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EXPLICIT COMPUTATION OF ORTHONORMAL SYMMETRIZED HARMONICS WITH APPLICATION TO THE IDENTITY REPRESENTATION OF THE ICOSAHEDRAL GROUP[*]

YIBIN ZHENG[†] AND PETER C. DOERSCHUK[‡]

Abstract. A novel method to explicitly compute orthonormal symmetrized harmonics is presented and the method is applied to the identity representation of the icosahedral group. Spherical viruses have icosahedral symmetry and the motivating application is the parametric representation of spherical viruses for use in inverse problems based on x-ray scattering data and cryoelectron microscopy images. The symmetrized harmonics are computed in the form of linear combinations of spherical harmonics of one order and therefore have simple rotational properties which is valuable in the electron microscopy application. The method is based on equating the expansions of a symmetrized delta function in spherical and in symmetrized harmonics from which bilinear equations for the weights in the linear combinations can be derived. The explicit character of the calculation is reflected in the fact that both explicit expressions and an efficient recursive algorithm are derived for computing the weights in the linear combinations.

Key words. symmetric harmonics, icosahedral harmonics

AMS subject classifications. 33C55, 20C40, 20H15, 20G45, 92B05

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1. Introduction.

An important problem in biophysics is the determination of the three-dimensional distribution of electron density in so-called "spherical" viruses [1] from x-ray scattering and electron microscopy data [2]. This is a large class of viruses, including both viruses of plants and animals, where all viral particles of a particular viral type are identical, each viral type has a particle diameter of 10^2–10^3Å, and each viral particle has all the symmetries of the icosahedron. Two approaches to analyzing such data are to represent the electron density either as a truncated orthonormal expansion [3, 4] or as a piecewise-constant function with icosahedrally symmetric boundaries that are described using truncated orthonormal expansions [5] and then solve a nonlinear least squares problem for the coefficients in the expansion. Because the viral particles are roughly spherical in shape and the icosahedral symmetry is a rotational symmetry, it is natural to use spherical coordinates and express the basis functions in the orthonormal expansion of the electron density as products of functions on the sphere and radial functions. Similarly, for the approach based on the piecewise-constant function, it is natural to describe the boundary by its radius from the origin as a function of the angles, in which case the basis functions in the expansion are functions on the sphere.

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[†] GE Corporate Research and Development, KWC-605, One Research Circle, Niskayuna, NY 12309 (zheng@crd.ge.com). Part of this work was done while this author was affiliated with Purdue University.

[‡] School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907-1285 (doerschu@ecn.purdue.edu).

In this paper we describe a new method for explicitly[1] computing sets of functions that are representations of rotational groups in three dimensions and demonstrate the method on the identity representation of the icosahedral group, i.e., we explicitly compute a complete orthonormal basis for icosahedrally symmetric functions on the sphere. We call the functions in this basis "icosahedrally symmetric basis functions" (abbreviated ISBFs) and are not yet specific about which basis we will explicitly compute (see section 2). Using the ISBFs in the orthonormal expansions involved in the biophysics problems of the previous paragraph is much superior to the natural alternative of using spherical harmonics (denoted by $Y_{l,m}(\theta,\phi)$, where, here and elsewhere, (θ,ϕ) are spherical coordinates). For example: (1) The constraint that the particle has icosahedral symmetry is built into the functions rather than having to be added as a constraint in the nonlinear least squares problem. (2) There are many fewer ISBFs than $Y_{l,m}$ functions so many fewer coefficients have to be determined by nonlinear least squares in order to determine the electron density at a given level of resolution. (3) By incorporating the icosahedral symmetry directly in the mathematical description of the electron density by use of the ISBFs, we remove certain nonuniqueness problems in the nonlinear least squares problems.

There has been extensive work on ISBFs [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19], which are basis functions for the identity representation of the icosahedral group (the only representation needed in our application), and also on the more general problem of basis functions for all five irreducible representations of the icosahedral group [9, 17]. Sometimes ISBFs are called "icosahedral harmonics" [12, 20, 14] but, in analogy with spherical harmonics terminology, we reserve "icosahedral harmonics" for a collection of basis functions for all five irreducible representations. In the majority of previous work, ISBFs are described as linear combinations of spherical harmonics of fixed order which leads to simple rotational properties which are important for our electron microscopy applications. In this framework, the only task is to determine the coefficients of the linear combination. In a minority of previous work (e.g., [14]), ISBFs are described as polynomials in the rectangular coordinates.

Although extensive work has been done, existing results are limited in two aspects that are important for our application: (1) Explicit expressions in terms of standard operations (+, −, ×, ÷, and complex exponentiation) for ISBFs of arbitrary order are not provided. (2) The algorithms provided to derive an ISBF for some particular order are laborious, especially for orders greater than 29 when there can be two or more ISBFs of a single order. Reflecting these limitations, the most extensive tables of which we are aware [12, 18] tabulate ISBFs only up to order 30 (and in fact only one of two functions of order 30 is tabulated) or 44, respectively, while in a medium resolution x-ray diffraction interpolation problem we have required functions of order roughly 85. In the previous work [18] most closely related to the present paper, the derivation is unnecessarily complicated and not rigorous due to the "Q" operator in [18], implementation of the resulting algorithm requires symbolic derivatives in

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[1] By "explicit" we mean relationships from which formulas such as those given in section 7 can be computed. This is a weaker notion of "explicit" than is standard in, for example, spherical harmonics, where [6, Eqs. (3.53) and (3.50)]

$$Y_{l,m}(\theta,\phi)=\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_{l,m}(\cos\theta)\exp(im\phi),$$

$$P_{l,m}(x)=\frac{(-1)^m}{2^l l!}(1-x^2)^{m/2}\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}(x^2-1)^l.$$

order to compute the "$c_{p,q}$" numbers in [18] (numerical approximations of the derivatives are essentially impossible because determination of an lth order ISBF requires derivatives through lth order), the resulting algorithm in [18] is very slow compared to the algorithm of this paper, and the matrix-factorization implications of (15) in [18] are not appreciated or exploited. In another related work [19], the authors base their approach on projection operators applied to spherical harmonics (as in equation (1) of the present paper) followed by Gram–Schmidt orthogonalization and do all of the necessary integrals numerically to machine precision by noting that the integrands of interest are polynomials and that, therefore, suitably high-order Gaussian quadrature formulas can compute the integrals to machine precision. These machine precision results are then represented using square roots and rational numbers, and tables to order 15 are provided. In contrast with the approach of [19], we apply projection operators to delta functions rather than spherical harmonics, expand the result in spherical harmonics and in ISBFs, and by equating the two expansions derive a bilinear system of equations from which the weights in the expansion of an ISBF in terms of spherical harmonics can be derived symbolically rather than numerically to machine precision. In summary, in this paper we remove the limitations indicated above and the resulting algorithm is highly suitable for computer implementation in either numerical or symbolic programming languages; software is available from the authors.

