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Explicit Orthonormal Fixed Bases for Spaces of Functions that are Totally Symmetric Under the Rotational Symmetries of a Platonic Solid†

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Abstract

Explicit complete orthonormal fixed bases are computed for subspaces of the space of square-integrable functions on the sphere where the subspaces contain functions that are totally symmetric under the rotational symmetries of a Platonic solid. Each function in the fixed basis is a linear combination of spherical harmonics of fixed l. For each symmetry (icosahedral/dodecahedral, octahedral/cubic, tetrahedral), the calculation has three steps: First, a bilinear equation is derived for the coefficients in the linear combination by equating the expansion of a symmetrized δ function in both spherical harmonics and the fixed basis functions for the appropriate subspace. The equation is parameterized by the location (θ_0, φ_0) of the δ function and must be satisfied for all locations. Second, the dependence on the δ-function location is expressed in a Fourier (φ_0) and a Taylor (θ_0) series and thereby a new system of bilinear equations is derived by equating selected coefficients. Third, a recursive solution of the new system is derived and the recursion is solved explicitly with the aid of symbolic computation. The results for the icosahedral case are important for structural studies of small spherical viruses.

1. Introduction

Let $L^2(\theta, \varphi)$ denote the Hilbert space of square-integrable functions on the sphere. We describe a method for computing orthonormal fixed bases for subspaces of $L^2(\theta, \varphi)$ where each subspace contains basis functions that transform as a particular row of a particular unitary irreducible representation of a group $\mathcal{G}$ of rotations in $\mathcal{R}^3$. We demonstrate the method by applying it to the identity representation of the icosahedral group. This particular example is of great interest in virus structural studies (Liljas, 1991; Zheng, Doerschuk & Johnson, 1995). We also state the results for the identity representations of the groups of the other Platonic solids.

In a virus structure problem, the electron density is assumed to be invariant under every rotation of the icosahedral group. Such functions form a subspace of $L^2(\theta, \varphi)$ and a natural way to describe the electron density is as a weighted sum of fixed basis functions for this subspace, where the fixed basis functions are orthonormal in addition to being totally symmetric under the rotations of the icosahedral group. Let the fixed basis functions be denoted by $T_\alpha(\theta, \varphi)$, where α is an index. Because the spherical harmonics (Jackson, 1975), denoted by $Y_{l,m}(\theta, \varphi)$, are a complete orthonormal fixed basis for $L^2(\theta, \varphi)$, it is natural to express $T_\alpha(\theta, \varphi)$ as

$$T_\alpha(\theta, \varphi) = \sum_{l=0}^{+\infty} \sum_{m=-l}^{+l} a_{\alpha,l,m} Y_{l,m}(\theta, \varphi).$$

Then, the goal is to determine $a_{\alpha,l,m}$.

The $T_\alpha(\theta, \varphi)$ functions are sometimes referred to as 'icosahedral harmonics' (*e.g.* Finch & Holmes, 1967; Jack & Harrison, 1975; Laporte, 1948). This terminology is somewhat different from the terminology used for spherical harmonics: for each l, the finite set of spherical harmonics $Y_{l,m}(\theta, \varphi)$ for $m = -l, \ldots, +l$ are basis functions of a particular representation of the special orthogonal group SO_3, while the countably infinite set of $T_\alpha(\theta, \varphi)$ functions are basis functions of only the identity representation of the icosahedral group.

Work on the construction of basis functions for various representations of the icosahedral group, including the $T_\alpha(\theta, \varphi)$ functions for the identity representation, has been done previously by Altmann (1957), Cohan (1958), Elcoro, Perez-Mato & Madariaga (1994), Heuser-Hofmann & Weyrich (1985), Jack & Harrison (1975), Kara & Kurki-Suonio (1981), Laporte (1948), Liu, Ping & Chen (1990), McLellan (1961) and Meyer (1954), among others. The approaches used include group-theoretical approaches and approaches through combining primitive invariant polynomials in the Cartesian coordinates. The construction process is very laborious, especially for large l, and no explicit formulae for $T_\alpha(\theta, \varphi)$, or equivalently for $a_{\alpha,l,m}$, could be given. The work described in this paper differs from the previous work in the following respects: each $T_\alpha(\theta, \varphi)$ is a linear combination of $Y_{l,m}(\theta, \varphi)$ for a single fixed l; the $a_{\alpha,l,m}$ coefficients of the combination are given by explicit formulae in terms of α, l and m; $T_\alpha(\theta, \varphi)$ and $T_{\alpha'}(\theta, \varphi)$ are orthogonal if $\alpha \neq \alpha'$. Other authors, *e.g.*

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Von der Lage & Bethe (1947), have also studied basis functions that are a linear combination of $Y_{l,m}(\theta, \varphi)$ for a single fixed l.

A standard group-theoretical approach to determine $T_\alpha(\theta, \varphi)$ is to apply projection operators (Cornwell, 1984, pp. 92–94) to the spherical harmonics. For the identity representation of the icosahedral group, the projection operator has a simple form and a candidate for $T_\alpha(\theta, \varphi)$, that is, the projection operator applied to a particular spherical harmonic, is

$$T_\alpha(\theta, \varphi) = \tfrac{1}{60} \sum_{k=0}^{59} P(T_k) Y_{l,m}(\theta, \varphi), \tag{1}$$

where T_k is the kth rotation of the icosahedral group, which has order 60, and the scalar transformation operator $P(T)$ applied to a function $\Psi(\mathbf{r})$ is defined by $P(T)\Psi(\mathbf{r}) = \Psi(T^{-1}\mathbf{r})$. [We are using the notation of Cornwell (1984).] While this method appears to be direct, it has some serious difficulties: First,

$$P(T_k) Y_{l,m}(\theta, \varphi) = \sum_{m'=-l}^{+l} D_{l,m,m'}(T_k) Y_{l,m'}(\theta, \varphi),$$

where the $D_{l,m,m'}(T_k)$ are the complicated Wigner D coefficients (see theorem 1), so it is difficult to perform the sum of (1) analytically for general l and m. Second, for a fixed l, Laporte's results (see theorem 2) state that there are only $N_l \leq 2l+1$ linearly independent $T_\alpha(\theta, \varphi)$ that can be constructed from $Y_{l,m}(\theta, \varphi)\,(m = -l, \ldots, +l)$ while (1) generates $2l+1$ candidates. Therefore, N_l functions must be chosen from among the $2l+1$ candidates. Furthermore, no set of N_l functions from among the candidates are guaranteed to be orthonormal, so a set of N_l linearly independent functions must then be orthogonalized by the Gram–Schmidt procedure. This orthogonalization is also difficult to perform analytically for general l and m. In summary, it is difficult to derive, by way of (1), expressions for an orthonormal set of $T_\alpha(\theta, \varphi)$ that are explicit functions of the indices.

Our approach is also based on projections. However, rather than projecting a spherical harmonic, as in (1), we project a delta function located at spherical coordinates (θ_0, φ_0), *i.e.* $\delta(\cos\theta - \cos\theta_0)\delta(\varphi - \varphi_0)$. The result of the projection is a symmetrized delta function denoted by $\Delta(\theta_0, \varphi_0; \theta, \varphi)$:

$$\Delta(\theta_0, \varphi_0; \theta, \varphi) = \tfrac{1}{60} \sum_{k=0}^{59} P(T_k)[\delta(\cos\theta - \cos\theta_0)\delta(\varphi - \varphi_0)]. \tag{2}$$

This projection is easy to compute because the result of applying a rotation to a delta function is just another delta function at different coordinates. Furthermore, it is straightforward to expand the symmetrized delta function $\Delta(\theta_0, \varphi_0; \theta, \varphi)$ as a weighted sum of spherical harmonics:

$$\Delta(\theta_0, \varphi_0; \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} w_{l,m}(\theta_0, \varphi_0) Y_{l,m}^*(\theta, \varphi).$$

In addition, because the $T_\alpha(\theta, \varphi)$ are a complete orthonormal fixed basis for the subspace of totally symmetric functions, we know the expansion of $\Delta(\theta_0, \varphi_0; \theta, \varphi)$ as a weighted sum of $T_\alpha(\theta, \varphi)$:

$$\Delta(\theta_0, \varphi_0; \theta, \varphi) = \sum_\alpha T_\alpha^*(\theta_0, \varphi_0) T_\alpha(\theta, \varphi). \tag{3}$$

Finally, by equating (1) and (3), we can derive nonlinear equations for the desired weights $a_{\alpha,l,m}$ and these nonlinear equations can be solved recursively to give explicit formulae for the $a_{\alpha,l,m}$.

