COMPUTATION OF REAL BASIS FUNCTIONS FOR THE 3-D ROTATIONAL POLYHEDRAL GROUPS T, O, AND I∗

NAN XU† AND PETER C. DOERSCHUK‡

Abstract. Basis functions which are invariant under the operations of a rotational polyhedral group $G$ are able to describe any 3-D object which exhibits the rotational symmetry of the corresponding Platonic solid. However, in order to characterize the spatial statistics of an ensemble of objects in which each object is different but the statistics exhibit the symmetry, a larger set of basis functions is required. In particular, for each irreducible representation (irrep) of $G$, it is necessary to include basis functions that transform according to that irrep. This larger set of basis functions is a basis for square-integrable functions on the surface of the sphere in 3-D. Because the objects are real-valued, it is convenient to have real-valued basis functions. In this paper the existence of such real-valued bases is proven and an algorithm for their computation is provided for the icosahedral $I$ and the octahedral $O$ symmetries. Furthermore, it is proven that such a real-valued basis cannot exist for the tetrahedral $T$ symmetry because some irreps of $T$ are essentially complex. The importance of these basis functions to computations in single-particle cryo electron microscopy is described.

Key words. rotational polyhedral groups, finite subgroups of $SO_3$, rotational groups of Platonic solids, real-valued matrix irreducible representations, numerical computation of similarity transformations, basis functions that transform as a row of an irreducible representation of a rotation group

AMS subject classifications. 2604, 2004, 57S17, 57S25

1. Introduction. 3-D rotational symmetry under a finite group $G$ of rotations arises in several situations such as quasi-crystals, fullerenes, and viruses. One method for representing such objects is an orthonormal expansion in basis functions where each basis function has a specific behavior under the operations of $G$. If the object is invariant under the operations of $G$, then each basis function should transform according to the identity irreducible representation (irrep) of $G$ (“invariant basis”) and such basis functions have been extensively studied [17, 34, 1, 31, 10, 15, 23, 25, 27, 28, 11, 38, 47, 16]. In more complicated situations, the object is not invariant under the operations of $G$ and a larger set of basis functions is needed, specifically, a set that includes functions that transform according to each of the irreps of $G$ (“all irreps basis”) and such basis functions have also been studied [10, 34, 11, 38]. Our motivating problem, a structural biology problem described in Section 2, is an example of the more complicated situation. We provide a practical computational algorithm for a set of basis functions with the following properties:

1. Each function in the basis is a linear combination of spherical harmonics$^1$ of a fixed degree $l$.
2. Each function in the basis is real-valued.
3. The basis functions are orthonormal.
4. Under the rotations of a finite symmetry group, each function in the basis transforms according to one row of the corresponding irreducible representation (irrep) matrices.

$^∗$This work was supported by NSF 1217867.
$^†$School of Electrical and Computer Engineering, Cornell University, Ithaca, NY, USA, ID (nx25@cornell.edu).
$^‡$School of Electrical and Computer Engineering, Nancy E. and Peter C. Meinig School of Biomedical Engineering, Cornell University, Ithaca, NY, USA, ID (pd83@cornell.edu).

$^1$Throughout this paper, spherical harmonics are denoted by $Y_{l,m}(\theta, \phi)$ where the degree $l$ satisfies $l \in \{0, 1, \ldots \}$, the order $m$ satisfies $m \in \{-l, \ldots, l\}$ and $(\theta, \phi)$ are the angles of spherical coordinates with $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$ [35, Section 14.30, pp. 378–379].
Because our structural biology problem includes the structure of viruses, which often exhibit the symmetry of a Platonic solid [13], we focus on the three rotational polyhedral groups, the tetrahedral $T$, octahedral $O$, and icosahedral $I$ groups. In the cases of the octahedral and icosahedral groups, it is possible to find a set of basis functions which is complete in the space of square-integrable functions on the surface of the sphere and which satisfies Properties 1–4. However, in the case of the tetrahedral group, it is not possible to find a set of basis functions that is both complete and which satisfies Properties 1–4 (Section 4) and one way in which to achieve completeness is to added additional complex-valued functions which is an undesirable situation for our structural biology application (Section 2). The finite subgroups of $SO_3$ are $T$, $O$, $I$, the cyclic groups $C_n$, and the dihedral groups $D_n$ [4, Theorem 19.2, p. 105]. The $T$, $O$, and $I$ basis functions can naturally and efficiently be computed in spherical coordinates with spherical harmonics and that is the focus of this paper. It is likely that the $C_n$ basis functions, and possibly the $D_n$ basis functions, are more naturally and efficiently computed in cylindrical coordinates with cylindrical harmonics and for that reason also they are not discussed.

In the majority of existing literature, basis functions of a symmetry group have been generated as a linear combination of spherical harmonics of a single degree [1, 2, 3, 33, 37, 34, 17, 47, 48], because of the importance of rotations and the relative simplicity of rotating spherical harmonics. Spherical harmonics have been widely applied in structural biology, e.g., the fast rotation function [14]. Other work express the basis functions of a rotational polyhedral group as multipole expansions in rectangular coordinates [26, 22]. Previous work uses a variety of techniques and often has a restriction on the value $l$ of the spherical harmonics [1, 2, 3, 33, 37, 10, 34, 11, 38]. For instance, Refs. [1, 2, 3] consider a range of point groups and use the techniques of projection operators and Wigner $D$ transformations to compute basis functions up to degree $l = 12$, while Ref. [10] uses similar techniques restricted to the icosahedral group to provide basis functions up to degree $l = 15$. Refs. [33, 37] use the method of representation transformation to compute the invariant basis functions of the cubic group up to degree $l = 30$; the work of Ref. [34] extends this computation to all irreps basis functions. Refs. [11, 38] propose a method for deriving all irreps basis functions of the cubic and the icosahedral groups for a specific degree $l$. However, for computation which needs all irreps basis functions for a large range of $l$ values (e.g., from 1 to 55), the one-by-one derivation is cumbersome. Later work [17, 47, 48] release this restriction on the degree $l$ and allow for the computation of the invariant basis functions of any rotational polyhedral group. However, the recursions in [47, 48] appear to be unstable in computational experiments.

In this paper we derive an algorithm for efficiently computing the all irreps basis functions for the tetrahedral, octahedral, and icosahedral groups for arbitrary value of $l$. The algorithm is not recursive, so stability is not an issue, and the most burdensome calculation in the algorithm is to determine the eigenvectors of a real symmetric matrix that is of dimension $2d_p$ where $d_p$ is the dimension of the $p$th irrep which, for the groups we consider, is no larger than 5. To compute functions satisfying Properties 1–4, we determine real-valued generalized projection operators [12, p. 93] and apply them to real-valued spherical harmonics (Section 4). To determine real-valued generalized projection operators, we first determine real-valued irrep matrices. Standard approaches exist, e.g., Young diagrams [19]. However, taking advantage of existing complex-valued irrep matrices [5, 29], we derive an algorithm to find a similarity matrix that transforms the potentially-real complex-valued irrep matrices to real-valued irrep matrices (Section 3). We also demonstrate that functions satisfying
Properties 1–4 exist if and only if real-valued irrep matrices exist (Section 5) and provide numerical examples (Section 6).

The following notation is used throughout the paper. Let \( M \) be a matrix. Then \( M^* \) is the complex conjugate of \( M \), \( M^T \) is the transpose of \( M \), and \( M^H \) is the Hermitian transpose of \( M \), i.e., \( (M^T)^* \). \( I_n \in \mathbb{R}^{n \times n} \) is the identity matrix. \( \mathbb{R} \) and \( \mathbb{I} \) are the real and imaginary parts, respectively, of their arguments. “Representation” and “Irreducible representation” are abbreviated by “rep” and “irrep”, respectively. For 3-D vectors, \( x = \|x\|_2 \) and \( x/x \) is shorthand for the \((\theta, \phi)\) angles in the spherical coordinate system. Integration of a function \( f: \mathbb{R}^3 \to \mathbb{C} \) over the surface of the sphere in \( \mathbb{R}^3 \) is denoted by \( \int f(x) d\Omega \) meaning \( \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} f(x, \theta, \phi) \sin \theta d\theta d\phi \). The Kronecker delta function is denoted by \( \delta_{i,j} \) and has value 1 if \( i = j \) and value 0 otherwise.