2. Approach. Our goal is to determine ISBFs such that (1) each function is real valued, (2) the set of functions are a complete orthonormal basis for smooth icosahedrally symmetric functions on the sphere, and (3) each function is a linear combination of $Y_{l,m}$ for some fixed l. Let $\int \mathrm{d}\Omega$ mean $\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\sin(\theta)\mathrm{d}\theta\mathrm{d}\phi$. Then the orthonormality referred to in the second property is $\int I_{\alpha}^{*}(\theta,\phi)I_{\alpha'}(\theta,\phi)\mathrm{d}\Omega = \delta_{\alpha,\alpha'}$, where I_α denotes an ISBF from a not-yet-specified basis. Since rotation of $Y_{l,m}$ gives a function that is a linear combination of $\{Y_{l,m'} : m' = -l,\ldots,+l\}$ [21], the third property assures that the ISBFs will have simple properties under rotations, which is important in electron microscopy [2].

Goals (1)–(3) of the previous paragraph do not uniquely define the ISBFs when there are two or more ISBFs (denoted by $I_{\alpha_1},\ldots,I_{\alpha_p}$) in the subspace $\mathcal{S}_l$ spanned by $\{Y_{l,m} : m = -l,\ldots,+l\}$. In particular, if $O \in \mathcal{R}^{p\times p}$ is an orthonormal matrix, then the p functions $(I_{\alpha_1},\ldots,I_{\alpha_p})^T$ could be replaced by the p functions $O(I_{\alpha_1},\ldots,I_{\alpha_p})^T$ and still satisfy goals (1)–(3). A method to chose the basis in the subspace $\mathcal{S}_l$ so that the basis has meaningful representation-theoretic or spectral-theoretic properties is an open question. In this paper (see section 6) the basis is chosen so that the matrix of expansion coefficients, expanding ISBFs in terms of spherical harmonics, is triangular. This choice of basis minimizes the number of terms when computing ISBFs from spherical harmonics. Except for sections 6–8, all results in the paper are true for any basis satisfying goals (1)–(3).

A standard group-theoretic approach to determine the ISBFs is to apply projection operators [22, pp. 92–94] to the spherical harmonics. For the identity representation of a group, the projection operator has a simple form and a candidate ISBF, that is, the projection operator applied to the (l,m)th spherical harmonic, is

$$J_{l,m}(\theta,\phi) = \frac{1}{g}\sum_{k=0}^{g-1} P(T_k)Y_{l,m}(\theta,\phi), \tag{1}$$

where $g = 60$ is the order of the icosahedral group, T_k is the kth rotation of the icosahedral group, 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 [22].) While this method appears to be direct, it has some serious difficulties: First,

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

where the $D_{l,m,m'}(T_k)$ are the complicated Wigner's D coefficients [21], 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 3.1) state that there are only $N_l \leq 2l+1$ linearly independent ISBFs that can be constructed from $\{Y_{l,m} : m = -l, \dots, +l\}$) while (1) will generate $2l+1$ 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 is 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 ISBFs 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., $\delta(\cos\theta-\cos\theta_0)\delta(\phi-\phi_0)$. The result of the projection is a symmetrized delta function denoted by $\Delta(\theta_0,\phi_0;\theta,\phi)$:

$$\Delta(\theta_0,\phi_0;\theta,\phi) = \frac{1}{g}\sum_{k=0}^{g-1} P(T_k)[\delta(\cos\theta-\cos\theta_0)\delta(\phi-\phi_0)].$$

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: $P(T_k)[\delta(\cos\theta - \cos\theta_0)\delta(\phi-\phi_0)] = \delta(\cos\theta-\cos\theta_k)\delta(\phi-\phi_k)$. Furthermore, it is straightforward to expand the symmetrized delta function $\Delta(\theta_0,\phi_0;\theta,\phi)$ as a weighted sum of spherical harmonics:

$$\Delta(\theta_0,\phi_0;\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} w_{l,m}(\theta_0,\phi_0)Y_{l,m}(\theta,\phi),$$

specifically,

$$\Delta(\theta_0,\phi_0;\theta,\phi) = \frac{1}{g}\sum_{k=0}^{g-1}\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k,\phi_k)Y_{l,m}(\theta,\phi). \tag{2}$$

In addition, because the ISBFs are a complete orthonormal fixed basis for the subspace of totally symmetric functions, we know the expansion of $\Delta(\theta_0,\phi_0;\theta,\phi)$ as a weighted sum of ISBFs:

$$\Delta(\theta_0,\phi_0;\theta,\phi) = \sum_{\alpha} I^*_{\alpha}(\theta_0,\phi_0)I_{\alpha}(\theta,\phi). \tag{3}$$

In order to assure that each ISBF is a linear combination of $Y_{l,m}$ for fixed l we constrain the ISBF, denoted by $I_{l,n}$, to have the form

$$I_{l,n}(\theta,\phi) = \sum_{m=-l}^{+l} b_{l,n,m}Y_{l,m}(\theta,\phi), \tag{4}$$

where $l \in \{0, 1, \dots\}$, $n \in \{0, 1, \dots, N_l - 1\}$ (see Theorem 3.1 for the value of N_l), and the weights $b_{l,n,m}$ are unknown and are in fact the goal of these calculations. It is the matrix constructed from $b_{l,n,m}$ (l fixed) that will be made triangular in section 6, thereby selecting a particular orthonormal basis as described above. Finally, by equating (2) and (3) and using (4), we can derive nonlinear equations for the weights $b_{l,n,m}$ and these nonlinear equations can be solved recursively to give explicit formulas for the $b_{l,n,m}$.

3. Preliminaries.

For the spherical harmonics $Y_{l,m}$ we use the conventions of [6] and exploit the standard result [6, Eq. (3.53)] that $Y_{l,m}(\theta,\phi) = N_{l,m}P_{l,m}(\cos\theta)e^{im\phi}$, where $P_{l,m}(x)$ are the associated Legendre functions [6, Eq. (3.49)] and

$$N_{l,m} = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}.$$

Laporte [14] proves the following result regarding N_l.

THEOREM 3.1 (Laporte [14]). *For l even, the number N_l (denoted by $N_l^{(\mathrm{e})}$) satisfies the relationship*

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

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

$$N_l^{(\mathrm{o})} = \begin{cases} N_{l-15}^{(\mathrm{e})}, & l \geq 15, \\ 0, & 0 \leq l < 15. \end{cases}$$

For our concrete calculations, we choose the coordinate system used by Altmann [7] and Laporte [14] in which the z axis passes through two opposite vertices and the xz plane includes one edge of the icosahedron.