In more detail, the program has the following steps:

(i) Show that the $T_\alpha(\theta, \varphi)$ can be indexed by two integers and expressed in the form

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

where $l = 0, 1, \ldots$ and $n = 0, \ldots, N_l - 1$. The goal of the calculation is to compute $b_{l,m,n}$.

(ii) Express a delta function that is totally symmetric under the rotations of the icosahedral group in terms of $Y_{l,m}(\theta, \varphi)$ and in terms of $T_{l,n}(\theta, \varphi)$.

(iii) Equate the two expansions.

(iv) 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).

(v) 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 doubly infinite sums. Corresponding coefficients in the two sums must be equal.

(vi) By equating corresponding coefficients of $\theta_0^j \exp(ik\varphi_0)$ for certain (j, k), derive a second system of bilinear equations for the $b_{l,n,m}$ coefficients. This system of equations does not depend on (θ_0, φ_0).

(vii) Derive a recursive solution for the second set of bilinear equations.

(viii) With the aid of *Mathematica*, solve the recursions to give exact values for the $b_{l,n,m}$ coefficients.

The remainder of the paper is organized in the following fashion. In §§2–6, we derive an orthonormal fixed basis for the subspace spanned by basis functions that transform as the identity representation of the icosahedral group. In §7, we state the corresponding results for the groups of the other Platonic solids. Finally, in §8, we show how similar ideas could be used to compute an orthonormal fixed basis for the subspace spanned by basis functions that transform as a particular row of a particular unitary irreducible representation of the icosahedral group. Such fixed orthonormal bases are of interest in a wider range of problems concerning the icosahedral group, such as fullerenes (Kratschmer, Lamb, Fostiropoulos & Huffman, 1990) and quasicrystals

(Elcoro, Perez-Mato & Madariaga, 1994). The results of this paper are described in greater detail in Zheng & Doerschuk (1994).

2. The relationship between the icosahedral fixed basis functions and spherical harmonics

Let $Y_{l,m}(\theta, \varphi)$, for $l = 0, 1, \ldots$ and $m = -l, \ldots, +l$, be spherical harmonics [we use the conventions of Jackson (1975)]. It is well known [Jackson, 1975, equation (3.53)] that $Y_{l,m}(\theta, \varphi) = N_{l,m} P_{l,m}(\cos\theta)\exp(im\varphi)$, where $P_{l,m}(x)$ are the associated Legendre functions [Jackson, 1975, equation (3.49)] and

$$N_{l,m} = \{[(2l+1)/4\pi][(l-m)!/(l+m)!]\}^{1/2}.$$

Spherical harmonics are closely related to rotations. Let T be a rotation of three-dimensional space described in terms of the Euler angles α, β, γ and having inverse T^{-1}.

Theorem 1. Any rotational operation on a spherical harmonic $Y_{l,m}(\theta, \varphi)$ will yield a linear combination of spherical harmonics of only the same l, that is,

$$P(T)Y_{l,m}(\theta, \varphi) = \sum_{m'=-l}^{+l} D_{l,m,m'}(\alpha, \beta, \gamma) Y_{l,m'}(\theta, \varphi),$$

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

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

$$\begin{aligned} d_{l,m,m'}(\beta) = \sum_{k=0}^{l+m} & (-1)^k [(l+m)!(l-m)!(l+m')! \\ & \times (l-m')!]^{1/2} / \{(l-m'-k)! \\ & \times (l+m-k)!(m'-m+k)!k!\} \\ & \times [\cos(\beta/2)]^{2l+m-m'-2k} \\ & \times [-\sin(\beta/2)]^{m'-m+2k}. \end{aligned}$$

Proof: See Rose (1957).

Our goal is to determine a set of functions $T_\alpha(\theta, \varphi)$ where the set is a real-valued complete orthonormal fixed basis for the subspace of $L^2(\theta, \varphi)$ containing functions that are totally symmetric under the rotations of the icosahedral group. The orthonormality condition is $\int T_\alpha^*(\theta, \varphi) T_{\alpha'}(\theta, \varphi)\, \mathrm{d}\Omega = \delta_{\alpha,\alpha'}$, where the complex conjugation is optional since the $T_\alpha(\theta, \varphi)$ are real and $\mathrm{d}\Omega = \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\varphi$ in spherical coordinates. Furthermore, we desire that each $T_\alpha(\theta, \varphi)$ function is a linear combination of $Y_{l,m}(\theta, \varphi)$ for fixed l, as allowed by theorem 1. Let N_l be the number of $T_\alpha(\theta, \varphi)$ that are linear combinations of $Y_{l,m}(\theta, \varphi)$ ($m = -l, \ldots, +l$) and therefore $N_l \leq 2l + 1$. We define the index α to be l, n, where $l = 0, 1, \ldots$ and $n = 0, \ldots, N_l - 1$, and therefore the functions have the general form

$$T_{l,n}(\theta, \varphi) = \sum_{m=-l}^{+l} b_{l,n,m} Y_{l,m}(\theta, \varphi). \quad (4)$$

The task of this paper is to find the $b_{l,n,m}$ coefficients in (4). For each $l = 0, 1, \ldots$, there are N_l sets of $2l + 1$ coefficients.

Laporte (1948) proves the following result regarding N_l:

Theorem 2. For l even, the number N_l is given by the generating function

$$1/[(1-x^6)(1-x^{10})] = \sum_{l=0}^{\infty} N_{2l} x^{2l},$$

while, for l odd, the number N_l is

$$N_l = \begin{cases} N_{l-15}, & l \geq 15 \\ 0, & 0 \leq l < 15. \end{cases} \quad (5)$$

The first fact about the $b_{l,n,m}$ coefficients can be determined simply from the choice that $T_{l,n}(\theta, \varphi)$ are real and $Y_{l,-m}(\theta, \varphi) = (-1)^m Y_{l,m}^*(\theta, \varphi)$ [Jackson, 1975, equation (3.54)].