2. Motivation. Single-particle cryo electron microscopy (cryo EM) [6, 9, 8] provides essentially a noisy 2-D projection in an unknown direction of the 3-D electron scattering intensity of a \( 10^1-10^2 \) nm biological object such as a ribosome or a virus. For studies with high spatial resolution, only one image is taken of each instance of the object because the electron beam rapidly damages the object. There are multiple software systems, e.g., Refs. [18, 30, 40], for computing a 3-D reconstruction of the object from sets of images of different instances of the object and these systems include the possibility that the instances come from a small set of classes where all instances within one class are identical (discrete heterogeneity). Not only may there be multiple classes of heterogeneity, but each instance within a class may vary due to, for example, flexibility (continuous heterogeneity). By describing the electron scattering intensity by a real-valued Fourier series with coefficients which are random variables and solving a maximum likelihood estimation problem for the mean vector and covariance matrix of the coefficients, we have a theory [49] and several examples [44, 43, 21] demonstrating the ability to characterize the continuous heterogeneity.

Symmetry is sometimes an important feature of a biological object. An important example for viruses is icosahedral symmetry [7]. If all instances are identical or if all instances within each class are identical (discrete heterogeneity), it is natural to impose the symmetry on the electron scattering intensity of the object. However, if each instance in the class is different (continuous heterogeneity) it is more natural to impose the symmetry on the statistics of the electron scattering intensity rather than imposing the symmetry on the electron scattering intensity itself [49, Eqs. 55–56]. A sufficient method to achieve symmetric statistics in the case of icosahedral symmetry is to use basis functions in the Fourier series such that each basis function has icosahedral symmetry. Such basis functions are known [48] and were used in the examples [44, 43, 21] referred to above. However, this is not a necessary and sufficient approach to achieving symmetric statistics. In particular, using basis functions where each function has the symmetry implies that each instance of the object has the symmetry while it is more natural to assume that the instances lack the symmetry and the symmetry only appears in the expectations that lead to the statistics. This requires constraints on the mean and covariance of the coefficients and the constraints are simplest if each basis function transforms under rotations of the group as some row of some irreducible representation of the group (Eq. 8) and if all of the basis functions are real valued (Eq. 10) [45] and these two goals are the primary topic of this paper. Using harmonic functions (Eq. 9) helps characterize the spatial resolution of the estimated electron scattering intensity and leads to simple formulas for both the electron scattering intensity and the 3-D Fourier transform of the electron scattering intensity. Using orthonormal functions (Eq. 11) improves the numerical properties of
the inverse problem.

Our focus on real-valued basis functions comes from the fact that the electron scattering intensity is real valued and therefore, if the basis functions are also real valued, then the coefficients can be real valued which simplifies the statistical estimation problem in two ways. Suppose $c$ (a column vector containing the coefficients) must be complex. The first complication is that it is necessary to estimate both the expectation of $cc^T$ and of $cc^H$. The second complication is that it is necessary to account for constraints on the allowed values of $c$, much like a 1-D Fourier series for a real-valued function that is periodic with period $T$ requires that the coefficients (denoted by $c_n$) satisfy $c_n = c_{-n}^*$ when the basis functions for the Fourier series are $\exp(i2\pi/Tnt)$. Our focus on real-valued basis functions which allow real-valued coefficients permits us to avoid both of these complications for the important case of the icosahedral group.

3. Computation of real irrep matrices. Starting from a set of matrices that make up a complex-valued unitary irrep, the goal of this section is to compute, if possible, a similarity transformation such that the similarity transformation applied to the known complex-valued unitary irrep is a real-valued orthonormal irrep. The question of existence is answered by the Frobenious-Schur theory [12, p. 129, Theorem III] as follows. Let $\Gamma_c^p$ of the icosahedral group.

for the case of potentially real irreps: $S^p \in \mathbb{C}^{d_p \times d_p}$ for the case of potentially real irreps:

1. For any such unitary matrix $S^p$, show that the complex irrep $\Gamma_c^p$ is similar to its complex conjugate $(\Gamma_c^p)^*$ with the similarity transformation $S^p(\Gamma_c^p)^T$.
2. Find a matrix $C^p$, which is an explicit function of $\Gamma_c^p$, and is a similarity matrix relating the two sets of matrices $\Gamma_c^p$ and $(\Gamma_c^p)^*$. 
3. Factor $C^p$ to compute a particular $S^p$.

Step 1 is achieved by Lemma 1.

LEMMA 1. Suppose that $\Gamma_c^p(g)$ $(g \in G)$ are complex unitary irrep matrices for the $p$th rep of the group $G$ which is potentially real. Let $S^p \in \mathbb{C}^{d_p \times d_p}$ denote a unitary matrix. The following two statements are equivalent:

(1) For all $g \in G$, $\Gamma_c^p(g) = (S^p)^H \Gamma_c^p(g) S^p$ such that $\Gamma_c^p(g) \in \mathbb{R}^{d_p \times d_p}$.

(2) For all $g \in G$, $[S^p(\Gamma_c^p)^T]^{-1}\Gamma_c^p(g)[S^p(\Gamma_c^p)^T] = (\Gamma_c^p(g))^*$. 

Please see Appendix A for the proof.

Step 2 computes a non-unitary symmetric matrix $(Z^p)$ (Lemma 2), which is then normalized $(C^p)$ to be unitary (Corollary 3).
Lemma 2. Suppose that $\Gamma_c^p(g) \ (g \in G)$ are complex unitary irrep matrices for the $p$th rep of the group $G$ which is potentially real. Let $A^p \in \mathbb{C}^{d_p \times d_p}$ be a nonsingular transpose-symmetric matrix (i.e., $(A^p)^T = A^p$) and $Z^p$ be defined by Eq. 3, specifically,

$$Z^p = \frac{1}{N_g} \sum_{g \in G} \Gamma_c^p(g) A^p ((\Gamma_c^p(g))^*)^{-1}.$$

If $Z^p$ is nonzero, then $Z^p$ has the following properties:
1. $(Z^p)^T = Z^p$.
2. $(Z^p)^* Z^p = c_Z I_{d_p}$ where $c_Z \in \mathbb{R}^+$. 
3. For all $g \in G$, $(\Gamma_c^p(g))^* = (Z^p)^* \Gamma_c^p(g) Z^p$.

Please see Appendix A for the proof.

It is important to find a matrix $A^p$ such that the matrix $Z^p$ is nonzero. For the three rotational polyhedral groups that we consider in this paper, this issue is discussed in Section 6.1.

Corollary 3. Define $C^p$ by

$$C^p = Z^p / \sqrt{c_Z}.$$

Then $C^p$ has the following properties:
1. $(C^p)^T = C^p$.
2. $(C^p)^* C^p = I_{d_p}$.
3. For all $g \in G$, $(\Gamma_c^p(g))^* = (C^p)^* \Gamma_c^p(g) C^p$.

The matrix $S^p$ in the definition of potentially real is not unique. Comparing Property 3 of Corollary 3 and Eq. 2, $S^p$ can be restricted to satisfy

$$C^p = S^p (S^p)^T$$

noting, however, that even with this restriction, $S^p$ is still not unique. Because Lemma 1 is "if and only if", any unitary matrix $S^p$ that satisfies Eq. 5 is a satisfactory similarity matrix. The existence of the unitary factorization described by Eq. 5 is guaranteed by the Takagi Factorization (Ref. [24, Corollary 4.4.6, p. 207]).

Step 3 is to perform the factorization of $C^p$ and a general algorithm is provided by Lemma 4 which is based on the relationship between the coneigenvectors of a unitary symmetric matrix $Q$ and the eigenvectors of its real representation matrix $B$, which is defined by $B = \begin{bmatrix} \Re Q & \Im Q \\ \Im Q & -\Re Q \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$.