4. The bilinear equations for $b_{l,n,m}$.

The first proposition about the $b_{l,n,m}$ coefficients can be determined simply from the choice that $I_{l,n}$ are real and $Y_{l,-m}(\theta,\phi) = (-1)^m Y^*_{l,m}(\theta,\phi)$ [6, Eq. (3.54)].

PROPOSITION 4.1. *For each $l = 0, 1, \dots,$ $n = 0, \dots, N_l - 1$, and $m = -l, \dots, +l$,*

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

The second proposition, based on the orthonormality of the $Y_{l,m}$, relates the orthonormality of the $b_{l,n,m}$ coefficients to the orthonormality of the $I_{l,n}$.

PROPOSITION 4.2. *$I_{l,n}$ and $I_{l',n'}$ ($l \neq l'$; $l, l' = 0, 1, \dots$; $n = 0, \dots, N_l - 1$; $n' = 0, \dots, N_{l'} - 1$) are orthonormal for any choice of $b_{l,n,m}$. For fixed $l = 0, 1, \dots$ the $I_{l,n}$ ($n = 0, \dots, N_l - 1$) are orthonormal if and only if*

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

Let (θ_0, ϕ_0) be the (arbitrary) spherical coordinates of a delta function within the first asymmetric unit. Let $\{(\theta_k, \phi_k) : k = 1, 2, \dots, 59\}$ 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 Proposition 4.3 below.

PROPOSITION 4.3. *As a function of the parameters θ_0 and ϕ_0, the* 60 *symmetry-related positions on the unit sphere are*

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

where ϕ_k, γ_k, and α_k $(k=0,1,\ldots,4)$ are related to θ_0 and ϕ_0 by

$$\begin{aligned}
\phi_k &= \phi_0 + k\frac{2\pi}{5},\\
\cos\gamma_k &= \frac{1}{\sqrt{5}}(\cos\theta_0 + 2\sin\theta_0\cos\phi_k),\\
\cos\alpha_k &= \frac{2-\sin\theta_0\cos\phi_k}{\sqrt{5-(\cos\theta_0+2\sin\theta_0\cos\phi_k)^2}}.
\end{aligned}$$

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

PROPOSITION 4.4. *For any θ_0 and ϕ_0,*

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

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

Equate the expressions for $\Delta(\theta_0,\phi_0;\theta,\phi)$ in terms of spherical harmonics (2) and ISBFs (3) to find that

$$\sum_{l=0}^{\infty}\sum_{n=0}^{N_l-1} I_{l,n}(\theta_0,\phi_0) I_{l,n}(\theta,\phi) = \frac{1}{60}\sum_{k=0}^{59}\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k,\phi_k) Y_{l,m}(\theta,\phi). \tag{5}$$

Replace $I_{l,n}(\theta,\phi)$ by its expansion in terms of $Y_{l,m}(\theta,\phi)$ (4), multiply by $Y^*_{l',m'}(\theta,\phi)$, integrate over solid angles in θ and ϕ, and use the orthonormality of the spherical harmonics to obtain (after renaming the indices $l' \to l$, $m' \to m$) one form (Proposition 4.5, equation (6)) of the fundamental equation for determining the $b_{l,n,m}$ coefficients. Use Proposition 4.4 in (6) or (4) in (6) to obtain two alternative forms ((7) and (8), respectively). The results are summarized in the following proposition.

Proposition 4.5. *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:

$$\sum_{n=0}^{N_l-1} b_{l,n,m} I_{l,n}(\theta_0, \phi_0) = \frac{1}{60} \sum_{k=0}^{59} Y_{l,m}^*(\theta_k, \phi_k), \tag{6}$$

$$\sum_{n=0}^{N_l-1} b_{l,n,m} I_{l,n}(\theta_0, \phi_0)$$

$$= \begin{cases} \frac{1}{12} N_{l,m} \Big[P_{l,m}(\cos\theta_0) \left(e^{im\phi_0} + (-1)^l e^{-im\phi_0}\right) \\ \quad + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k) \left(e^{im\alpha_k} + (-1)^l e^{-im\alpha_k}\right) \Big]^*, & m = 5\mu \textit{ with } \mu \in \mathcal{Z}, \\ 0 & \textit{otherwise}, \end{cases} \tag{7}$$

$$\sum_{n=0}^{N_l-1} \sum_{m'=-l}^{+l} b_{l,n,m'} b_{l,n,m} Y_{l,m'}(\theta_0, \phi_0) = \frac{1}{60} \sum_{k=0}^{59} Y_{l,m}(\theta_k, \phi_k) \tag{8}$$

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

Notice that there is no coupling between different values of l in (6), (7), and (8).

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

Proposition 4.6.

1. *If* $m \neq 5\mu$ *with* $\mu \in \mathcal{Z}$, *then* $b_{l,n,m} = 0$.
2. *For* l *even,* $b_{l,n,m}$ *is real. For* l *odd,* $b_{l,n,m}$ *is imaginary.*
3. $b_{l,n,m} = b_{l,n,-m}(-1)^{l+m}$.
4. *For* l *odd,* $b_{l,n,0} = 0$.

Using these properties, we can simplify the expression for the $I_{l,n}$ as follows.

Proposition 4.7.

$$I_{l,n}(\theta, \phi) = \begin{cases} \sum_{m=0}^{+l} \frac{2}{1+\delta_{m,0}} N_{l,m} b_{l,n,m} P_{l,m}(\cos\theta) \cos m\phi, & l \textit{ even}, \\ \sum_{m=1}^{+l} 2 N_{l,m} i b_{l,n,m} P_{l,m}(\cos\theta) \sin m\phi, & l \textit{ odd}. \end{cases} \tag{9}$$

Proposition 4.7 implies that the ISBFs are completely determined by the $b_{l,n,m}$ coefficients for which $m \geq 0$. Therefore in the remainder of the paper, we assume $m \geq 0$ and $m' \geq 0$. Also, we absorb the "i" that occurs for l odd into $b_{l,n,m}$ so that the new definition of $b_{l,n,m}$ is always real (Proposition 4.6(2)). 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.

Notice in equation (8) that the $b_{l,n,m}$ coefficients enter only through the quantity $\sum_{n=0}^{N_l-1} b_{l,n,m} b_{l,n,m'}$. Therefore, define

$$C_{l,m,m'} = \sum_{n=0}^{N_l-1} b_{l,n,m} b_{l,n,m'}. \tag{10}$$

The remainder of the calculation is in two parts: (1) explicit computation of the $C_{l,m,m'}$ constants and (2) factorization of (10) to determine the $b_{l,n,m}$ coefficients.