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

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

The second fact, based on the orthonormality of the $Y_{l,m}(\theta, \varphi)$, relates the orthonormality of the $b_{l,n,m}$ coefficients to the orthonormality of the $T_{l,n}(\theta, \varphi)$:

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

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

3. The fundamental bilinear equation for $b_{l,n,m}$

For our calculations, we choose the coordinate system used by Altmann (1957) and Laporte (1948) in which the z axis 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 $\{(\theta_k, \varphi_k) : k = 1, 2, \ldots, 59\}$ 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:

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

$$\begin{aligned} \{(\theta_k, \varphi_k) &: k = 0, 1, \ldots, 59\} \\ &= \{(\theta_0, \varphi_k) : k = 0, 1, \ldots, 4\} \\ & \quad \bigcup \left(\bigcup_{n=0}^{4} \{[\gamma_n, \alpha_n + k(2\pi/5)] : k = 0, 1, \ldots, 4\} \right) \\ & \quad \bigcup \left(\bigcup_{n=0}^{4} \{[\pi - \gamma_n, \pi - \alpha_n \right. \\ & \quad \left. + k(2\pi/5)] : k = 0, 1, \ldots, 4\} \right) \\ & \quad \bigcup \{(\pi - \theta_0, \pi - \varphi_k) : k = 0, 1, \ldots, 4\}, \end{aligned}$$

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

$$\varphi_k = \varphi_0 + k(2\pi/5)$$
$$\cos\gamma_k = \cos\beta\cos\theta_0 + \sin\beta\sin\theta_0\cos\varphi_k$$
$$\sin\alpha_k = -(\sin\theta_0\sin\varphi_k)/\sin\gamma_k, \quad k = 0, 1, \ldots, 4$$

and

$$\beta = \arctan 2$$

Explicitly, the icosahedral delta function of (2) is

$$\Delta(\theta_0, \varphi_0; \theta, \varphi) = \tfrac{1}{60}\sum_{k=0}^{59} \delta(\cos\theta - \cos\theta_k)\delta(\varphi - \varphi_k),$$

where $\delta(x)$ is the Dirac δ function and (θ_k, φ_k) are given by fact 3.

The relationship between $\Delta(\theta_0, \varphi_0; \theta, \varphi)$ and the $T_{l,n}(\theta, \varphi)$ is described by the following fact:

Fact 4. The functions $T_{l,n}(\theta,\varphi)$ $(l = 0, 1, \ldots, n = 0, \ldots, N_l - 1)$ are a complete orthonormal fixed basis for the subspace of $L^2(\theta, \varphi)$ that contains functions that are totally symmetric with respect to the rotations of the icosahedral group if and only if

$$\Delta(\theta_0, \varphi_0; \theta, \varphi) = \sum_{l=0}^{\infty}\sum_{n=0}^{N_l-1} T_{l,n}(\theta_0, \varphi_0)T_{l,n}(\theta, \varphi).$$

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

Fact 5. For any θ_0 and φ_0,

$$\sum_{k=0}^{59} Y_{l,m}(\theta_k, \varphi_k) = \begin{cases} 5N_{l,m}\{P_{l,m}(\cos\theta_0)[\exp(im\varphi_0) \\ \quad +(-1)^l\exp(-im\varphi_0)] \\ \quad +\sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)[\exp(im\alpha_k) \\ \quad +(-1)^l\exp(-im\alpha_k)]\}, & m = 5\mu \text{ with } \mu \in Z \\ 0, & \text{otherwise,} \end{cases}$$

where Z are integers.

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

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

$$\sum_{n=0}^{N_l-1} b_{l,n,m}T_{l,n}(\theta_0, \varphi_0) = \tfrac{1}{60}\sum_{k=0}^{59} Y^*_{l,m}(\theta_k, \varphi_k), \tag{6}$$

$$\sum_{n=0}^{N_l-1} b_{l,n,m}T_{l,n}(\theta_0, \varphi_0) = \begin{cases} \tfrac{1}{12}N_{l,m}\{P_{l,m}(\cos\theta_0)[\exp(im\varphi_0) \\ \quad +(-1)^l\exp(-im\varphi_0)] \\ \quad +\sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)[\exp(im\alpha_k) \\ \quad +(-1)^l\exp(-im\alpha_k)]\}^*, & m = 5\mu \text{ with } \mu \in Z \\ 0, & \text{otherwise,} \end{cases} \tag{7}$$

$$\sum_{n=0}^{N_l-1}\sum_{m'=-l}^{+l} b_{l,n,m'}b_{l,n,m}Y_{l,m'}(\theta_0, \varphi_0) = \tfrac{1}{60}\sum_{k=0}^{59} Y_{l,m}(\theta_k, \varphi_k) \tag{8}$$

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

Proof: Write $\Delta(\theta_0, \varphi_0; \theta, \varphi)$ in terms of both the fixed basis functions and spherical harmonics and equate the two expressions:

$$\begin{aligned} &\sum_{l=0}^{\infty}\sum_{n=0}^{N_l-1} T_{l,n}(\theta_0, \varphi_0)T_{l,n}(\theta, \varphi) \\ &= \Delta(\theta_0, \varphi_0; \theta, \varphi) \\ &= \tfrac{1}{60}\sum_{k=0}^{59}\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k, \varphi_k)Y_{l,m}(\theta, \varphi). \end{aligned} \tag{9}$$

Substitute (4) into (9) to obtain

$$\begin{aligned} &\sum_{l=0}^{\infty}\sum_{n=0}^{N_l-1}\sum_{m=-l}^{+l} T_{l,n}(\theta_0, \varphi_0)b_{l,n,m}Y_{l,m}(\theta, \varphi) \\ &= \tfrac{1}{60}\sum_{k=0}^{59}\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k, \varphi_k)Y_{l,m}(\theta, \varphi). \end{aligned} \tag{10}$$

Multiply (10) by $Y^*_{l',m'}(\theta, \varphi)$, integrate over solid angles in θ and φ $(d\Omega_{\theta,\varphi})$ and use the orthonormality of the spherical harmonics to obtain (after renaming the indices $l' \to l, m' \to m$) (6). Use fact 5 in (6) to obtain (7). Use (4) in (6) to obtain (8).

The purpose of (8) is to demonstrate explicitly the bilinear nature of the equations. Notice, for example, from (8), that there is no coupling between different values of l.

From (7), we immediately obtain the following properties of the $b_{l,m,n}$ coefficients:

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

(ii) For l even, $b_{l,n,m}$ is real. For l odd, $b_{l,n,m}$ is imaginary.

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

(iv) For l odd, $b_{l,n,0} = 0$.

Using these properties, we can simplify the expression for the $T_{l,n}(\theta, \varphi)$:

Fact 8.

$$T_{l,n}(\theta,\varphi)=\begin{cases}\sum_{m=0}^{+l}[2/(1+\delta_{m,0})]N_{l,m}b_{l,n,m} \\ \quad\times P_{l,m}(\cos\theta)\cos m\varphi, & l\text{ even} \\ \sum_{m=1}^{+l}2N_{l,m}ib_{l,n,m}P_{l,m}(\cos\theta)\sin m\varphi, \\ & l\text{ odd.}\end{cases}$$

Fix the value of l. To this point, the only restriction on $T_{l,n}(\theta,\varphi)$ for $n=0,\ldots,N_l-1$ that 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 9. 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

$$t_{l,0}<t_{l,1}<\ldots<t_{l,N_l-1}, \tag{11}$$

where the inequalities are strict. In a basis satisfying (11), 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 1 and 3. 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 that satisfies (11) by applying Gaussian elimination. However, the intermediate basis need not be an orthonormal basis. Therefore, apply Gram–Schmidt orthogonalization, starting with the N_lth row, to transform to an orthonormal basis while still satisfying (11). The final claim (*i.e.* $b_{l,n,m}=0$ for $m<5n$) follows from the strict inequalities and fact 1.

We now modify the $b_{l,n,m}$ notation slightly to incorporate results to this point. First, facts 3 and 8 imply that the fixed basis functions 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 2). In summary, the new definition, for $l=0,1,\ldots,n=0,\ldots,N_l-1$ and $m=0,\ldots,l$, is

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

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 13.