Lemma 4. Let $Q \in \mathbb{C}^{n \times n}$ be a unitary symmetric matrix, i.e., $Q^T = Q$ and $QQ^* = I_n$. Let $B \in \mathbb{R}^{2n \times 2n}$ be the real representation of $Q$, i.e., $B = \begin{bmatrix} \Re Q & \Im Q \\ \Im Q & -\Re Q \end{bmatrix} \in \mathbb{R}^{2n \times 2n}$. Then, the following properties hold:
1. $B$ is nonsingular and has $2n$ real eigenvalues and $2n$ orthonormal eigenvectors.
2. The eigenvectors and eigenvalues of $B$ are in pairs, specifically,
$$B \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix} \text{ if and only if } B \begin{bmatrix} y \\ -x \end{bmatrix} = -\lambda \begin{bmatrix} y \\ x \end{bmatrix}.$$
3. Let $\begin{bmatrix} x_{y1} \\ -y_1 \end{bmatrix}, \ldots, \begin{bmatrix} x_{yn} \\ -y_n \end{bmatrix}$ be the orthonormal eigenvectors of $B$ associated with $n$ positive eigenvalues of $\lambda_1, \ldots, \lambda_n$. (Since $B$ is nonsingular, there are no
zero eigenvalues.) Then $x_1 - iy_1, \ldots, x_n - iy_n$ are the set of orthonormal coneigenvectors of $Q$ associated with the $n$ coneigenvalues of $Q(x_k - iy_k) = \lambda_k(x_k - iy_k)$ for $k = 1, \ldots, n$.

4. $\lambda_1 = \ldots = \lambda_n = 1$.

5. Define $u_k = x_k - iy_k$ and $U = [u_1, \ldots, u_n] \in \mathbb{C}^{n \times n}$. Then $U$ is unitary.

6. $Q = UU^T$.

Please see Appendix A for the proof.

Applying Lemma 4 to $C_p$ results in a particular matrix $S^p$ which is the $U$ matrix of Property 5. The complete algorithm is summarized in Theorem 5.

**Theorem 5.** A unitary matrix, $S^p \in \mathbb{C}^{d_p \times d_p}$, which is a similarity transformation between the provided potentially-real complex unitary irrep and a real orthonormal irrep, can be computed by the following steps:

1. Compute $Z^p$ by Eq. 3.
2. Compute $cZ$ by Lemma 2 Property 3 and compute $C^p$ by Eq. 4.
3. Compute the eigenvectors and eigenvalues of

   $$(7) \quad B^p = \begin{bmatrix} \Re C^p & \Im C^p \\ \Im C^p & -\Re C^p \end{bmatrix} \in \mathbb{R}^{2d_p \times 2d_p}.$$  

4. Form the matrix $V^p \in \mathbb{R}^{2d_p \times d_p}$ whose columns are the $d_p$ eigenvectors of $B^p$ that have positive eigenvalues.
5. Then $S^p = [I_{d_p}, iI_{d_p}]V^p$.

**4. Computation of real basis functions.** In this section, formulas corresponding to the four goals in Section 1 are stated in Eqs. 9–12 and the computation of basis functions satisfying these formulas is then described. The mathematical goal corresponding to Item 4 in Section 1 requires the following definition:

**Definition 6.** ([12, Eq. 1.26, p. 20]) A basis function that transforms as the $n$th row ($n \in \{1, \ldots, d_p\}$) of the $p$th rep ($p \in \{1, \ldots, N_{\text{rep}}\}$) of the finite group $G$, denoted by $F_{p,n} \in \mathbb{C}$, is a function such that

$$F_{p,n}(R_g^{-1}x/x) = \sum_{m=1}^{d_p} (\Gamma^p(g))_{m,n}F_{p,m}(x/x) \text{ for all } g \in G,$$

where $R_g \in \mathbb{R}^{3 \times 3}$ is the 3-D rotation matrix corresponding to $g \in G$ and $\Gamma^p(g)_{g \in G}$ are the unitary irrep matrices of the $p$th rep.

The basis functions which satisfy the four goals in Section 1 have four indices: which irreducible representation ($p$), which subspace defined by spherical harmonics of fixed order $l$ ($l$), which vector ($n$), and which component of the vector ($j$). Let $F_{p,l,n,j}$ be a basis function that transforms as the $j$th row of the irrep matrices and $F_{p,l,n} = (F_{p,l,n,j=1}, \ldots, F_{p,l,n,j=d_p})^T$. Let $Y_{l,m}(\theta, \phi)$ be the spherical harmonic of degree $l$ and order $m$ [35, Section 14.30, pp. 378–379]. Then the goals are to obtain
a set of functions such that

\[ F_{p,l,n,j}(\theta, \phi) = \sum_{m=-l}^{+l} c_{p,l,n,j,m} Y_{l,m}(\theta, \phi) \]  

(9)

\[ F_{p,l,n,j}(\theta, \phi) \in \mathbb{R} \]  

(10)

\[
\delta_{p,p'}\delta_{l,l'}\delta_{n,n'}\delta_{j,j'} = \int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} F_{p,l,n,j}(\theta, \phi) F_{p',l',n',j'}(\theta, \phi) \sin \theta \, d\theta \, d\phi  
\]  

(11)

\[ F_{p,l,n}(R_g^{-1}x/x) = (\Gamma^p(g))^T F_{p,l,n}(x/x). \]  

(12)

The computation is performed by the projection method of Ref. [12, p. 94] in which various projection operators (Definition 7) are applied to each function of a complete basis for the space of interest. When the various projection operators are defined using real-valued orthonormal irrep matrices (as computed in Section 3) and are applied to a real-valued complete orthonormal basis in the subspace spanned by spherical harmonics of degree \( l \) (which has dimension \( 2l+1 \)) then the resulting basis for the same subspace is real-valued, complete, and orthonormal [12, Theorems I and II, pp. 92-93].

The remainder of this section has the following organization. First, the projection operators are defined (Definition 7). Second, the initial basis in the subspace is described. Third, the results of applying the projection operators to the basis functions are described in terms of individual functions (Lemma 8) and in terms of sparse matrices of order \( (2l+1) \times (2l+1) \). Fourth, normalization is discussed (Eq. 23). Fifth, too many basis functions are computed by this process, i.e., more than \( 2l+1 \), so Gram-Schmidt orthogonalization is used to extract a subset containing \( 2l+1 \). Finally, sixth, comments are made on the non-uniqueness of the final basis.

**Definition 7.** The projection operators \( P_{j,k}^p \) are defined by [12, Eq. 5.2, p. 93]

\[ P_{j,k}^p = \frac{d_p}{N_g} \sum_{g \in G} (\Gamma^p(g))_{j,k}^* P(g) \]  

(13)

where \( \Gamma^p(g) \in \mathbb{C}^{d_p \times d_p} \) for all \( g \in G \) are the irrep matrices and \( P(g) \) is the abstract rotation operator, specifically,

\[ P(g)f(x) = f(R_g^{-1}x) \]  

(14)

where \( R_g \in \mathbb{R}^{3 \times 3} \) with \( R_g^{-1} = R_g^T \) and \( \det R_g = +1 \) is the rotation matrix corresponding to \( g \in G \). When \( P(g) \) is applied to a vector-valued function, it operates on each component of the vector.

The projection operator is applied to a set of basis functions. One natural choice is the set of spherical harmonics [35, Eq. 14.30.1, p. 378] (denoted by \( Y_{l,m}(\theta, \phi) \), where the arguments will routinely be suppressed) because \( Y_{l,m} \) have simple rotational properties. However, except for \( Y_{l,m=0} \), spherical harmonics are complex valued. Older literature [32, Eq. 10.3.25, p. 1264] used real-valued definitions, e.g.,

\[ \hat{Y}_{l,m}(\theta, \phi) = \begin{cases} 
\sqrt{2}3Y_{l,m}(\theta, \phi), & m < 0 \\
Y_{l,0}(\theta, \phi), & m = 0 \\
\sqrt{2}Y_{l,m}(\theta, \phi), & m > 0
\end{cases} \]  

(15)

which retain simple rotational properties. We will derive basis functions that satisfy the four goals of Section 1 in terms of \( \hat{Y}_{l,m} \), because they are real-valued, but also
describe our results in terms of \( Y_{l,m} \), because much standard software is available. Both \( Y_{l,m} \) and \( \bar{Y}_{l,m} \) are orthonormal systems of functions. The \( Y_{l,m} \) functions have the symmetry property \( Y_{l,-m}(\theta, \phi) = (-1)^m Y_{l,m}^*(\theta, \phi) \) [35, Eq. 14.30.6, p. 378] and the rotational property

\[
P(R) Y_{l,m}(\theta, \phi) = \sum_{m'=-l}^{+l} D_{l,m,m'}(R) Y_{l,m'}(\theta, \phi)
\]

where (1) \( R \) is a rotation matrix (\( R \in \mathbb{R}^{3 \times 3} \) with \( R^{-1} = R^T \) and \( \det R = +1 \)), (2) \( D_{l,m,m'}(R) \) are the Wigner \( D \) coefficients [39, Eq. 4.8, p. 52], and (3) \( P(R) \) is the rotation operator \( P(R)f(x) = f(R^{-1}x) \).

