch.*, 40a:99–111, 1985.

[7] A. Jack and S. C. Harrison. On the interpretation of small-angle x-ray solution scattering from spherical viruses. J. Mol. Biol., 99:15–25, 1975.

[8] J. D. Jackson. Classical Electrodynamics. John Wiley, second edition, 1975.

[9] M. Kara and K. Kurki-Suonio. Symmetrized multipole analysis of orientational distributions. Acta *Cryst.*, A37:201–210, 1981.

[10] W. Kratschmer, L. D. Lamb, K. Fostiropoulos, and D. R. Huffman. Solid C_{60}: a new form of carbon. Nature (London), 347:354–357, 1990.

[11] E. Kreyszig. Introductory Functional Analysis With Applications. John Wiley and Sons, 1978.

[12] 0 . Laporte. Polyhedral harmonics. *Z. Naturforschg.*, 3a:447–456, 1948.

[13] L. Liljas. Structure of spherical viruses. Int. J. Biol. Macrornol., 13:273–280, October 1991

[14] F. Liu, J.-L. Ping, and C. Jin-Quan. Application of the eigenfunction method to the icosahedral group. J. Math. Phys., 31(5):1065–1075, 1990.

[15] A. G. McLellan. Eigenfunctions for integer and half-odd integer values of J symmetrized according to the icosahedral group and the group C_{3v}. J. Chem. Phys., 34(4):1350–1359, 1961.

[16] M. E. Rose. Elementary Theory of Angular Momentum. John Wiley and Sons, 1957.

[17] W. Rudin. Real *and* Complex Analysis. McGraw-Hill Book Company, second edition, 1974