The remainder of the calculation of the $b_{l,n,m}$ coefficients is the same in plan but different in detail for l even *versus* l odd. We will show the l-even case and then state the results for l odd. First, specialize fact 6 using facts 8 and 9 to find:

Fact 10. 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:

$$\begin{aligned}\sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)} & b_{l,n,m}[2/(1+\delta_{m',0})]N_{l,m'}b_{l,n,m'} \\ \times P_{l,m'}(\cos\theta_0)\cos m'\varphi_0 & \\ =\tfrac{1}{6}N_{l,m}\Bigg[P_{l,m}(\cos\theta_0)\cos m\varphi_0 & \\ +\sum_{k=0}^{4}P_{l,m}(\cos\gamma_k)\cos m\alpha_k\Bigg]. &\end{aligned} \tag{12}$$

4. Series expansions

For each l, (12) 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.* $\exp(ik\varphi_0)$] 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 $\theta_0^m\exp(\pm im\varphi_0)$. 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 that computes the coefficients of the terms $\theta_0^m\exp(\pm im\varphi_0)$ will lead to the same results.

Our approach, which we only sketch here, is based on two ideas: a particular function space, denoted by $\mathcal{P}$, and a particular operator, denoted by $\mathcal{Q}$, on the function space $\mathcal{P}$. We first describe $\mathcal{P}$. Let f be a smooth function on the sphere. The Fourier–Taylor coefficients of f are

$$d_{m,k}=\frac{1}{k!}\left[\frac{\mathrm{d}^k}{\mathrm{d}\theta^k}\left(\frac{1}{2\pi}\right)\int_0^{2\pi}f(\theta,\varphi)\exp(-im\varphi)\,\mathrm{d}\varphi\right]\Bigg|_{\theta=0}$$

for $m=\ldots,-1,0,+1,\ldots$ and $k=0,1,\ldots$ and the reconstructed function is

$$f(\theta,\varphi)=\sum_{m=-\infty}^{\infty}\sum_{k=0}^{\infty}d_{m,k}\theta^{k}\exp(im\varphi).$$

The function space $\mathcal{P}$ is a subspace of smooth functions on the sphere that is defined by the fact that $d_{m,k}=0$ for $0\le k\le |m|$. Therefore, f can alternatively be written

$$f(\theta,\varphi)=\sum_{m=-\infty}^{\infty}\sum_{k=|m|}^{\infty}d_{m,k}\theta^{k}\exp(im\varphi).$$

The operator Q, applied to $f\in\mathcal{P}$, is defined by

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

Applied to functions $f\in\mathcal{P}$, the operator Q has a variety of properties of which the most important is that $Q[g(f)]=Q[g(Q[f])]$, where g is any polynomial. We conjecture and use that the same formula applies when g is a smooth function.

The operator Q is important because if $f\in\mathcal{P}$ and you can explicitly compute the power series of $Q[f]$, then you have explicit formulae for a certain subset of the Fourier–Taylor coefficients for f. We apply exactly this program to (12). First, we verify that the left-hand side of (12) is in $\mathcal{P}$. Second, we apply Q to both sides in order to get a new equation where on both sides there is a series with terms of the type $a_m\theta_0^{|m|}\cos m\varphi_0$, where a_m are coefficients independent of θ_0 and φ_0. Third, we equate coefficients of $\theta_0^{|m|}\cos m\varphi_0$ on left- and right-hand sides to arrive at an equation that is independent of θ_0 and φ_0 and which, in terms of

$$g_{l,m}=\begin{cases}(-1)^m(l+m)!/[2^m(l-m)!m!], & m\ge 0\\ 2^m/[(-m)!], & m<0,\end{cases}$$

is described in the following fact:

Fact 11. For $l=0,2,4,\ldots$ and $m=5\mu\ (0\le m\le +l)$,

$$\sum_{m'=0}^{l}\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)}[2/(1+\delta_{m',0})]\times b_{l,n,m'}b_{l,n,m}N_{l,m'}g_{l,m'}\theta_0^{m'}\cos m'\varphi_0$$
$$=\tfrac{1}{6}N_{l,m}\Bigg\{g_{l,m}\theta_0^{m}\cos m\varphi_0+\sum_{\substack{\mu'=0\\ m'=5\mu'}}^{\infty}\theta_0^{m'}5\cos m'\varphi_0\times[2^{1-m'}/(1+\delta_{0,m'})]\sum_{k=0}^{m'}(1/k!)P_{l,m}^{(k)}(\cos\beta)\sin^k\beta\times\sum_{r=0}^{\lfloor(m'-k)/2\rfloor}c_{m'-k-2r,2r}(-1)^r\Bigg\},$$

where $P_{l,m}^{(k)}(x)=\mathrm{d}^kP_{l,m}(x)/\mathrm{d}x^k$ and where the $c_{p,q}$ coefficients are defined by

$$\cos\big(m\sin^{-1}\{y/[1-(\cos\beta+x\sin\beta)^2]^{1/2}\}\big)=\sum_{p=0}^{\infty}\sum_{q=0}^{\infty}c_{p,q}x^py^q.$$

For $m'=5\mu'\ (0\le m'\le +l)$, equate the coefficient of $\theta_0^{m'}$ on both sides of fact 11 to get

$$\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)}[2/(1+\delta_{m',0})]\times b_{l,n,m'}b_{l,n,m}N_{l,m'}g_{l,m'}\cos m'\varphi_0$$
$$=\tfrac{1}{6}N_{l,m}\Bigg\{\delta_{m,m'}g_{l,m}\cos m\varphi_0+5\cos m'\varphi_0[2^{1-m'}/(1+\delta_{0,m'})]\times\sum_{k=0}^{m'}(1/k!)P_{l,m}^{(k)}(\cos\beta)\sin^k\beta\times\sum_{r=0}^{\lfloor(m'-k)/2\rfloor}c_{m'-k-2r,2r}(-1)^r\Bigg\},$$

which must hold for $l=0,2,4,\ldots,$ $m=5\mu$ $(0\le m\le +l)$ and $m'=5\mu'$ $(0\le m'\le +l)$. Division of both sides by $[2/(1+\delta_{m',0})]N_{l,m'}g_{l,m'}\cos m'\varphi_0$ results in

Fact 12. For l even, $m=5\mu$ $(0\le m\le +l)$ and $m'=5\mu'$ $(0\le m'\le +l)$,

$$\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)}b_{l,n,m'}b_{l,n,m}=C_{l,m,m'},\qquad(13)$$

where

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

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

Fact 13. For l odd, $m=5\mu$ $(0\le m\le +l)$ and $m'=5\mu'$ $(0\le m'\le +l)$,

$$\sum_{n=0}^{\min(N_l-1,\lfloor m/5\rfloor,\lfloor m'/5\rfloor)}b_{l,n,m'}b_{l,n,m}=C_{l,m,m'},\qquad(14)$$

where

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

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

$$- \sin\left(m \sin^{-1}\{y/[1-(\cos\beta + x\sin\beta)^2]^{1/2}\}\right) = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} s_{p,q} x^p y^q.$$

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

5. Recursive solution

Equations (13) and (14) 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 sides of (13) and (14) in m' and m implies that $C_{l,m,m'} = C_{l,m'm}$ and that we need only consider $m \geq m'$ so (13) and (14) simplify to

$$\sum_{n=0}^{\min(N_l-1,\lfloor m'/5\rfloor)} b_{l,n,m'} b_{l,n,m} = C_{l,m,m'} \qquad 0 \leq m' \leq l,\ m' \leq m \leq l. \qquad (15)$$

We now describe an algorithm for solving (15). Based on fact 1, 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 an $N_l \times (\lfloor l/5 \rfloor + 1)$ 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 9, this array has the form shown in Fig. 1. Equation (15) describes a sum over elements in one (if $m = m'$) or two (if $m \neq m'$) columns. Suppose 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 (15) becomes

$$b_{l,0,10}^2 + b_{l,1,10}^2 + b_{l,2,10}^2 = C_{l,10,10}. \qquad (16)$$

Since $b_{l,0,10}$ and $b_{l,1,10}$ are known, (16) can be solved for $b_{l,2,10}$:

$$b_{l,2,10} = (C_{l,10,10} - b_{l,0,10}^2 - b_{l,1,10}^2)^{1/2}.$$

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

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

Fig. 1. The $b_{l,n,m}$ array for fixed l. '0' indicates a guaranteed 0 element while '*' indicates a possibly nonzero element.