Standard computations based on the properties described in the previous paragraph result in Lemma 8.

**Lemma 8.** Suppose that the \( p \)th rep of a group \( G \) is potentially real with the real-valued orthogonal irrep matrices \( \Gamma^p_r(g) \in \mathbb{R}^{d_p \times d_p} \) for all \( g \in G \). Then, the projection operation on real spherical harmonics \( Y_{l,m} \) for \( m \in \{-l, \ldots, l\} \) and \( l \in \mathbb{N} \) can be determined by

\[
\mathcal{P}^p_{j,k} \bar{Y}_{l,m}(\theta, \phi) = \sum_{m'=-l}^{+l} \mathcal{D}^p_{j,k;m,m'} \bar{Y}_{l,m'}(\theta, \phi)
\]

where

\[
\mathcal{D}^p_{j,k;l,m;m'} = \frac{d_p}{N_g} \sum_{g \in G} (\Gamma^p_r(g))_{j,k} D_{l,m,m'}(R_g),
\]

\[
\bar{D}_{l,m,m'} = \left\{ \begin{array}{ll} -\frac{i}{\sqrt{2}} (D_{l,m,m'} - (-1)^m D_{l,-m,m'}), & m < 0 \\ \frac{1}{\sqrt{2}} (D_{l,0,m'} + (-1)^m D_{l,-m,m'}), & m = 0 \\ \frac{1}{\sqrt{2}} (D_{l,m,m'} + (-1)^m D_{l,-m,m'}), & m > 0 \end{array} \right.,
\]

and

\[
D_{l,m,m'} = \left\{ \begin{array}{ll} \frac{1}{2} \left[ D_{l,m,m'} - (-1)^m D_{l,-m,m'} - (-1)^m D_{l,-m,-m'} + (-1)^{m+m'} D_{l,-m,-m'} \right], & m < 0, m' < 0 \\ \frac{1}{2} \left[ D_{l,m,0} - (-1)^m D_{l,-m,0} \right], & m < 0, m' = 0 \\ \frac{1}{2} \left[ D_{l,m,m'} - (-1)^m D_{l,-m,m'} + (-1)^m D_{l,m,-m'} - (-1)^{m+m'} D_{l,m,-m'} \right], & m < 0, m' > 0 \\ \frac{1}{2} \left[ D_{l,0,m'} - (-1)^m D_{l,0,m'} \right], & m = 0, m' < 0 \\ \frac{1}{2} \left[ D_{l,m,0} + (-1)^m D_{l,-m,0} \right], & m = 0, m' = 0 \\ \frac{1}{2} \left[ D_{l,m,m'} + (-1)^m D_{l,m,-m'} + (-1)^m D_{l,-m,m'} - (-1)^{m+m'} D_{l,-m,-m'} \right], & m > 0, m' < 0 \\ \frac{1}{2} \left[ D_{l,m,0} + (-1)^m D_{l,-m,0} \right], & m > 0, m' = 0 \\ \frac{1}{2} \left[ D_{l,m,m'} + (-1)^m D_{l,m,-m'} + (-1)^m D_{l,-m,m'} + (-1)^{m+m'} D_{l,-m,-m'} \right], & m > 0, m' > 0 \end{array} \right..
\]
An alternative view of Lemma 8 is described in this paragraph. Define the vectors \( Y_l = (Y_{l-1}, \ldots, Y_{l+l})^T \in \mathbb{C}^{2l+1} \) and \( \tilde{Y}_l = (\tilde{Y}_{l-1}, \ldots, \tilde{Y}_{l+l})^T \in \mathbb{R}^{2l+1} \). There exists a unitary matrix \( U_l \in \mathbb{C}^{(2l+1)\times(2l+1)} \) such that \( \tilde{Y}_l(\theta, \phi) = U_l^H Y_l(\theta, \phi) \) where \( U_l \) has at most two non-zero entries in any row or any column. The Wigner D coefficient can be grouped into a matrix \( D_l(R) \in \mathbb{C}^{(2l+1)\times(2l+1)} \) such that \( P(R) Y_l(\theta, \phi) = D_l(R) Y_l(\theta, \phi) \) where \( D_l(R) \) is typically a full matrix. In terms of these two matrices, (1) \( P(R) Y_l(\theta, \phi) = D_l(R) Y_l(\theta, \phi) \) where \( D_l(R) \in \mathbb{C}^{(2l+1)\times(2l+1)} \) is defined by \( D_l(R) = U_l^H D_l(R) U_l \). The matrix equations \( D_l(R) = U_l^H D_l(R) U_l \) are equivalent to Eqs. 21 and 22, respectively, but Eqs. 21 and 22 are less expensive to compute because of the sparseness of \( U_l \).

A vector of \( d_p \) normalized real basis functions, denoted by \( C_{k,l,m}^p(\theta, \phi) \in \mathbb{R}^{d_p} \) and expressed in terms of \( Y_{l,m} \) (not \( \tilde{Y}_{l,m} \)), can be computed from Lemma 8 (Eq. 18) as follows [12, p. 94],

\[
C_{k,l,m}^p(\theta, \phi) = \frac{1}{\hat{c}_{k,l,m}^P} \begin{bmatrix} P_{k,l,m}^p Y_{l,m} Y_{l,m} \\ \vdots \\ P_{d_p,k,l,m}^p Y_{l,m} Y_{l,m} \end{bmatrix} = \hat{D}_{l,m}^p Y_l(\theta, \phi),
\]

where \( (\hat{D}_{l,m})_{j,m'} = \hat{D}_{j,k,l,m,m'}^p / \hat{c}_{k,l,m}^P \) for \( j \in \{1, \ldots, d_p\} \), \( m' \in \{-l, \ldots, l\} \), and \( \hat{c}_{k,l,m}^P = \sqrt{\sum_{m'=-l}^{l} |D_{j,k,l,m,m'}^p |^2} \) all for some \( k \in \{1, \ldots, d_p\} \) such that \( \hat{c}_{k,l,m}^P > 0 \).

Note that this procedure computes \( 2l+1 \) coefficient matrices by varying \( m \) through the set \( \{-l, \ldots, +l\} \), so that a total of \( (2l+1)d_p \) basis functions are computed, which is more than is necessary for a basis since the subspace of square-integrable functions on the surface of the sphere where the subspace is defined by degree \( l \in \mathbb{N} \) is spanned by \( (2l+1) \) basis functions. Through Gram-Schmidt orthogonalization, the set of coefficient matrices, \( \hat{D}_{l,m}^p \) for \( m \in \{-l, \ldots, l\} \), shrinks to a smaller set of coefficient matrices, \( \hat{H}_{l,n}^p \) for \( n \in \{1, \ldots, N_{p,l} < 2l+1\} \). The value of \( N_{p,l} \in \mathbb{N} \) is determined by this process. Replacing \( Y_{l,m} \) (\( \tilde{Y}_{l,m} \)) by \( \hat{H}_{l,n}^p \) (\( \tilde{Y}_{l,n}^p \)) and using Lemma 8 (Eq. 17) instead of Lemma 8 (Eq. 18) leads via the same ideas to a set of real orthonormal coefficient matrices \( \{ \hat{H}_{l,n}^p \}_{n=1}^{N_{p,l}} \). Finally, two expressions for the vector of \( d_p \) orthonormal real basis functions, \( F_{p,l,n}(\theta, \phi) \), are

\[
F_{p,l,n}(\theta, \phi) = \hat{H}_{l,n}^p \tilde{Y}_{l,n} \text{ or } \hat{H}_{l,n}^p Y_l(\theta, \phi), \text{ for } n \in \{1, \ldots, N_{p,l}\}
\]

which differ in whether real- or complex-valued spherical harmonics are used.