5. Calculation of $C_{l,m,m'}$. Denote the integer part function by $\lfloor\cdot\rfloor$. Use Proposition 4.7 in Proposition 4.5 and specialize to the case of l even, $m = 5\mu$ with $\mu = 0, \ldots, \lfloor l/5\rfloor$ and $m' = 5\mu'$ with $\mu' = 0, \ldots, \lfloor l/5\rfloor$ to get the result that

$$\begin{aligned}&\sum_{m'=0}^{l} C_{l,m,m'} \frac{2N_{l,m'}}{1+\delta_{m',0}} P_{l,m'}(\cos\theta_0)\cos m'\phi_0\\ &= \frac{1}{6}N_{l,m}\left[P_{l,m}(\cos\theta_0)\cos m\phi_0 + \sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)\cos m\alpha_k\right].\end{aligned}\tag{11}$$

Multiply both sides of (11) by $\cos m''\phi_0$, integrate from 0 to 2π with respect to ϕ_0, and then divide by 2π. After using the orthonormality of $\cos m\phi_0$ and renaming m'' to m' we obtain Proposition 5.1, which is the basis for computing the $C_{l,m,m'}$.

Proposition 5.1. *For l even, $m = 5\mu$ with $\mu = 0, \ldots, \lfloor l/5\rfloor$ and $m' = 5\mu'$ with $\mu' = 0, \ldots, \lfloor l/5\rfloor$,*

$$\begin{aligned}N_{l,m'}C_{l,m,m'}P_{l,m'}(\cos\theta_0) &= \frac{1}{6}N_{l,m}\left[P_{l,m'}(\cos\theta_0)\delta_{m,m'}\frac{1+\delta_{m',0}}{2}\right.\\ &\left.+\frac{1}{2\pi}\int_0^{2\pi}\sum_{k=0}^{4} P_{l,m}(\cos\gamma_k)\cos(m\alpha_k)\cos(m'\phi_0)\mathrm{d}\phi_0\right].\end{aligned}\tag{12}$$

Equation (12) is of the form $C_{l,m,m'}f_{l,m'}(\theta_0) = h_{l,m,m'}(\theta_0)$. Therefore, for fixed l, m, and m', the functions $f_{l,m'}(\cdot)$ and $h_{l,m,m'}(\cdot)$ are proportional and $C_{l,m,m'}$ is the constant of proportionality. We are unable to compute the value of the integral contained in $h_{l,m,m'}(\cdot)$. However, we can compute $\lim_{\theta_0\to 0}(1/m'!)\mathrm{d}^{m'}/\mathrm{d}\theta_0^{m'}$ of both $f_{l,m'}(\cdot)$ and $h_{l,m,m'}(\cdot)$ and the resulting functions continue to have the same constant of proportionality. Define constants $g_{l,m'}$ and $D_{l,m,m'}$ by

$$g_{l,m'} = \left[\frac{1}{m'!}\frac{\mathrm{d}^{m'}}{\mathrm{d}\theta_0^{m'}}P_{l,m'}(\cos\theta_0)\right]_{\theta_0=0},\tag{13}$$

$$D_{l,m,m'} = \sum_{k=0}^{4}\left[\frac{1}{m'!}\frac{\mathrm{d}^{m'}}{\mathrm{d}\theta_0^{m'}}\frac{1}{2\pi}\int_0^{2\pi} P_{l,m}(\cos\gamma_k)\cos(m\alpha_k)\cos(m'\phi_0)\mathrm{d}\phi_0\right]_{\theta_0=0}.\tag{14}$$

Substitute these definitions into the limit of the m'th derivative of (12) to obtain the final equation for determining $C_{l,m,m'}$ in terms of $g_{l,m'}$, $D_{l,m,m'}$, and the standard formula for $N_{l,m}$.

Proposition 5.2. *For l even, $m = 5\mu$ with $\mu = 0, \ldots, \lfloor l/5\rfloor$ and $m' = 5\mu'$ with $\mu' = 0, \ldots, \lfloor l/5\rfloor$,*

$$N_{l,m'}C_{l,m,m'}g_{l,m'} = \frac{1}{6}N_{l,m}\left[g_{l,m'}\delta_{m,m'}\frac{1+\delta_{m',0}}{2} + D_{l,m,m'}\right].\tag{15}$$

We are unable to directly evaluate the derivatives in (13) and (14) and then set $\theta_0 = 0$ so instead we use the following proposition.

Proposition 5.3. *Let $f(\cdot)$ be a function with continuous arbitrary order derivatives. If $\lim_{\theta\to 0} f(\theta)/\theta^m = C$ and $|C| < \infty$, then*

$$\left[\frac{1}{m!}\frac{\mathrm{d}^m}{\mathrm{d}\theta^m}f(\theta)\right]_{\theta=0} = \lim_{\theta\to 0}\frac{f(\theta)}{\theta^m} = C.\tag{16}$$