$$b_{l,0,10} b_{l,0,m} + b_{l,1,10} b_{l,1,m} + b_{l,2,10} b_{l,2,m} = C_{l,10,m} \qquad (17)$$

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 (17) can be solved for $b_{l,2,m}$:

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

An algorithm of the type sketched in the previous paragraph 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 $C_{15,5,5} \neq 0$. However, the algorithm of the previous paragraph can be generalized to deal with this problem by taking advantage of fact 9. 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 Fig. 2. Note two aspects of the algorithm of Fig. 2: 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 $\sum_{n'} b_{l,n',m'}^2$ 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 Fig. 2 in exact arithmetic, we have used the *Mathematica* symbolic computation system. The program for performing these calculations is listed in Appendix *B*.* 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 $P_{l,m}^{(k)}(\cos\beta) = P_{l,m}^{(k)}(1/5^{1/2})$, the following fact, proved by induction starting with equations 8.733–1,2 of Gradshteyn & Ryzhik (1980), is useful.

Fact 14. $P_{l,m}^{(k)}(x)$, where $|x| < 1$, can be expressed in the form

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

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

$$A_{k+1}(x) = A_k'(x) + \frac{lxA_k(x) + (l+m)B_k(x)}{1-x^2}$$

$$B_{k+1}(x) = B_k'(x) + \frac{lxB_k(x) + (l-m)A_k(x)}{-1+x^2}$$

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

6. Derivation of explicit forms of the icosahedral fixed basis functions

To substantiate the derivations in the previous sections, in this section we derive explicit expressions for those fixed basis functions that can be determined from (15) for $m' = 0$ (the so-called 'first set') or $m' = 5$ (the so-called 'second set'). (Recall that $m \geq m'$ always). Notice that

* Appendix *B* has been deposited with the IUCr (Reference: JS0012). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

the first and second sets do not correspond to $n = 0$ and $n = 1$. For instance, $N_{15} = 1$ so there is only an $n = 0$ fixed basis function for $l = 15$ but, because $b_{15,0,0} = 0$, it is necessary to consider $m' = 5$ in (15) so the single fixed basis function belongs to the second set.

In Appendix *A*, we list the coefficients for all fixed basis functions in the range $0 \le l < 45$. 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 PCD for machine-readable tables of coefficients and software.

6.1. *The first set of icosahedral fixed basis functions*

The first set of icosahedral fixed basis functions is the collection of $T_{l,n}(\theta, \varphi)$ for which $b_{l,n,0} \neq 0$. Specifically, the first set is those fixed basis functions that are computed by the $b_{l,n,m} = (C_{l,m',m} - \sum_{n'=0}^{n-1} b_{l,n'm'} \times b_{l,n'm})/b_{l,n,m'}$ statement in the algorithm of Fig. 2 with $n = m' = 0$. From fact 4, we know that $b_{l,n,0} = 0$ for l odd. Therefore, there are no l-odd fixed basis functions in the first set.

Set $m' = 0$ in (13) to get

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

```
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'} - Σ_{n'=0}^{n-1} b²_{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} - Σ_{n'=0}^{n-1} b_{l,n',m'} b_{l,n',m}) / b_{l,n,m'}
  }
  m'+ = 5
}
```

Fig. 2. An algorithm for the solution of equation (15) in the general case. The control structures are written in the C programming language.

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

$$b_{l,0,0} b_{l,0,m} = \tfrac{1}{6}[(l-m)!/(l+m)!]^{1/2}[\delta_{m,0} + 5P_{l,m}(1/5^{1/2})]. \tag{18}$$

Evaluate (18) at $m = 0$ to get

$$b^2_{l,0,0} = \tfrac{1}{6}[1 + 5P_{l,0}(1/5^{1/2})]. \tag{19}$$

Evaluation of (19) shows that $b_{l,0,0} = 0$ for $l = 2, 4, 8, 14$. Therefore, fixed basis functions of order $l = 2, 4, 8, 14$, if they exist, are not members of the first set and, in fact, (5) shows that they do not exist at all. [We have verified that fixed basis functions of order $l = 2, 4, 8, 14$ do not exist in the first or second set but in order to demonstrate that a fixed basis function of order l does not exist at all it is necessary to check through the $(l+1)$th set]. The first four unnormalized l-even fixed basis functions, obtained by exact numerical calculations from (18), are

$$\begin{aligned} T_{0,0}(\theta,\varphi) &= 1 \\ T_{6,0}(\theta,\varphi) &= 3960P_{6,0}(\cos\theta) - P_{6,5}(\cos\theta)\cos 5\varphi \\ T_{10,0}(\theta,\varphi) &= 896\,313\,600P_{10,0}(\cos\theta) \\ &\quad + 27\,360P_{10,5}(\cos\theta)\cos 5\varphi \\ &\quad + P_{10,10}(\cos\theta)\cos 10\varphi \\ T_{12,0}(\theta,\varphi) &= 14\,250\,297\,600P_{12,0}(\cos\theta) \\ &\quad - 55\,440P_{12,5}(\cos\theta)\cos 5\varphi \\ &\quad + P_{12,10}(\cos\theta)\cos 10\varphi. \end{aligned}$$

[Division of the stated formula by $(4\pi)^{1/2}$, $3600 \times (11\pi/13)^{1/2}$, $25\,920\,000(1729\pi)^{1/2}$, or $399\,168\,000 \times (595\pi)^{1/2}$ will normalize $T_{0,0}$, $T_{6,0}$, $T_{10,0}$ or $T_{12,0}$, respectively.] In Fig. 3, we show a spherical plot of $T_{10,0}$ which clearly exhibits the icosahedral symmetry of $T_{10,0}$.

6.2. *The second set of icosahedral fixed basis functions*

The second set of icosahedral fixed basis functions is the collection of $T_{l,n}(\theta, \varphi)$ for which $b_{l,n,0} = 0$ and $b_{l,n,5} \neq 0$. Specifically, the second set is those fixed basis

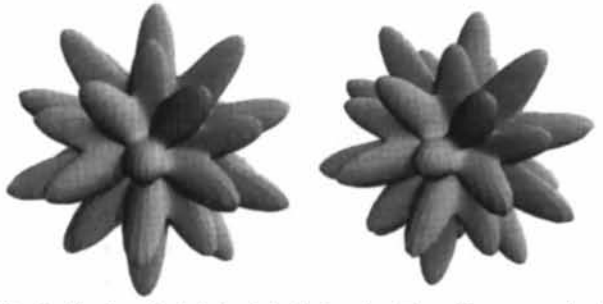

Fig. 3. The icosahedral fixed basis function $T_{10,0}$. The stereopair of plots shows a surface whose distance from the origin at particular θ and φ values is the value of $c_{10,0} + T_{10,0}(\theta,\varphi)$, where $c_{10,0} = 2\max_{\theta,\varphi}[|T_{10,0}(\theta,\varphi)|]$.