Note that the basis is not unique. In the approach of this paper, the nonuniqueness enters in several places, e.g., in the choice of \( A^P \) (Eq. 3), in the definition of the eigenvectors and the order of the loading of the eigenvectors into the matrix \( U \) (both Lemma 4), and in the creation of an orthonormal family of basis functions in the subspace of dimension \( 2l+1 \) which is spanned by the \( 2l+1 \) spherical harmonics of degree \( l \).

5. Real basis functions generate and require real irreps. The one result in this section, Lemma 9, states that a real-valued set of orthonormal basis functions of the \( p \)th irrep of the finite group exists if and only if a real irrep exists, independent of whether the basis functions are expressed as linear combinations of spherical harmonics of fixed degree \( l \).

**Lemma 9.** Real-valued orthonormal basis functions of the \( p \)th irrep of the finite group \( G \) exist if and only if the \( p \)th irrep of \( G \) is potentially real.
Proof. Real-valued functions imply real-valued irreps: Let \( F_{p,\zeta}(x/x) \) for \( \zeta \in \{1, \ldots, N\} \) be a vector of \( d_p \) real-valued orthonormal basis functions where the \( j \)th component is the basis function that transforms according to the \( j \)th row of the \( p \)th irrep matrices of \( G \). Therefore, Eq. 12 (the vector form of Eq. 8 in Definition 6) is

(25) \[ P(g)F_{p,\zeta}(x/x) = F_{p,\zeta}(R^{-1}_g x/x) = (\Gamma^p(g))^T F_{p,\zeta}(x/x). \]

Define \( J^{P'_p}_{\zeta',\zeta} \in \mathbb{R}^{d_p \times d_p} \) by

(26) \[ J^{P'_p}_{\zeta',\zeta} = \int [P(g)F_{p,\zeta}(x/x)] [P(g)F_{p',\zeta'}(x/x)]^T \, d\Omega. \]

Evaluate \( J^{P'_p}_{\zeta',\zeta} \) twice. In the first evaluation,

(27) \[ J^{P'_p}_{\zeta',\zeta} = \int F_{p,\zeta}(x/x) [F_{p',\zeta'}(x/x)]^T \, d\Omega = I_{d_p} \delta_{p,p'} \delta_{\zeta,\zeta'}. \]

where the first equality is due to rotation the coordinate system by \( R_g \), and the second equality is due to the fact that the \( \{F_{p,\zeta}\} \) are orthonormal.

In the second evaluation, use Eq. 25, rearrange, and use the orthonormality of \( \{F_{p,\zeta}\} \) to get

(28) \[ J^{P'_p}_{\zeta',\zeta} = \int (\Gamma^p(g))^T F_{p,\zeta}(x/x) \left[ (\Gamma^{p'}(g))^T F_{p',\zeta'}(x/x) \right]^T \, d\Omega \]

(29) \[ = (\Gamma^p(g))^T \left[ \int F_{p,\zeta}(x/x) [F_{p',\zeta'}(x/x)]^T \, d\Omega \right] \Gamma^{p'}(g) \]

(30) \[ = (\Gamma^p(g))^T I_{d_p} \delta_{p,p'} \delta_{\zeta,\zeta'} \Gamma^{p'}(g) \]

(31) \[ = (\Gamma^p(g))^T \Gamma^{p'}(g) \delta_{p,p'} \delta_{\zeta,\zeta'}. \]

Equating the two expressions for \( J^{P'_p}_{\zeta',\zeta} \) gives

(32) \[ (\Gamma^p(g))^T \Gamma^{p'}(g) = I_{d_p}. \]

Since \( \Gamma^p(g) \) is unitary, multiplying on the right by \( (\Gamma^p(g))^H \) implies that \( (\Gamma^p(g))^T = (\Gamma^p(g))^H \) so that \( \Gamma^p(g) \) is real.

Real-valued irreps imply real-valued functions: This follows from Lemma 8 and Eqs. 23–24. \( \square \)

6. Application to the rotational polyhedral groups. In this section, the theory of this paper is applied to the three rotational polyhedral groups, which are the tetrahedral \( T \), octahedral \( O \), and icosahedral \( I \) groups. Properties of each group and the parameter values which select a specific basis are described in Section 6.1 and the numerical results are presented in Section 6.2.

6.1. Irreps and rotation matrices of rotational polyhedral groups. Unitary complex-valued irrep matrices for the tetrahedral and octahedral groups are available at the Bilbao Crystallographic Server [5, 42, 41]. Unitary complex-valued irrep matrices for the icosahedral group are provided by [29]. The Frobenious-Schur indicator (Section 3) implies that all reps of the octahedral and the icosahedral groups are potentially real. Similarly, the tetrahedral group has irreps \( A \) and \( T \) that are potentially real and irreps \( 1E \) and \( 2E \) that are essentially complex. In the reminder of
the paper, we refer to the tetrahedral irreps $A_1, A_2, E$ and $T$ as the 1st, 2nd, 3rd and 4th irreps, respectively, and refer to the octahedral irreps $A_1, A_2, E, T_1$ and $T_2$ as the 1st, 2nd, 3rd, 4th and 5th irreps, respectively. The basic properties of the groups are tabulated in Table 1.

| Symmetry Groups | $N_g$ | $N_{\text{rep}}$ | $d_p$ | potentially real reps |
|-----------------|-------|------------------|-------|-----------------------|
| Tetrahedral     | 12    | 4                | $\{1, 1, 1, 3\}$ | 1,4 |
| Octahedral      | 24    | 5                | $\{1, 1, 2, 3, 3\}$ | 1,2,3,4,5 |
| Icosahedral     | 60    | 5                | $\{1, 3, 3, 4, 5\}$ | 1,2,3,4,5 |

Table 1: Basic properties of the rotational polyhedral groups: the group orders ($N_g$), the number of reps ($N_{\text{rep}}$), the dimension of the $p$th irrep ($d_p$ for $p \in \{1, \ldots, N_{\text{rep}}\}$), and the potentially real reps of each group.

For each symmetry operation, a rotation matrix ($R_g \in \mathbb{R}^{3 \times 3}$ for $g \in G$ which satisfies $R_T^g = R_g^{-1}$, det $R_g = +1$) is needed. The set of rotation matrices defines the relationship between the symmetries and the coordinate system. Any orthonormal real-valued irrep with $d_p = 3$ can serve as such a set of rotation matrices. For the tetrahedral and octahedral groups, rotation matrices are available at the Bilbao Crystallographic Server [5, 42, 41] although the matrices must be re-ordered in order to match the multiplication tables of the irrep matrices and, after reordering, they are the 4th irrep of the tetrahedral group and the 4th irrep of the octahedral group. For the icosahedral group, we desire to use the coordinate system in which the $z$-axis passes through two opposite vertices of the icosahedron and the $xz$ plane includes one edge of the icosahedron [28, 1, 48]. Rotation matrices in this coordinate system are available [46] although the matrices must be reordered to match the multiplication table of the irrep matrices [29]. The reordering and the similarity matrix to match the rotation matrices to either of the two $d_p = 3$ sets of irrep matrices are given in Appendix B. The calculations described in this paper use the rotation matrices reordered to match the multiplication table of the 2nd irrep.

For the particular irreps described above, it is necessary to give values for the $A^p$ matrices of Lemma 2. The identity matrix $I_{d_p}$ satisfies the nonsingular and transpose symmetric hypotheses of Lemma 2. However, for the $p = 4$ irrep of the icosahedral group for which $d_4 = 4$, $I_4$ leads to $Z^4 = 0$ by direct computation. It was not difficult to find a choice for $A^p$ such that all potentially-real irreps of the tetrahedral, octahedral, and icosahedral groups have nonzero $Z^p$. For instance, the choice of an “exchange permutation” matrix [20, Section 1.2.11, p. 20] for $A^p$, which is the anti-diagonal matrix with all ones on the anti-diagonal, leads to $Z^p = A^p$ by direct computation. This choice for $A^p$ was used in all computations in this paper.