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Initialization: $c_{l,m,-1} = 0, c_{m-1,m,m'} = 0$.
for( $m' = 0$ ; $m' \le M'$ ; $m' + +$ ){
        Compute $z_{m'}$ using equation (40);
        for( $m = m'$ ; $m \le L$ ; $m + +$ ){
            Compute $c_{m,m,m'}$ using equation (44);
            for( $l = m + 1$ ; $l \le L$ ; $l + +$ ){
                Compute $c_{l,m,m'}$ using equation (42);
            }
        }
}
```

FIG. 1. *Recursive algorithm to compute* $c_{l,m,m'}$.

Using Proposition 5.3 we can evaluate $g_{l,m'}$ and $D_{l,m,m'}$ (see Appendices A and B) with the results that

$$g_{l,m'} = \frac{(-1)^{m'}(l+m')!}{2^{m'}m'!(l-m')!},$$

$$D_{l,m,m'} = \frac{5}{2^{m'}} c_{l,m,m'},$$

where $c_{l,m,m'}$ can be computed either explicitly by

$$c_{l,m,m'} = 2^{-l} \sum_{i=\lfloor \frac{l+m}{2} \rfloor}^{l} (-1)^{l-i} \frac{(2i)!}{(l-i)!i!} \left(\frac{1}{\sqrt{5}} \right)^{2i-l-m} \sum_{j=0}^{2i-l-m} \frac{2^j}{(2i-l-m-j)!j!}$$

$$\times \sum_{p=0,2,\ldots}^{m} \frac{m!}{p!} \left(\frac{2}{\sqrt{5}} \right)^{m-p} \sum_{q=0}^{m-p} \left(-\frac{1}{2} \right)^{q} \frac{\delta_{m',j+p+q}}{(m-p-q)!q!}$$

or recursively as shown in Figure 1.

6. Factorization of $C_{l,m,m'}$ to compute $b_{l,n,m}$. Once we have $C_{l,m,m'}$, we use (10) to calculate $b_{l,n,m}$ using well-known matrix factorization algorithms. Note that there is no interaction between different values of l in (10) and so in this section l takes some fixed value and that value is suppressed in the matrix notation. Let $\mathbf{C}$ and $\mathbf{b}$ be matrices of dimensions $\lfloor l/5 \rfloor \times \lfloor l/5 \rfloor$ and $N_l \times \lfloor l/5 \rfloor$, respectively, in which the (n, μ)th elements are $C_{l,5n,5\mu}$ and $b_{l,n,5\mu}$, respectively. Equation (10) is then equivalent to

$$\mathbf{C} = \mathbf{b}^{\mathrm{T}}\mathbf{b}. \tag{17}$$

Therefore, $\mathbf{C}$ is symmetric and positive semidefinite. By orthonormality of ISBFs within the same l it follows that $\mathbf{b}\mathbf{b}^{\mathrm{T}} = \mathbf{I}_{N_l}$ (Proposition 4.2), where $\mathbf{I}_q$ is the $q \times q$ identity matrix and therefore $\mathbf{C}$ is also idempotent. Because $\mathbf{C}$ is idempotent, any factorization of $\mathbf{C}$ will be row orthonormal as described in Proposition 6.1.

PROPOSITION 6.1. *Let* $\mathbf{U} \in \mathcal{R}^{n \times n}$. *If* $\mathbf{V} \in \mathcal{R}^{m \times n}$ *is (row) full rank and* $\mathbf{U} = \mathbf{V}^{\mathrm{T}}\mathbf{V}$, *then* $\mathbf{V}$ *is row orthonormal if and only if* $\mathbf{U}$ *is idempotent.*

Note that if $\mathbf{b}$ is a solution to (17), then for any $N_l \times N_l$ orthogonal matrix $\mathbf{O}$, $\mathbf{b}' = \mathbf{O}\mathbf{b}$ is also a solution. For this reason we may add an additional constraint on $\mathbf{b}$ requiring it to be upper triangular, which implies $b_{l,n,5\mu} \equiv 0$ for $\mu < n$.

One algorithm to factor $\mathbf{C}$ is eigenvalue decomposition. Because $\mathbf{C}$ is idempotent $\mathbf{C}$ has only two eigenvalues, 0 and 1. Rows of $\mathbf{b}$ span the same space as eigenvectors of $\mathbf{C}$ with eigenvalues 1. Gram–Schmidt orthogonalization may be used on these eigenvectors to obtain orthogonal row vectors of $\mathbf{b}$. This algorithm requires all elements of $\mathbf{C}$ and it usually does not generate an upper triangular solution.

An alternative factorization algorithm is the Cholesky factorization, which is the algorithm we have used in computer codes. In this algorithm $b_{l,n,m}$ are computed by

$$\text{(18)}\quad b_{l,n,5n} = \sqrt{C_{l,5n,5n} - \sum_{n'=0}^{n-1} b^2_{l,n',5n}},$$

$$\text{(19)}\quad b_{l,n,5n'} = \frac{1}{b_{l,n,5n}}\left(C_{l,5n',5n} - \sum_{k=0}^{n-1} b_{l,k,5n} b_{l,k,5n'}\right), \quad n' = n+1, \dots, N_l - 1.$$

Equations (18) and (19) should be applied in the order $n = 0, 1, \dots, N_l - 1$ to ensure that the $b_{l,m,m'}$ that occur on the right-hand side are already determined by the time they are needed. This algorithm requires only elements of $C_{l,m,m'}$ for the index values $0 \le m' \le 5N_l$ and $m' \le m \le l$. This is a computational advantage because computation of $C_{l,m,m'}$ can be expensive especially for large l, m, m'. The algorithm generates an upper triangular $\mathbf{b}$.

7. Numerical example. For $l \in \{0, 1, \dots, 29\}$ there are either zero or one harmonic for each l and the cases with one harmonic are $l \in \{0, 6, 10, 12, 15, 16, 18, 20–22, 24–28\}$. By evaluating the recursions of this paper we have computed the harmonics through $l = 85$. Here we state only the first four harmonics in unnormalized form as computed symbolically by *Mathematica*:

$$\begin{aligned}
I_{0,0}(\theta,\phi) &= 1,\\
I_{6,0}(\theta,\phi) &= 2^3\cdot 3^2\cdot 5\cdot 11 P_{6,0}(\cos\theta) - P_{6,5}(\cos\theta)\cos 5\phi,\\