functions 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 Fig. 2 with $n = 0, 1$ and $m' = 5$. We now determine the $b_{l,n,m}$ coefficients. First consider the l-even fixed basis functions. Setting $m' = 5$ in (13), we obtain

$$\begin{aligned} & b_{l,0,5} b_{l,0,m} + b_{l,1,5} b_{l,1,m} \\ & \quad = [N_{l,m}/(12 N_{l,5})] \Big\{ \delta_{|m|,5} g_{l,m}/g_{l,5} + [5/(16 g_{l,5})] \\ & \quad \times \sum_{k=0}^{5} (1/k!) P_{l,m}^{(k)}(1/5^{1/2})(2/5^{1/2})^k \\ & \quad \times \sum_{r=0}^{\lfloor (5-k)/2 \rfloor} c_{5-k-2r,2r}(-1)^r \Big\} \end{aligned} \tag{20}$$

where, by applying (18) three times to achieve the second equality,

$$\begin{aligned} b_{l,0,5} b_{l,0,m} &= (b_{l,0,0} b_{l,0,5})(b_{l,0,0} b_{l,0,m})/b_{l,0,0}^2 \\ &= [(l-5)!(l-m)!/(l+5)!(l+m)!]^{1/2} \\ &\quad \times \big([25 P_{l,m}(1/5^{1/2}) P_{l,5}(1/5^{1/2})] \\ &\quad \times \{6[1 + 5 P_{l,0}(1/5^{1/2})]\}^{-1}\big). \end{aligned} \tag{21}$$

Using (21) in (20), we worked out the expression for the l-even second-set fixed basis functions with the aid of *Mathematica* and this is

$$\begin{aligned} b_{l,1,5} b_{l,1,m} &= \tfrac{1}{12}[(l-m)!(l+5)!/(l+m)!(l-5)!]^{1/2} \\ &\quad \times \big(\delta_{m,5} - [(l-5)!/(l+5)!] \\ &\quad \times \{2^5 5! u_{l,m} + [50 P_{l,m}(1/5^{1/2}) P_{l,5}(1/5^{1/2})] \\ &\quad \times [1 + 5 P_{l,0}(1/5^{1/2})]^{-1}\}\big), \end{aligned} \tag{22}$$

where

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

Evaluate (22) 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 $b_{l,1,5} \neq 0$ is $l = 30$, *i.e.* the lowest-order second-set l-even fixed basis function is $T_{30,1}(\theta, \varphi)$. By further calculations with *Mathematica*, we find that an unnormalized expression for $T_{30,1}$ is

$$\begin{aligned} & T_{30,1}(\theta, \varphi) \\ & \quad = 21\,575\,737\,826\,844\,783\,682\,237\,777\,575\,936\,000\,000 \\ & \qquad \times P_{30,5}(\cos\theta)\cos 5\varphi \\ & \qquad + 2\,404\,901\,042\,680\,144\,820\,126\,515\,200\,000 \\ & \qquad \times P_{30,10}(\cos\theta)\cos 10\varphi \\ & \qquad + 195\,936\,300\,573\,276\,856\,320\,000 \\ & \qquad \times P_{30,15}(\cos\theta)\cos 15\varphi \\ & \qquad + 7\,601\,550\,560\,755\,200 P_{30,20}(\cos\theta)\cos 20\varphi \\ & \qquad + (7\,075\,752\,000/11) P_{30,25}(\cos\theta)\cos 25\varphi \\ & \qquad + 12251 P_{30,30}(\cos\theta)\cos 30\varphi. \end{aligned}$$

[Division of the stated formula by $11\,587\,425\,684\,543\;700\,992\,000\,000\,000\,000$ $(28\,072\,776\,427\,766\,064\,319\,187\,390\,671\pi/61)^{1/2}$ will normalize $T_{30,1}$.] For comparison, an unnormalized expression for $T_{30,0}(\theta, \varphi)$, a member of the first set, is

$$\begin{aligned} & T_{30,0}(\theta, \varphi) \\ & \quad = 813\,279\,038\,255\,889\,216\,053\,348\,786\,362\,122\,240\,000\,000 \\ & \qquad \times P_{30,0}(\cos\theta) \\ & \qquad - 47\,353\,003\,689\,115\,160\,214\,196\,322\,304\,000\,000 \\ & \qquad \times P_{30,5}(\cos\theta)\cos 5\varphi \\ & \qquad + 1\,645\,439\,737\,221\,580\,537\,036\,800\,000 \\ & \qquad \times P_{30,10}(\cos\theta)\cos 10\varphi \\ & \qquad - 55\,708\,614\,976\,734\,720\,000 P_{30,15}(\cos\theta)\cos 15\varphi \\ & \qquad + 9\,702\,264\,499\,200 P_{30,20}(\cos\theta)\cos 20\varphi \\ & \qquad - 5\,407\,920 P_{30,25}(\cos\theta)\cos 25\varphi \\ & \qquad + P_{30,30}(\cos\theta)\cos 30\varphi. \end{aligned}$$

[Division of the stated formula by $41\,445\,759\,345\,654\;852\,911\,923\,200\,000\,000\,000\,000$ $(9\,198\,155\,739\pi/61)^{1/2}$ will normalize $T_{30,0}$.]

Now let us consider the second-set l-odd fixed basis functions. 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 (14), we get

$$\begin{aligned} b_{l,0,5} b_{l,0,m} &= \tfrac{1}{12}[(l-m)!(l+5)!/(l+m)!(l-5)!]^{1/2} \\ &\quad \times \{\delta_{m,5} - 3840[(l-5)!/(l+5)!] v_{l,m}\}, \end{aligned} \tag{23}$$

where

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

As before, by setting $m = 5$ in (23), 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 l-odd second-set fixed basis function is $T_{15,0}(\theta, \varphi)$, which has the unnormalized expression

$$T_{15,0}(\theta, \varphi) = -36\,306\,144\,000 P_{15,5}(\cos\theta)\sin 5\varphi - 62\,640 P_{15,10}(\cos\theta)\sin 10\varphi + P_{15,15}(\cos\theta)\sin 15\varphi.$$

[Division of the stated formula by $3\,919\,104\,000\,000\,(215\,656\,441\pi/31)^{1/2}$ will normalize $T_{15,0}$.] $T_{15,0}$ is, by (5), the lowest-order l-odd fixed basis function among any set.

6.3. *Symbolic verification of the icosahedral fixed basis functions*

As described in §4, we use $Q[g(f)] = Q[g(Q[f])]$ for smooth g but can only prove it for polynominal g. Therefore, 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 Jack & Harrison (1975). [For $l = 30$, Jack & Harrison (1975) list only one fixed basis function, which is our $T_{30,0}$, in spite of the fact that $N_{30} = 2$.] Second, for $l < 45$, we have verified that each $T_{l,n}(\theta, \varphi)$ is totally symmetric through symbolic calculations with *Mathematica* (Zheng & Doerschuk, 1995).

7. Other polyhedral symmetries

Using the same idea and techniques that have been applied in previous sections to the icosahedral symmetry, we can derive complete orthonormal fixed bases for the subspaces of functions in $L^2(\theta, \varphi)$ that are totally symmetric under octahedral or tetrahedral symmetries. Since the cube is dual to the octahedron and the dodecahedron is dual to the icosahedron, it is not necessary to consider the cubic or dodecahedral symmetries separately. Below, we only outline the calculations and have suppressed the details. Please contact PCD for machine-readable tables of coefficients and software.