6.2. Numerical results. For the tetrahedral group, the coefficient matrices $\mathcal{H}_{l,m}^{p}$ for degree $l \in \{1, \ldots, 45\}$, $p \in \{1, 4\}$ and $n \in \{1, \ldots, N_{p,l}\}$, were computed. The total number of rows in the coefficient matrices is $N_{p=1,l} + N_{p=4,l} < 2l + 1$ for each $l$, which is in agreement with the fact that only two of four irreps are potentially real and therefore only two of four irreps are included in our calculation. The resulting basis functions have been numerically verified to be real-valued and orthonormal.

For the octahedral and icosahedral cases, there are numerical checks that can be performed on the basis functions because all irreps are potentially real. Eq. 9 is achieved by construction. Eq. 10 is achieved by construction for $\mathcal{H}_{l,m}^{p}$ and by
testing an array of \((\theta, \phi)\) values for \(\hat{\mathbf{H}}_{l,m}^p\). Eq. 11 is verified by forming the matrices \(\mathbf{\hat{H}}_l = [(\mathbf{\hat{H}}_{l,1}^{p=1})^T, \ldots, (\mathbf{\hat{H}}_{l,N_{rep}}^{p=N_{rep}})^T]^T\) and \(\hat{\mathbf{H}}_l = [(\hat{\mathbf{H}}_{l,1}^{p=1})^T, \ldots, (\hat{\mathbf{H}}_{l,N_{rep}}^{p=N_{rep}})^T]^T\) and verifying that each is of dimension \((2l + 1) \times (2l + 1)\), which verifies that the correct number of basis functions have been found \((\sum_{p=1}^{N_{rep}} d_p N_p^l = 2l + 1)\), and verifying that \(\hat{\mathbf{H}}_l (\hat{\mathbf{H}}_l)\) is orthonormal (unitary) which verifies that the basis functions are orthonormal. Eq. 12 is verified by testing an array of \((\theta, \phi)\) values. The verifications were carried out for \(l \in \{0, \ldots, 45\}\).

Example basis functions are shown in Figure 1 by visualization of the function

\[
\xi_{p,l,n,j}(x) = \begin{cases} 
1, & x \leq \kappa_1 + \kappa_2 F_{p,l,n,j}(x/x) \\
0, & \text{otherwise}
\end{cases}
\]

where \(\kappa_1\) and \(\kappa_2\) are chosen so that \(0.5 \leq \kappa_1 + \kappa_2 I_{p,l,n,j}(x/x) \leq 1\).

Please contact the corresponding author for software.

Fig. 1: Examples of the real basis functions of the three rotational polyhedral groups. The surfaces of 3-D objects defined by Eq. 33 are visualized by UCSF Chimera [36] where the darkness indicates the distance from the center of the object. The darker the color is, the closer the point is to the center.

7. Conclusion. Motivated by cryo electron microscopy problems in structural biology, this paper presents a method for computing real-valued basis functions which transform as the various rows and irreducible representations of a rotational polyhedral group. The method has two steps: (1) compute real-valued orthonormal irreducible representation matrices (Section 3) and (2) use the matrices to define projection operators which are applied to a real-valued basis for the desired function space.
The method is applied to the icosahedral, octahedral, and tetrahedral groups where the second step is performed in spherical coordinates using the spherical harmonics basis. The most burdensome part of the calculation for the first step is the solution of a real symmetric eigenvector problem of dimension equal to twice the dimension of the irreducible representation matrices. For these three groups, the largest matrix is of dimension 5 so the calculations are straightforward. Of the remaining rotational polyhedral groups, basis functions for the cyclic groups are more naturally described in cylindrical coordinates using the complex exponential basis and possibly the same is true for the dihedral groups and so the calculations for the second step would be quite different from those described in this paper. However, the calculations in the first step, which apply to any potentially real irreducible representation, would remain relevant.

The resulting basis functions are described by linear combinations of spherical harmonics and a Mathematica program to compute the coefficients of the linear combination and a Matlab program to evaluate the resulting basis functions have been written and are available from the authors upon request.

**Appendix A. Proofs of Lemmas.**

*Proof of Lemma 1.* Eq. 1 implies Eq. 2) \( \Gamma^r_p \) is real by definition so that

\[
\Gamma^r_p(g) = (\Gamma^r_p(g))^*,
\]

Since \( \Gamma^r_p = (S^p)^H \Gamma^r_p(g) S^p \), it follows that

\[
\Gamma^r_p = (S^p)^H \Gamma^r_p(g) S^p = ((S^p)^H \Gamma^r_p(g) S^p)^* = (S^p)^T (\Gamma^r_p(g))^* (S^p)^*.
\]

Multiply on the left by \((S^p)^H\) and on the right by \((S^p)^T\) to get

\[
((S^p)^T)^{-1} (S^p)^H \Gamma^r_p(g) S^p (S^p)^T = (\Gamma^r_p(g))^*,
\]

which, since \((S^p)^H = (S^p)^{-1}\), implies that

\[
[S^p (S^p)^T]^{-1} \Gamma^r_p(g) [S^p (S^p)^T] = (\Gamma^r_p(g))^*.
\]

Therefore \( \Gamma^r_p(g) \) is similar to \( (\Gamma^r_p(g))^*\).

Eq. 2 implies Eq. 1) Multiplying by \((S^p)^T\) on the left and \((S^p)^*\) on the right of Eq. 2 gives

\[
(S^p)^T [S^p (S^p)^T]^{-1} \Gamma^r_p(g) [S^p (S^p)^T] (S^p)^* = (S^p)^T (\Gamma^r_p(g))^* (S^p)^*.
\]

which can be reorganized using the assumption that \( S^p \) is unitary to get

\[
[(S^p)^T (S^p)^*]^{-1} \Gamma^r_p(g) S^p [(S^p)^T (S^p)^*] = (S^p)^T (\Gamma^r_p(g))^* (S^p)^*.
\]

Then, also since \( S^p \) is unitary, it follows that

\[
(S^p)^{-1} \Gamma^r_p(g) S^p = [(S^p)^{-1} \Gamma^r_p(g) S^p]^*.
\]

Since the left and the right hand sides of the above equation are complex conjugates of each other, it follows that each is real, i.e., \( \Gamma^r_p(g) = (S^p)^{-1} \Gamma^r_p(g) S^p \) is a real-valued matrix.
Proof of Lemma 2. Property 1: Because the irrep is unitary, $Z^p$ can be written in the form

$$Z^p = \frac{1}{N_g} \sum_{g \in G} \Gamma_c^p(g) A^p(\Gamma_c^p(g))^T. \tag{34}$$

Then, Property 1 follows from a direct computation.

Properties 2 and 3: For any arbitrary $g' \in G$, we have

$$
\Gamma_c^p(g') Z^p (\Gamma_c^p(g'))^T = \frac{1}{N_g} \sum_{g \in G} \Gamma_c^p(g) A^p(\Gamma_c^p(g)) (\Gamma_c^p(g'))^T \\
= \frac{1}{N_g} \sum_{g \in G} \Gamma_c^p(g') A^p(\Gamma_c^p(g')) \Gamma_c^p(g) (\Gamma_c^p(g'))^T \\
= \frac{1}{N_g} \sum_{g \in G} \Gamma_c^p(g') A^p(\Gamma_c^p(g)) \\
= Z^p 
$$

where the forth equivalence follows from the Rearrangement Theorem [12, Theorem II, p. 24]. Because the irrep is unitary, rearranging Eq. 35 gives $\Gamma_c^p(g') Z^p = Z^p (\Gamma_c^p(g'))^*$. Because $g'$ is arbitrary,

$$\Gamma_c^p(g) Z^p = Z^p (\Gamma_c^p(g))^*, \quad \text{for all } g \in G. \tag{36}$$

Property 2 follows from Ref. [12, Theorem II, p. 128] because the irrep $\Gamma_c^p$ is potentially real.

Note that both $\Gamma_c^p$ and $(\Gamma_c^p)^*$ are unitary irreps of dimension $d_p$ of the group $G$. Schur’s Lemma [12, Theorem I, p. 80] applied to Eq. 36 implies that either $Z^p = 0$ or $\det Z^p \neq 0$. Because of the assumption $Z^p \neq 0$, $Z^p$ is nonsingular. Therefore, $Z^p$ is a similarity transform from $\Gamma_c^p(g)$ to $(\Gamma_c^p(g))^*$ for all $g \in G$ which proves Property 3. □

Proof of Lemma 4. For simplicity, let $Q_1 = \Re Q$ and $Q_2 = \Im Q$.