I_{10,0}(\theta,\phi) &= 2^8\cdot 3^4\cdot 5^2\cdot 7\cdot 13\cdot 19 P_{10,0}(\cos\theta) + 2^5\cdot 3^2\cdot 5\cdot 19 P_{10,5}(\cos\theta)\cos 5\phi\\
&\qquad + P_{10,10}(\cos\theta)\cos 10\phi,\\
I_{12,0}(\theta,\phi) &= 2^8\cdot 3^5\cdot 5^2\cdot 7^2\cdot 11\cdot 17 P_{12,0}(\cos\theta) - 2^4\cdot 3^2\cdot 5\cdot 7\cdot 11 P_{12,5}(\cos\theta)\cos 5\phi\\
&\qquad + P_{12,10}(\cos\theta)\cos 10\phi.
\end{aligned}$$

(Division of the stated formula by $\sqrt{2^2\pi}$, $2^4\cdot 3^2\cdot 5^2\sqrt{11\pi/13}$, $2^9\cdot 3^4\cdot 5^4\sqrt{7\cdot 13\cdot 19\pi}$, or $2^9\cdot 3^4\cdot 5^3\cdot 7\cdot 11\sqrt{5\cdot 7\cdot 17\pi}$ will normalize $I_{0,0}$, $I_{6,0}$, $I_{10,0}$, or $I_{12,0}$, respectively.) In Figure 2 we show a spherical plots of $I_{6,0}$ and $I_{12,0}$ which clearly exhibit the icosahedral symmetry of $I_{6,0}$ and $I_{12,0}$.

8. The *l* odd case. The calculations are similar to the case of l even. Here we list only the major results. The explicit expression for $c_{l,m,m'}$ (37) is modified to

$$c_{l,m,m'} = (-1)2^{-l} \sum_{i=\lfloor\frac{l+m}{2}\rfloor}^{l} (-1)^{l-i}\frac{(2i)!}{(l-i)!i!}\left(\frac{1}{\sqrt{5}}\right)^{2i-l-m} \sum_{j=0}^{2i-l-m} \frac{2^j}{(2i-l-m-j)!j!}$$
$$\times \sum_{p=1,3,\dots}^{m} \frac{m!}{p!}\left(\frac{2}{\sqrt{5}}\right)^{m-p} \sum_{q=0}^{m-p}\left(-\frac{1}{2}\right)^q \frac{\delta_{m',j+p+q}}{(m-p-q)!q!}.$$

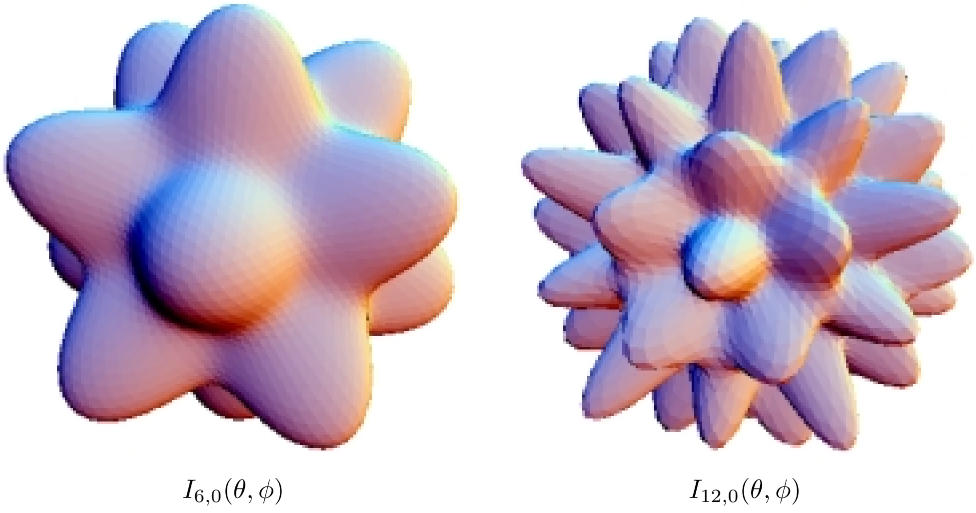

FIG. 2. *The ISBFs for* $(l,n)=(6,0)$ *and* $(l,n)=(12,0)$. *For each value of* θ *and* ϕ *the distance of the surface from the origin is* $c_{l,n}+I_{l,n}(\theta,\phi)$, *where* $c_{l,n}=2\max_{\theta,\phi}(|I_{l,n}(\theta,\phi)|)$.

For the recursive calculations, the initial conditions of z_m are modified to $z_1=1, z_2=-1$ and (44) is modified to

$$c_{m,m,m'}=\left(-\frac{1}{\sqrt{5}}\right)^{m-1}\frac{(2m)!}{m!}\left(\frac{1}{2}\right)\binom{m}{m'}z_{m'}.$$

9. Generalization to other representations and other rotational groups. The idea of applying the projection operator to the delta function can be applied to other finite groups of coordinate rotations and to higher dimensional representations.

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 $d_p=1,3,3,4,5$ [23, 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 which, for the icosahedral group, are tabulated in [15].

We continue to use the notation and results of [22] specialized to square integrable functions on the sphere which are indicated by $L^2(\theta,\phi)$. Let $f(\theta,\phi)\in L^2(\theta,\phi)$. By [22, Theorem I, p. 92] it follows that

$$f(\theta,\phi)=\sum_{p=0}^{N-1}\sum_{j=0}^{d_p-1}a_j^p f_j^p(\theta,\phi), \tag{20}$$

where $f_j^p(\theta,\phi)$ is a normalized basis function transforming as the jth row of the d_p-dimensional unitary irreducible representation Γ^p of $\mathcal{G}$, a_j^p are a set of complex numbers, and the sum on p is over all the inequivalent unitary irreducible representations of $\mathcal{G}$. Following [22, p. 93] we define the projection operator $\mathcal{P}^p_{j,j'}$ by

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

By [22, Theorem II, p. 93] it follows that

$$\mathcal{P}^p_{j,j} f(\theta,\phi) = a^p_j f^p_j(\theta,\phi),$$

where a^p_j and $f^p_j(\theta,\phi)$ are the coefficients and basis functions of the expansion of $f(\theta,\phi)$ (20) that relate to the jth row of Γ^p.

We apply these results to $\delta(\cos\theta - \cos\theta_0)\delta(\phi-\phi_0)$ to find that

$$\begin{aligned}
\delta(\cos\theta - \cos\theta_0)\delta(\phi-\phi_0) &= \sum_{p=0}^{N-1}\sum_{j=0}^{d_p-1} a^p_j \Delta^p_j(\theta_0,\phi_0;\theta,\phi),\\
a^p_j \Delta^p_j(\theta_0,\phi_0;\theta,\phi) &= \mathcal{P}^p_{j,j}\delta(\cos\theta - \cos\theta_0)\delta(\phi-\phi_0)\\
&= \frac{d_p}{g}\sum_{k=1}^{g}\Gamma^p(T_k)^*_{j,j}\delta(\cos\theta-\cos\theta_k)\delta(\phi-\phi_k), \qquad (21)
\end{aligned}$$

where (θ_k,ϕ_k) are the symmetry-related positions, e.g., for the icosahedral group, (θ_k,ϕ_k) are given by Proposition 4.3. The normalization a^p_j is set by the condition $\int \Delta^p_j(\theta_0,\phi_0;\theta,\phi)\mathrm{d}\Omega = 1$.

The symmetrized delta functions $\Delta^p_j(\theta_0,\phi_0;\theta,\phi)$ define subspaces, denoted by $(L^p_j)^2(\theta,\phi)$, of the Hilbert space $L^2(\theta,\phi)$ by

$$(L^p_j)^2(\theta,\phi) = \left\{ f(\theta,\phi)\in L^2(\theta,\phi) : f(\theta,\phi) = \int \Delta^p_j(\theta_0,\phi_0;\theta,\phi) f(\theta_0,\phi_0)\mathrm{d}\Omega_0 \right\}.$$

Each subspace contains only a certain type of basis function, the union of the subspaces is all of $L^2(\theta,\phi)$, 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 $I^p_j(\theta,\phi;\alpha)$ 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

$$I^p_j(\theta,\phi;l,n) = \sum_{m=-l}^{+l} b^p_j(l,n,m) Y_{l,m}(\theta,\phi).$$

Second, one can expand $\Delta^p_j(\theta_0,\phi_0;\theta,\phi)$ as a weighted sum of $Y_{l,m}(\theta,\phi)$:

$$\Delta^p_j(\theta_0,\phi_0;\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l} w^p_j(\theta_0,\phi_0;l,m) Y_{l,m}(\theta,\phi),$$

specifically (by using (21)),

$$\Delta^p_j(\theta_0,\phi_0;\theta,\phi) = \frac{d_p}{g a^p_j}\sum_{k=1}^{g}\Gamma^p(T_k)^*_{j,j}\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y^*_{l,m}(\theta_k,\phi_k)Y_{l,m}(\theta,\phi). \qquad (22)$$

Third, since $I^p_j(\theta,\phi;l,n)$ are a complete orthonormal fixed basis for $(L^p_j)^2(\theta,\phi)$, it follows that

$$\Delta^p_j(\theta_0,\phi_0;\theta,\phi) = \sum_{l=0}^{\infty}\sum_{n=0}^{N^p_j(l)} \left(I^p_j(\theta_0,\phi_0;l,n)\right)^* I^p_j(\theta,\phi;l,n). \qquad (23)$$

Fourth, by equating the expansions for $\Delta_j^p(\theta_0, \phi_0; \theta, \phi)$ provided by (22) and (23), one arrives at an equation that is exactly a generalization of (5). From this point forward, the $I_j^p(\theta, \phi; l, n)$ can be obtained by using the same methods already used for the identity representation of the icosahedral group.

10. Conclusion. We have described a novel method for explicitly computing orthonormal symmetrized harmonics and have applied the method to the identity representation of the icosahedral group. The work was motivated by the analysis of data from spherical viruses. Other applications of icosahedral symmetry include fullerenes [24] and quasi crystals [10]. A *Mathematica* program to obtain exact closed-form expressions for ISBFs of arbitrary order and a C program to calculate their numerical values are available from the authors upon request.

The same approach can be used to determine general explicit expressions for other groups and the particular examples of tetrahedrally and octahedrally symmetric basis functions have been done by the authors. Moreover, since the icosahedrally symmetric delta function can be viewed as the result of applying the projection operator of the identity representation of the icosahedral group to the regular delta function, we believe the same technique can be employed to calculate basis functions for the other four irreducible representations of the icosahedral group. These functions are of great interest in quantum mechanical problems with an icosahedrally symmetric potential, of which one example is the C_{60} molecule. Work in this direction is already in progress and will be reported in a future publication.

Appendix A. Computation of $g_{l,m'}$. Since

$$P_{l,m}(x) = \frac{(-1)^m (1-x^2)^{m/2}}{2^l l!} \frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}} (x^2-1)^l = (-1)^m (1-x^2)^{m/2} G_{l,m}(x), \tag{24}$$

where

$$G_{l,m}(x) = \frac{1}{2^l l!} \frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}} (x^2-1)^l \tag{25}$$

is a polynomial of order $l - m$, we find that

$$P_{l,m'}(\cos\theta_0) = (-1)^{m'} (\sin\theta_0)^{m'} G_{l,m'}(\cos\theta_0).$$

Using Proposition 5.3 we obtain

$$g_{l,m'} = \lim_{\theta_0 \to 0} \frac{P_{l,m'}(\cos\theta_0)}{\theta_0^{m'}} = (-1)^{m'} G_{l,m'}(1) = \frac{(-1)^{m'} (l+m')!}{2^{m'} m'! (l-m')!}.$$

Appendix B. Computation of $D_{l,m,m'}$. We begin the calculation of $D_{l,m,m'}$ by recalling the trigonometric and polynomial definitions of the Chebyshev polynomials of the first kind:

$$T_m(x) = \cos(m \arccos x) = \sum_{p=0,2,\dots}^{m} \binom{m}{p} x^{m-p} (x^2-1)^{p/2}. \tag{26}$$

Define $R_{l,m}(x,y)$ by

$$\begin{aligned}R_{l,m}(x,y) &= P_{l,m}\big((y+2x)/\sqrt{5}\,\big)\cos\Big(m\arccos\Big((2-x)/\sqrt{5-(y+2x)^2}\Big)\Big)\\ &= \Big(-\frac{1}{\sqrt{5}}\Big)^m G_{l,m}\Big(\frac{1}{\sqrt{5}}(y+2x)\Big)\\ &\quad\times\sum_{p=0,2,\ldots}^{m}\binom{m}{p}(2-x)^{m-p}[5x^2+y^2-1+4x(y-1)]^{p/2},\end{aligned} \tag{27}$$

where we have used (25) and (26). $R_{l,m}(x,y)$ derives its importance from the fact that $R_{l,m}(\sin\theta_0\cos\phi_k,\cos\theta_0) = P_{l,m}(\cos\gamma_k)\cos(m\alpha_k)$ which is central in the definition of $D_{l,m,m'}$ (14). Since $R_{l,m}(x,y)$ is a polynomial of order l in x and y it can be written in the form

$$R_{l,m}(x,y) = \sum_{m''=0}^{l} c_{l,m,m''}(y)x^{m''}, \tag{28}$$

where $c_{l,m,m''}(y)$ is a polynomial in y of order at most l.

Proposition B.1. *Define* $A_{m'',m'}$ *by*

$$A_{m'',m'} = \frac{1}{2\pi}\int_0^{2\pi}(\cos\phi_k)^{m''}\cos(m'\phi_0)\mathrm{d}\phi_0. \tag{29}$$

Then

1. *if* $m'' < m'$, *then* $A_{m'',m'} = 0$,
2. $A_{m',m'} = (1/2^{m'})\cos\frac{2\pi}{5}km'$.

Define $Q_{l,m,m'}(\theta_0)$ by

$$Q_{l,m,m'}(\theta_0) = \frac{1}{2\pi}\int_0^{2\pi} R_{l,m}(\sin\theta_0\cos\phi_k,\cos\theta_0)\cos(m'\phi_0)\mathrm{d}\phi_0,$$

which is the first step on the path from $R_{l,m}(\sin\theta_0\cos\phi_k,\cos\theta_0)$ to $D_{l,m,m'}$. Note that all dependence of $R_{l,m}(\sin\theta_0\cos\phi_k,\cos\theta_0)$ on ϕ_k (and thus on ϕ_0) comes from the first argument x. Using Proposition B.1 and (28) we obtain

$$Q_{l,m,m'}(\theta_0) = \sum_{m''=m'}^{l} c_{l,m,m''}(\cos\theta_0)(\sin\theta_0)^{m''}A_{m'',m'}. \tag{30}$$