7.1. *Octahedral/cubic symmetries*

This case has been previously studied by Von der Lage & Bethe (1947) under the name Kubic harmonics for $l \le 6$ and for all representations rather than just the identity representation. Choose appropriate coordinates such that the spherical coordinates of the vertices of the underlying octahedron are

$$\{(0,0), (\tfrac{\pi}{2}, 0), (\tfrac{\pi}{2}, \tfrac{\pi}{2}), (\tfrac{\pi}{2}, \pi), (\tfrac{\pi}{2}, \tfrac{3\pi}{2}), (\pi, 0)\}.$$

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

for l even,

$$\sum_{m' \ge 0}\sum_{4n<m'} b_{l,n,m}[2/(1+\delta_{m',0})]N_{l,m'}b_{l,n,m'} \times P_{l,m'}(\cos\theta_0)\cos m'\varphi_0 = \tfrac{1}{3}N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\varphi_0 + \tfrac{1}{2}\sum_{k=0}^{3} P_{l,m}(\cos\gamma_k)\cos m\alpha_k\right], \quad m = 4\mu;$$

for l odd,

$$\sum_{m' > 0}\sum_{4n<m'} b_{l,n,m}N_{l,m'}b_{l,n,m'}P_{l,m'}(\cos\theta_0)\cos m'\varphi_0 = \tfrac{1}{3}N_{l,m}\left[P_{l,m}(\cos\theta_0)\sin m\varphi_0 + \tfrac{1}{2}\sum_{k=0}^{3} P_{l,m}(\cos\gamma_k)\sin m\alpha_k\right], \quad m = 4\mu;$$

where α_k, γ_k have the same definitions as in the icosahedral case with $\beta = \pi/2$ and $\varphi_k = \varphi_0 + k\pi/2$. Using the series-expansion techniques, we obtain expressions for determining the coefficients $b_{l,n,m}$:

for l even,

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

for l odd,

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

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

$$\sum_{p=0}^{\infty}\sum_{q=0}^{\infty} c_{p,q}x^p y^q = \cos\{m \arcsin[y/(1-x^2)^{1/2}]\}$$

$$\sum_{p=0}^{\infty}\sum_{q=0}^{\infty} s_{p,q}x^p y^q = -\sin\{m \arcsin[y/(1-x^2)^{1/2}]\}.$$

7.2. *Tetrahedral symmetry*

The spherical coordinates of the vertices of the underlying tetrahedron are

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

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

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

so that the coefficients $b_{l,n,m}$ can be chosen real (or pure imaginary) as in the icosahedral case. Let $\Delta^{(p)}(\theta_0,\varphi_0;\theta,\varphi)$ be the delta function associated with the primal tetrahedron and let $\Delta^{(d)}(\theta_0,\varphi_0;\theta,\varphi)$ be the delta function associated with the dual tetrahedron. Further, let

$$\Delta^{(+)}(\theta_0,\varphi_0;\theta,\varphi)=\Delta^{(p)}(\theta_0,\varphi_0;\theta,\varphi)+\Delta^{(d)}(\theta_0,\varphi_0;\theta,\varphi)$$
$$\Delta^{(-)}(\theta_0,\varphi_0;\theta,\varphi)=\Delta^{(p)}(\theta_0,\varphi_0;\theta,\varphi)-\Delta^{(d)}(\theta_0,\varphi_0;\theta,\varphi).$$

Instead of expanding $\Delta^{(p)}(\theta_0,\varphi_0;\theta,\varphi)$, we expand $\Delta^{(\pm)}(\theta_0,\varphi_0;\theta,\varphi)$ in terms of both spherical harmonics and the unknown tetrahedral fixed basis functions. This will give us two independent sets of tetrahedral fixed basis functions. The master equations for determining the coefficients are:

for l even,

$$\sum_{m'\geq 0}\sum_{3n<m'} b^{(+)}_{l,n,m}[2/(1+\delta_{m',0})]N_{l,m'}b^{(+)}_{l,n,m'} \times P_{l,m'}(\cos\theta_0)\cos m'\varphi_0 = \tfrac{1}{4}N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\varphi_0 + \sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\cos m\alpha_k\right]$$

$$\sum_{m'\geq 0}\sum_{3n<m'} b^{(-)}_{l,n,m}[2/(1+\delta_{m',0})] \times N_{l,m'}b^{(-)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\sin m'\varphi_0 = \tfrac{1}{4}N_{l,m}\left[P_{l,m}(\cos\theta_0)\sin m\varphi_0 + \sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\sin m\alpha_k\right], \quad m=3\mu;$$

for l odd,

$$\sum_{m'\geq 0}\sum_{3n<m'} b^{(+)}_{l,n,m}N_{l,m'}b^{(+)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\sin m'\varphi_0 = \tfrac{1}{4}N_{l,m}\left[P_{l,m}(\cos\theta_0)\sin m\varphi_0 + \sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\sin m\alpha_k\right]$$

$$\sum_{m'\geq 0}\sum_{3n<m'} b^{(-)}_{l,n,m}N_{l,m'}b^{(-)}_{l,n,m'}P_{l,m'}(\cos\theta_0)\cos m'\varphi_0 = \tfrac{1}{4}N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\varphi_0 + \sum_{k=0}^{2}P_{l,m}(\cos\gamma_k)\cos m\alpha_k\right], \quad m=3\mu;$$

where α_k,γ_k are defined as before [with the new value of β and $\varphi_k=\varphi_0+k(2\pi/3)$]. The final expressions for determining $b_{l,n,m}$ coefficients are:

for l even,

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

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

for l odd,

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

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

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

8. Application to other representations of the icosahedral group and other rotational groups

The idea of applying the projection operator to the delta function can be applied to other (*i.e.* higher-dimensional) representations of the icosahedral group, as well as to other finite groups of coordinate rotations.

Let g be the order of the finite group $\mathcal{G}$ of coordinate rotations, N be the number of irreducible representations and d_p, for $p = 0, \ldots, N-1$, be the dimension of the pth irreducible representation. For the icosahedral group, these values are $g = 60$, $N = 5$ and $d_p = 1, 3, 3, 4, 5$ (Artin, 1991, p. 324). Let $\Gamma^p(T_k)_{j,j'}$ for $p = 0, \ldots, N-1$, $k = 0, \ldots, g-1$ and $j, j' = 1, \ldots, d_p$ be the matrix elements of the kth member of the group in the pth unitary irreducible representation. For the icosahedral group, these matrices are known (Liu, Ping & Chen, 1990).

By applying two theorems and a definition in Cornwell (1984) to $L^2(\theta, \varphi)$, we have the following two theorems and definition:

Theorem 3 (Cornwell, 1984, p. 92, Theorem I). Any function $f(\theta, \varphi) \in L^2(\theta, \varphi)$ can be expressed as a linear combination of basis functions of the unitary irreducible representations of a group $\mathcal{G}$ of coordinate rotations in $\mathcal{R}^3$. That is,

$$f(\theta, \varphi) = \sum_{p=0}^{N-1} \sum_{j=0}^{d_p-1} a_j^p f_j^p(\theta, \varphi), \tag{24}$$

where $f_j^p(\theta, \varphi)$ is a normalized basis function transforming as the jth row of the d_p-dimensional unitary irreducible representation Γ^p of $\mathcal{G}$, the a_j^p are a set of complex numbers and the sum of p is over all the inequivalent unitary irreducible representations of $\mathcal{G}$.

Definition 1 (Cornwell, 1984, p. 93). Projection operators: Let Γ^p be a unitary irreducible representation of dimension d_p of a finite group of coordinate transformations $\mathcal{G}$ of order g. Then, the projection operators are defined by

$$\mathcal{P}_{j,j'}^p = (d_p/g) \sum_{T \in \mathcal{G}} \Gamma^p(T)_{j,j'}^* P(T).$$

Theorem 4 (Cornwell, 1984, p. 93, Theorem II). For any function $f(\theta, \varphi) \in L^2(\theta, \varphi)$,

$$\mathcal{P}_{j,j}^p f(\theta, \varphi) = a_j^p f_j^p(\theta, \varphi),$$

where a_j^p and $f_j^p(\theta, \varphi)$ are the coefficients and basis functions of the expression of $f(\theta, \varphi)$ [(24)] that relate to the jth row of Γ^p.