Property 1: The matrices $Q_1$, $Q_2$, and $B$ are all real and symmetric. Since $B \in \mathbb{R}^{2n \times 2n}$ and $B^T = B$, $B$ has $2n$ real eigenvalues (possibly repeated) and $2n$ real orthonormal eigenvectors [24, Theorem 2.5.6, p. 104]. Define $M$ by

$$M = \begin{bmatrix} I & -iI \\ 0 & I \end{bmatrix} B \begin{bmatrix} I & 0 \\ iI & I \end{bmatrix} = \begin{bmatrix} 0 & Q_2 + iQ_1 \\ Q_2 - iQ_1 & -Q_1 \end{bmatrix}. $$

Then,

$$\det(B) = \det(M) = \det((Q_2 + iQ_1)(Q_2 - iQ_1) - 0(-Q_1)) = \det(QQ^*) = |\det(Q)|^2 > 0$$

because $Q$ is non-singular. Hence, $B$ is non-singular.

Property 2:

$$B \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix} \iff \begin{cases} Q_1 x - Q_2 y = \lambda x \\ Q_2 x + Q_1 y = -\lambda y \end{cases} \iff \begin{cases} Q_2 y - Q_1 x = -\lambda x \\ Q_2 x + Q_1 y = -\lambda y \end{cases}$$
\[ \iff B \begin{bmatrix} x \\ y \end{bmatrix} = -\lambda \begin{bmatrix} x \\ y \end{bmatrix}. \]

Property 3: Define the matrices
\[ X = [x_1, \ldots, x_n] \in \mathbb{R}^{n \times n} \]
\[ Y = [y_1, \ldots, y_n] \in \mathbb{R}^{n \times n} \]
\[ \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n \times n} \]
\[ U = X - iY \in \mathbb{C}^{n \times n}. \]

The equation
\[ B \begin{bmatrix} x_k \\ -y_k \end{bmatrix} = \lambda_k \begin{bmatrix} x_k \\ -y_k \end{bmatrix} \text{ for } k \{1, \ldots, n\} \]
is equivalent to
\[ B \begin{bmatrix} X \\ -Y \end{bmatrix} = \begin{bmatrix} Q_1 & Q_2 \\ Q_2 & -Q_1 \end{bmatrix} \begin{bmatrix} X \\ -Y \end{bmatrix} \Lambda \]
which is equivalent to
\[ \begin{cases} Q_1X - Q_2Y = \Lambda X \\ Q_2X + Q_1Y = -Y \Lambda. \end{cases} \]

Multiplying the second equation by \( i \) and adding to the first equation gives
\[ U\Lambda = (X - iY)\Lambda = (Q_1X - Q_2Y) + i(Q_2X + Q_1Y) = (Q_1 + iQ_2)X + (Q_1 + iQ_2)iY = (Q_1 + iQ_2)(X + iY) = QU^*. \]

Therefore \( x_k - iy_k \) and \( +\lambda_k \) are the coneigenvectors and coneigenvalues of \( Q \), respectively.

Property 4: Because \( QQ^* = I_n \) by assumption, the eigenvalues of \( QQ^* \) are the eigenvalues of \( I_n \) which all have value 1. By Ref. [24, Proposition 4.6.6, p. 246], \( \xi \) is an eigenvalue of \( QQ^* \) if and only if \( +\sqrt{\xi} \) is a coneigenvalue of \( Q \). Therefore, all the coneigenvalues of \( Q \) have value 1.

Property 5: Let the columns of \( V \in \mathbb{R}^{2n \times 2n} \) be the 2n real orthonormal eigenvectors of \( B \), i.e.,
\[ (38) \quad V = \begin{bmatrix} [x_1, y_1] & \cdots & [x_n, y_n] \\ [x_1, -y_1] & \cdots & [x_n, -y_n] \end{bmatrix}. \]

Then, \( VTV = VTV^T = I_{2n} \) and \( VHV = VH^H = I_{2n}. \)

Define \( L \in \mathbb{C}^{n \times 2n} \) by \( L = [I_n, iI_n] \) and \( \tilde{U} \in \mathbb{C}^{2 \times 2n} \) by \( \tilde{U} = LV \). Then
\[ \tilde{U}\tilde{U}^H = (LV)(LV)^H = LVV^H L^H = LL^H = I_n + I_n = 2I_n. \]

Appendix B. Relationships between icosahedral \( d_3 = 3 \) irreps. Let \( R_g \) be the rotation matrices of Ref. [46] which are also a real orthonormal irrep of dimension 3. Let \( \Gamma_p(g) \) be the complex unitary irreps of Ref. [29] where \( p = 2 \) and
\( p = 3 \) are of dimension 3. With different permutations, \( R_g \) can be made similar to both \( \Gamma^p=2(g) \) and \( \Gamma^p=3(g) \). In particular, \( \Gamma^p(g) = (S^p)^H R_{\gamma^p(g)} S^p \) for \( p \in \{2, 3\} \) where the permutation \( \gamma^p(g) \) and the complex unitary matrices \( S^p \in \mathbb{C}^{3 \times 3} \) are given in Table 2 and Eq. 39, respectively.

\[
(39) \quad S^{p=2} = \begin{bmatrix}
-1/\sqrt{2} & 0 & -1/\sqrt{2} \\
-1/\sqrt{2} & 0 & i/\sqrt{2} \\
0 & 1 & 0
\end{bmatrix} \quad S^{p=3} = \begin{bmatrix}
-1/\sqrt{2} & 0 & -1/\sqrt{2} \\
i/\sqrt{2} & 0 & -i/\sqrt{2} \\
0 & 1 & 0
\end{bmatrix} .
\]

| \( g \) | \( \gamma^2(g) \) | \( \gamma^3(g) \) |
|------|----------------|----------------|
| 1    | 2              | 5              |
| 2    | 3              | 4              |
| 3    | 4              | 5              |
| 4    | 6              | 10             |
| 5    | 7              | 8              |
| 6    | 9              | 10             |
| 10   | 1              | 2              |

\[ g_{11} \ldots g_{20} \] \[ \gamma^2_{20} \ldots \gamma^3_{20} \]

Table 2: Permutations relating the 3 dimensional icosahedral irreps of Refs. [46, 29].

Acknowledgments. We are grateful for helpful discussions with Prof. Dan Mihai Barbasch (Department of Mathematics, Cornell University) about representation theory and the method for generating real irreducible representation matrices in Section 3.

REFERENCES

[1] S. L. Altmann, On the symmetries of spherical harmonics, Proc. Camb. Phil. Soc., 53 (1957), pp. 343–367.
[2] S. L. Altmann and C. J. Bradley, The band structure of hexagonal close-packed metals: I. The cellular method, Proceedings of the Physical Society, 86 (1965), p. 915, http://stacks.iop.org/0370-1328/86/i=5/a=303.
[3] S. L. Altmann and A. P. Cracknell, Lattice harmonics I. Cubic groups, Rev. Mod. Phys., 37 (1965), pp. 19–32, http://dx.doi.org/10.1103/RevModPhys.37.19, http://link.aps.org/doi/10.1103/RevModPhys.37.19.
[4] M. A. Armstrong, Groups and Symmetry, Springer, 1997.
[5] M. I. Aboyo, A. Kirov, C. Capillas, J. M. Perez-Mato, and H. Wondratschek, Bilbao crystallographic server. II. Representations of crystallographic point groups and space groups, Acta Cryst., A62 (2006), pp. 115–128. http://dx.doi.org/10.1107/S0108767305040286.
[6] X.-C. Bai, G. McMullan, and S. H. W. Scheres, How cryo-EM is revolutionizing structural biology, Trends in Biochemical Sciences, 40 (2015), pp. 49–57. http://dx.doi.org/10.1016/j.tibs.2014.10.005.

[7] D. L. D. Caspar and A. Klug, Physical principles in the construction of regular viruses, Cold Spring Harbor Symposium on Quantitative Biology, 27 (1962), pp. 1–24.