Furthermore, by Proposition 5.3 and (30),

$$\left[\frac{1}{m'!}\frac{\mathrm{d}^{m'}}{\mathrm{d}\theta_0^{m'}}Q_{l,m,m'}(\theta_0)\right]_{\theta_0=0} = \lim_{\theta_0\to 0}\frac{Q_{l,m,m'}(\theta_0)}{\theta_0^{m'}} = c_{l,m,m'}(1)\frac{1}{2^{m'}}\cos\frac{2\pi}{5}km'. \tag{31}$$

In addition, if m' is an integer multiple of 5, then $\sum_{k=0}^{4}\cos\frac{2\pi}{5}km' = 5$. Using this fact and (31) in the definition of $D_{l,m,m'}$ (14) we obtain

$$D_{l,m,m'} = \frac{5}{2^{m'}}c_{l,m,m'}(1). \tag{32}$$

It remains only to calculate $c_{l,m,m'}(1)$. In the following two subsections we provide two methods, a finite summation and a recurrence, both based on the observation that

$$R_{l,m}(x,1) = \sum_{m'=0}^{l} c_{l,m,m'}(1)x^{m'}. \tag{33}$$

That is, $c_{l,m,m'}(1)$ is the coefficient of the term $x^{m'}$ in the lth order polynomial $R_{l,m}(x,1)$. For notational convenience, from now on we shall rewrite $c_{l,m,m'}(1)$ as $c_{l,m,m'}$ and $R_{l,m}(x,1)$ as $R_{l,m}(x)$.

B.1. Explicit expression for $\boldsymbol{c_{l,m,m'}}$. Substituting $y = 1$ into (27) we obtain

$$R_{l,m}(x) = \Big(-\frac{2}{\sqrt{5}}\Big)^m G_{l,m}\Big(\frac{1}{\sqrt{5}}(1+2x)\Big)H_m(x), \tag{34}$$

where

$$H_m(x) = (1-x-x^2)^{m/2}T_m\Big(\frac{2-x}{2\sqrt{1-x-x^2}}\Big) = \sum_{p=0,2,\ldots}^{m}\binom{m}{p}\Big(1-\frac{x}{2}\Big)^{m-p}\Big(\frac{\sqrt{5}}{2}x\Big)^p. \tag{35}$$

The function $G_{l,m}(\cdot)$ can be evaluated for an arbitrary argument from its definition in (25): take the derivative term by term of the binomial expansion of $(x^2-1)^l$ to obtain

$$G_{l,m}(x) = \frac{1}{2^l l!}\sum_{i=\lfloor\frac{l+m}{2}\rfloor}^{l}\binom{l}{i}(-1)^{l-i}\frac{(2i)!}{(2i-l-m)!}x^{2i-l-m}.$$

By further use of the binomial expansion, we can obtain the following expression for $R_{l,m}(x)$:

$$\begin{aligned}R_{l,m}(x) = 2^{-l}&\sum_{i=\lfloor\frac{l+m}{2}\rfloor}^{l}(-1)^{l-i}\frac{(2i)!}{(l-i)!i!}\Big(\frac{1}{\sqrt{5}}\Big)^{2i-l-m}\sum_{j=0}^{2i-l-m}\frac{2^j x^j}{(2i-l-m-j)!j!}\\ &\times\sum_{p=0,2,\ldots}^{m}\frac{m!}{p!}\Big(\frac{2}{\sqrt{5}}\Big)^{m-p}x^p\sum_{q=0}^{m-p}\Big(-\frac{1}{2}\Big)^q\frac{x^q}{(m-p-q)!q!}.\end{aligned} \tag{36}$$

From (36) and (33) it is clear that an explicit expression for $c_{l,m,m'}$ is

$$\begin{aligned}c_{l,m,m'} = 2^{-l}&\sum_{i=\lfloor\frac{l+m}{2}\rfloor}^{l}(-1)^{l-i}\frac{(2i)!}{(l-i)!i!}\Big(\frac{1}{\sqrt{5}}\Big)^{2i-l-m}\sum_{j=0}^{2i-l-m}\frac{2^j}{(2i-l-m-j)!j!}\\ &\times\sum_{p=0,2,\ldots}^{m}\frac{m!}{p!}\Big(\frac{2}{\sqrt{5}}\Big)^{m-p}\sum_{q=0}^{m-p}\Big(-\frac{1}{2}\Big)^q\frac{\delta_{m',j+p+q}}{(m-p-q)!q!}.\end{aligned} \tag{37}$$

B.2. Recursive calculation of $\boldsymbol{c_{l,m,m'}}$. Using the recursive relation for Chebyshev polynomials

$$T_{m+1}(x) - 2xT_m(x) + T_{m-1}(x) = 0$$

and (35) we can derive the following recursive relation for $H_m(x)$:

$$H_{m+1}(x) + (x-2)H_m(x) + (1-x-x^2)H_{m-1}(x) = 0 \tag{38}$$

with the initial condition $H_0(x) = 1, H_1(x) = 1 - x/2$. The solution of (38) is

$$\begin{aligned} H_m(x) &= \frac{1}{2}\left[\left(1 + \frac{-1+\sqrt{5}}{2}x\right)^m + \left(1 - \frac{\sqrt{5}+1}{2}x\right)^m\right] \\ &= \frac{1}{2}\sum_{m'=0}^{m} \binom{m}{m'} z_{m'} x^{m'}, \end{aligned} \tag{39}$$

where

$$z_{m'} = \left(\frac{-1+\sqrt{5}}{2}\right)^{m'} + (-1)^{m'}\left(\frac{\sqrt{5}+1}{2}\right)^{m'}.$$

Note that $z_{m'}$ satisfies the recursion

$$z_{m'+1} + z_{m'} - z_{m'-1} = 0 \tag{40}$$

with the initial condition $z_0 = 2$ and $z_1 = -1$.

Using (34), (24), and the recursion for $P_{l,m}(x)$ in l

$$(l+1-m)P_{l+1,m}(x) - (2l+1)xP_{l,m}(x) + (l+m)P_{l-1,m}(x) = 0,$$

we can derive a recursion for $R_{l,m}(x)$ in l:

$$(l+1-m)R_{l+1,m}(x) - (2l+1)\frac{1}{\sqrt{5}}(1+2x)R_{l,m}(x) + (l+m)R_{l-1,m}(x) = 0. \tag{41}$$

Substitute (33) into (41). The coefficient of each power of x must vanish separately, which leads to the recursion

$$(l+1-m)c_{l+1,m,m'} - (2l+1)\frac{1}{\sqrt{5}}(c_{l,m,m'} + 2c_{l,m,m'-1}) + (l+m)c_{l-1,m,m'} = 0. \tag{42}$$

To initialize (42) to compute $c_{l,m,m'}$, note that $c_{l,m,-1} = 0$ and $c_{m-1,m,m'} = 0$. We still need $c_{m,m,m'}$ to start the recursion, but

$$\sum_{m'=0}^{m} c_{m,m,m'} x^{m'} = R_{m,m}(x) = \left(-\frac{1}{\sqrt{5}}\right)^m \frac{(2m)!}{m!} H_m(x) \tag{43}$$

so by (39)

$$c_{m,m,m'} = \left(-\frac{1}{\sqrt{5}}\right)^m \frac{(2m)!}{m!}\left(\frac{1}{2}\right)\binom{m}{m'} z_{m'}. \tag{44}$$

Given an integer L, Figure 1 shows an algorithm, with control structures written in the C programming language, to calculate all $c_{l,m,m'}$ for $l \le L, m' \le M' = 5N_L, m' \le m \le l$. Because the factorization algorithm described in section 6 uses only $C_{l,m,m'}$ for which $0 \le m' \le 5N_l, m' \le m \le l$, it follows that for any single l we need only to compute $c_{l,m,m'}$ for $0 \le m' \le 5N_l, m' \le m \le l$.

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