We apply these results to $\delta(\cos\theta - \cos\theta_0)\delta(\varphi - \varphi_0)$ to find that

$$\delta(\cos\theta - \cos\theta_0)\delta(\varphi - \varphi_0) = \sum_{p=0}^{N-1} \sum_{j=0}^{d_p-1} a_j^p \Delta_j^p(\theta_0, \varphi_0; \theta, \varphi)$$

$$\begin{aligned} a_j^p \Delta_j^p(\theta_0, \varphi_0; \theta, \varphi) &= \mathcal{P}_{j,j}^p \delta(\cos\theta - \cos\theta_0)\delta(\varphi - \varphi_0) \\ &= (d_p/g) \sum_{k=1}^{g} \Gamma^p(T_k)_{j,j}^* P(T_k) \delta(\cos\theta - \cos\theta_0)\delta(\varphi - \varphi_0) \\ &= (d_p/g) \sum_{k=1}^{g} \Gamma^p(T_k)_{j,j}^* \delta(\cos\theta - \cos\theta_k)\delta(\varphi - \varphi_k), \end{aligned} \tag{25}$$

where (θ_k, φ_k) are the symmetry-related positions, *e.g.* for the icosahedral group (θ_k, φ_k) are given by fact 3.

The symmetrized delta functions $\Delta_j^p(\theta_0, \varphi_0; \theta, \varphi)$ define subspaces, denoted by $(L_j^p)^2(\theta, \varphi)$, of the Hilbert space $L^2(\theta, \varphi)$ by

$$(L_j^p)^2(\theta, \varphi) = \Big\{ f(\theta, \varphi) \in L^2(\theta, \varphi) : f(\theta, \varphi) = \int \Delta_j^p(\theta_0, \varphi_0; \theta, \varphi) f(\theta_0, \varphi_0)\, \mathrm{d}\Omega_0 \Big\}.$$

Each subspace contains only a certain type of basis function, the union of the subspaces is all of $L^2(\theta; \varphi)$, and the only function in the intersection of any pair of the subspaces is the zero function.

The goal is to determine a complete orthonormal fixed basis in each subspace. Denote the fixed basis functions by $T_j^p(\theta, \varphi; \alpha)$, where α is an index. We proceed exactly as in the previous sections of the paper devoted to the identity representation of the icosahedral group. First, one can show that α can be written as l, n and

$$T_j^p(\theta, \varphi; l, n) = \sum_{m=-l}^{+l} b_j^p(l, n, m) Y_{l,m}(\theta, \varphi).$$

Second, one can expand $\Delta_j^p(\theta_0, \varphi_0; \theta, \varphi)$ as a weighted sum of $Y_{l,m}(\theta, \varphi)$ by using (25):

$$\begin{aligned} \Delta_j^p(\theta_0, \varphi_0; \theta, \varphi) &= \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} w_j^p(\theta_0, \varphi_0; l, m) Y_{l,m}(\theta, \varphi) \\ w_j^p(\theta_0, \varphi_0; l, m) &= \int \Delta_j^p(\theta_0, \varphi_0; \theta, \varphi) Y_{l,m}^*(\theta, \varphi)\, \mathrm{d}\Omega \\ &= \int (d_p/g a_j^p) \sum_{k=1}^{g} \Gamma^p(T_k)_{j,j}^* \delta(\cos\theta - \cos\theta_k)\delta(\varphi - \varphi_k) Y_{l,m}^*(\theta, \varphi)\, \mathrm{d}\Omega \\ &= (d_p/g a_j^p) \sum_{k=1}^{g} \Gamma^p(T_k)_{j,j}^* Y_{l,m}^*(\theta_k, \varphi_k). \end{aligned} \tag{26}$$

Third, since $T_j^p(\theta, \varphi; l, n)$ are a complete orthonormal fixed basis for $(L_j^p)^2(\theta, \varphi)$, it follows that

$$\Delta_j^p(\theta_0, \varphi_0; \theta, \varphi) = \sum_{l=0}^{\infty} \sum_{n=0}^{N_j^p(l)} [T_j^p(\theta_0, \varphi_0; l, n)]^* T_j^p(\theta, \varphi; l, n). \tag{27}$$

Fourth, by equating the expansions for $\Delta_j^p(\theta_0, \varphi_0; \theta, \varphi)$ provided by (26) and (27), one arrives at an equation that is exactly a generalization of (9) in fact 6. From this point forward, the $T_j^p(\theta, \varphi; l, n)$ can be obtained by using the same methods already used for the identity representation of the icosahedral group.

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Note added in proof: We have simplified the calculations of §4 so that Q is unnecessary. Equation (12) can be written

$$\sum_{m'=0}^{l} e_{l,m,m'} h_{l,m'} P_{l,m'}(\cos\theta_0) \cos m'\varphi_0 = f_{l,m}(\theta_0, \varphi_0),$$

where $f_{l,m}(\theta_0, \varphi_0)$ is the right-hand side of (12), $h_{l,m'} = 2N_{l,m'}/(1+\delta_{m',0})$ and the definition of $e_{l,m,m'}$ can be inferred from (12). Multiplication by $\cos m''\varphi_0$, integration of φ_0 from 0 to 2π and renaming m'' as m' leads to

$$e_{l,m,m'} h_{l,m'} P_{l,m'}(\cos\theta_0)\pi = \int_0^{2\pi} f_{l,m}(\theta_0, \varphi_0) \cos m'\varphi_0 \, d\varphi_0. \tag{28}$$

Differentiation m' times with respect to θ_0, evaluation of the resulting equation at $\theta_0 = 0$ and use of $[\partial^{m'} P_{l,m'}(\cos\theta_0)/\partial\theta_0^{m'}]_{\theta_0=0} = g_{l,m'}$, where $g_{l,m'}$ is defined in §4 leads to the result that

$$e_{l,m,m'} h_{l,m'} g_{l,m'} \pi = \int_0^{2\pi} [\partial^{m'} f_{l,m}(\theta_0, \varphi_0)/\partial\theta_0^{m'}]_{\theta_0=0} \cos m'\varphi_0 \, d\varphi_0. \tag{29}$$

While the right-hand side of (28) is very complicated, the right-hand side of (29) can be evaluated explicitly. In fact, (29) divided by $h_{l,m'} g_{l,m'} \pi$ is (13). The reason that this simplification can be achieved is that $f_{l,m}$ lies in a subspace of $\mathcal{P}$:

$$f_{l,m}(\theta_0, \varphi_0) \in \text{span}\{Y_{l,m'}(\theta_0, \varphi_0), \quad m' = -l, \ldots, +l\} \subset \mathcal{P}.$$

APPENDIX *A*
Tables of icosahedral fixed basis functions

Table 1. *Table of $b_{l,n,m}$ coefficients for $T_{l,n}(\theta, \varphi)$ for $n = 0$ and $l \in \{0, 1, \ldots, 44\}$*

	$l = 0$	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			$5.23470931063209 \times 10^{-10}$
	$l = 12$	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		$5.458054970675743 \times 10^{-17}$	$-1.17921811835546 \times 10^{-17}$
	$l = 18$	20	21
$m = 0$	$9.002655639988 \times 10^{-1}$	$1.974780890363718 \times 10^{-1}$	
5	$-4.983700158317558 \times 10^{-7}$	$3.407144393312143 \times 10^{-7}$	$4.092807665027534 \times 10^{-7}$
10	$2.95803665617139 \times 10^{-13}$	$2.227863454007644 \times 10^{-13}$	$-3.010993744539446 \times 10^{-14}$
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			$6.664202520526863 \times 10^{-33}$

Table 1 *(cont.)*

	$l = 26$	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	$3.242397542911047 \times 10^{-33}$	$-1.826761158766107 \times 10^{-32}$	$-9.29118303087409 \times 10^{-33}$
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 2. *Table of $b_{l,n,m}$ coefficients for $T_{l,n}(\theta, \varphi)$ for $n = 1$ 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	$9.13353520771848 \times 10^{-62}$		

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