[8] Y. Cheng, Single-particle cryo-EM at crystallographic resolution, Cell, 161 (2015), pp. 450–457. http://dx.doi.org/10.1016/j.cell.2015.03.049.

[9] Y. Cheng, N. Gregorrieff, P. A. Penczek, and T. Walz, A primer to single-particle cryo-electron microscopy, Cell, 161 (2015), pp. 438–449. http://dx.doi.org/10.1016/j.cell.2015.03.050.

[10] N. V. Cohan, The spherical harmonics with the symmetry of the icosahedral group, Proc. Camb. Phil. Soc., 54 (1958), pp. 28–38.

[11] R. Conte, J. Raynal, and E. Soulie, Determination of point group harmonics for arbitrary j by a projection method. I. Cubic group, quantization along an axis of order 4, J. Math. Phys., 25 (1984), pp. 1176–1186.

[12] J. F. Cornwell, Group Theory in Physics, vol. 1, Academic Press, London, 1984.

[13] F. H. C. Crick and J. D. Watson, Structure of small viruses, Nature, 177 (1956), pp. 473–475. http://dx.doi.org/10.1038/177473a0.

[14] R. A. Crowther, The fast rotation function, in The Molecular Replacement Method: A Collection of Papers on the Use of Non-Crystallographic Symmetry, M. G. Rossmann, ed., Gordon and Breach, 1972, pp. 173–178.

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

[16] G. W. Fernando, M. Weinert, R. E. Watson, and J. W. Davenport, Point group symmetries and Gaussian integration, J. Computational Physics, 112 (1994), pp. 282–290.

[17] K. Fox and I. Ozier, Construction of tetrahedral harmonics, The Journal of Chemical Physics, 52 (1970), pp. 5044–5056.

[18] J. Frank, M. Radermacher, P. Penczek, J. Zhu, Y. Li, M. Ladjadj, and A. Leith, SPIDER and WEB: Processing and visualization of images in 3D electron microscopy and related fields, J. Struct. Biol., 116 (1996), pp. 190–199.

[19] W. Fulton, Young tableaux: with applications to representation theory and geometry, vol. 35, Cambridge University Press, 1997.

[20] G. H. Golub and C. F. Van Loan, Matrix Computations, The Johns Hopkins University Press, Baltimore, 4th ed., 2013.

[21] Y. Gong, D. Veesler, P. C. Doerschuk, and J. E. Johnson, Effect of the viral protease on the dynamics of bacteriophage HK97 maturation intermediates characterized by variance analysis of cryo EM particle ensembles, Journal of Structural Biology, 193 (2016), pp. 188–195.

[22] K. T. Hecht, Vibration-rotation energies of tetrahedral XY4 molecules, Journal of Molecular Spectroscopy, 5 (1961), pp. 390–404, http://dx.doi.org/10.1016/0022-2852(61)90103-5, http://www.sciencedirect.com/science/article/pii/0022285261901035.

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

[24] R. A. Horn and C. R. Johnson, Matrix Analysis, Cambridge University Press, 1985.

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

[26] H. A. Jahn, A new coriolis perturbation in the methane spectrum. I. Vibrational-rotational hamiltonian and wave functions, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 168 (1938), pp. 469–495. http://dx.doi.org/10.1098/rspa.1938.0187, http://rspa.royalsocietypublishing.org/content/168/935/469, arXiv:http://rspa.royalsocietypublishing.org/content/168/935/469.full.pdf.

[27] M. Kara and K. Kurki-Suonio, Symmetrized multipole analysis of orientational distributions, Acta Cryst., A37 (1981), pp. 201–210.

[28] O. Laporte, Polyhedral harmonics, Z. Naturforsch., 3a (1948), pp. 447–456.

[29] F. Liu, J.-L. Ping, and J.-Q. Chen, Application of the eigenfunction method to the icosahedral group, J. Math. Phys., 31 (1990), pp. 1065–1075.

[30] S. J. Ludtke, P. R. Baldwin, and W. Chiu, EMAN: semiautomated software for high-resolution single-particle reconstructions, J. Struct. Biol., 128 (1999), pp. 82–97.

[31] B. Meyer, On the symmetries of spherical harmonics, Canadian J. Math., 135 (1954), pp. 135–
[32] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill, New York, 1953.

[33] F. M. Mueller and M. G. Priestley, *Inversion of cubic de Haas-van Alphen data, with an application to palladium*, Phys. Rev., 148 (1966), pp. 638–643, http://dx.doi.org/10.1103/PhysRev.148.638, http://link.aps.org/doi/10.1103/PhysRev.148.638.

[34] J. Muggli, *Cubic harmonics as linear combinations of spherical harmonics*, Zeitschrift für angewandte Mathematik und Physik ZAMP, 23 (1972), pp. 311–317.

[35] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, *NIST Handbook of Mathematical Functions*, Cambridge University Press, Cambridge, UK, 2010, http://dlmf.nist.gov.

[36] E. F. Pettersen, T. D. Goddard, C. C. Huang, G. S. Couch, D. M. Greenblatt, E. C. Meng, and T. E. Ferrin, *UCSF Chimera—A visualization system for exploratory research and analysis*, J. Comput. Chem., 25 (2004), pp. 1605–1612.

[37] H. Puff, *Contribution to the theory of cubic harmonics*, Physica Status Solidi (B), 41 (1970), pp. 311–317.

[38] J. Raynal and R. Conte, *Determination of point group harmonics for arbitrary j by a projection method III. Cubic group, quantization along a ternary axis*, J. Math. Phys., 25 (1984), pp. 3375–3381.

[39] M. E. Rose, *Elementary Theory of Angular Momentum*, John Wiley and Sons, New York, 1957.

[40] S. H. W. Scheres, *RELION: Implementation of a Bayesian approach to cryo-EM structure determination*, J. Struct. Biol., 180 (2012), pp. 519–529.

[41] B. C. Server, *The octahedral group tables*. http://www.cryst.ehu.es/cgi-bin/rep/programs/sam/point.py?sg=207&num=30. Accessed: 2015-06-03.

[42] B. C. Server, *The tetrahedral group tables*. http://www.cryst.ehu.es/cgi-bin/rep/programs/sam/point.py?sg=195&num=28. Accessed: 2015-06-03.

[43] J. Tang, B. M. Kearney, Q. Wang, P. C. Doerschuk, T. S. Baker, and J. E. Johnson, *Dynamic and geometric analyses of Nudaurelia capensis ω virus maturation reveal the energy landscape of particle transitions*, Journal of Molecular Recognition, 27 (2014), pp. 230–237.

[44] Q. Wang, T. Matsui, T. Domitrovic, Y. Zheng, P. C. Doerschuk, and J. E. Johnson, *Dynamics in cryo EM reconstructions visualized with maximum-likelihood derived variance maps*, Journal of Structural Biology, 181 (2013), pp. 195–206.

[45] N. Xu and P. C. Doerschuk, *Reconstruction for stochastic 3-D signals with symmetric statistics in noise: electron microscopy of virus particles*, in Proceedings of ICIP 2015, IEEE International Conference on Image Processing, Québec City, Canada, 27–30 September 2015, IEEE, pp. 1444–1447, http://dx.doi.org/10.1109/ICIP.2015.7351039.

[46] Y. Zheng and P. C. Doerschuk, *Symbolic symmetry verification for harmonic functions invariant under polyhedral symmetries*, Comput. in Phys., 9 (1995), pp. 433–437.

[47] Y. Zheng and P. C. Doerschuk, *Explicit orthonormal fixed bases for spaces of functions that are totally symmetric under the rotational symmetries of a Platonic solid, Acta Crystallographica, A52 (1996), pp. 221–235.

[48] Y. Zheng and P. C. Doerschuk, *Explicit computation of orthonormal symmetrized harmonics with application to the identity representation of the icosahedral group*, SIAM Journal on Mathematical Analysis, 32 (2000), pp. 538–554.

[49] Y. Zheng, Q. Wang, and P. C. Doerschuk, *3-D reconstruction of the statistics of heterogeneous objects from a collection of one projection image of each object*, Journal of the Optical Society of America A, 29 (2012), pp. 959–970.