Orientational Sampling Schemes Based on Four Dimensional Polytopes

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Abstract: The vertices of regular four-dimensional polytopes are used to generate sets of uniformly distributed three-dimensional rotations, which are provided as tables of Euler angles. The spherical moments of these orientational sampling schemes are treated using group theory. The orientational sampling sets may be used in the numerical computation of solid-state nuclear magnetic resonance spectra, and in spherical tensor analysis procedures.

Keywords: polytope; polychora; group theory; Schlafli symbols; powder averaging; orientational sampling; solid-state nuclear magnetic resonance

1. Introduction

In general, physical properties are anisotropic, meaning that they depend on the orientation of the object of interest in three-dimensional space, defined with respect to an external reference frame. For example, the magnetic resonance response of solid samples depends on the orientation of the molecules with respect to the applied magnetic field [1,2]. Similar considerations apply to many other physical quantities and spectroscopic properties.

If the physical system is macroscopically isotropic (for example, a finely-divided powdered solid), all molecular orientations are encountered with equal probability. The physical response of such systems is an average over all molecular orientations.

Suppose that a computational method exists for estimating the value of a particular macroscopic observable for a single molecular orientation. To estimate the powder response, it is necessary to
average the results of such computations over a large number of distinct orientations. This is called powder averaging, and is a common procedure in, for example, the computation of solid-state magnetic resonance observables [3–6]. In general, the computational cost of powder averaging is proportional to the number of sampled orientations. It is clearly desirable to use an orientational sampling scheme that gives an acceptable approximation to the isotropic result using the minimum number of orientations. The problem of optimum orientational sampling has been a recurring feature of the solid-state nuclear magnetic resonance (NMR) literature for many years [3–6].

In addition, there are experimental procedures that require repetition of an experiment for a set of different physical orientations of the system (or parts of the system), in order to estimate the values of anisotropic physical quantities. Physical manipulations of this kind are found, for example, in the NMR of microscopically oriented samples such as single crystals or oriented materials [1].

There are also experiments of this type in which the sample remains fixed in space, but the orientations of the nuclear spin polarizations are manipulated using applied radio-frequency pulse sequences. For example, in the class of experiments known as spherical tensor analysis [7–9], the orientational space of the nuclear spins is sampled in order to derive the spherical tensor components of the quantum statistical operator describing the state of the nuclear spin ensemble. In all such experimental procedures, it is desirable that the orientation sampling scheme is as efficient as possible.

### 1.1. Gaussian Spherical Quadrature

An approach to the orientational sampling problem, using the concept of Gaussian spherical quadrature, was described by Edén et al. in 1998 [4]. This approach may be summarized as follows: An orientational sampling scheme \( S \) consists of a finite set \( \Omega_S \) of \( N_S \) distinct orientations \( \Omega_j^S \) in three-dimensional space, and a set \( w^S \) of weights \( w_j^S \) with the property \( \sum_{j=1}^{N_S} w_j^S = 1 \). Both sets have the same number of elements \( N_S \). The isotropic average \( \langle Q \rangle \) of a physical observable \( Q \) is estimated by computing \( Q \) for each orientational sampling point \( \Omega_j^S \) and superposing the results according to:

\[
\langle Q \rangle_{est}^S = \sum_{j=1}^{N_S} w_j^S Q(\Omega_j^S)
\]  

(1)

The performance of a sampling scheme may be characterized by its spherical moments, which are defined as follows:

\[
\sigma_{\ell m m'}^S = \sum_{j=1}^{N_S} w_j^S D_{\ell m m'}^{\ell m m'}(\Omega_j^S)
\]  

(2)

Here \( D_{\ell m m'}^{\ell m m'}(\Omega_j^S) \) is an element of the Wigner matrix [10] of integer rank \( \ell \), evaluated at orientation \( \Omega_j^S \). The Wigner matrices are representations of the group of the three-dimensional rotations \( SO(3) \), with the Wigner matrices of integer rank \( \ell \) spanning the irreducible representation of \( SO(3) \) of dimension \( 2\ell + 1 \). If the rotation \( \Omega_j^S \) is parametrized using the three Euler angles \( \{ \alpha_j^S, \beta_j^S, \gamma_j^S \} \), representing consecutive rotations about the z, y and z-axes of 3D space, all Wigner matrix elements may be written as follows:

\[
D_{\ell m m'}^{\ell m m'}(\Omega_j^S) = e^{-im\alpha_j^S}d_{\ell m m'}^{\ell m m'}(\beta_j^S)e^{-im'\gamma_j^S}
\]  

(3)

where \( d_{\ell m m'}^{\ell m m'}(\beta_j^S) \) is an element of the reduced Wigner matrix and the indices \( m \) and \( m' \) span the integers in the range \( -\ell, \ldots, \ell \). By definition, the zero-rank spherical moment is given by \( \sigma_{000}^S = 1 \).
As discussed by Edén et al. [4], orientational sampling schemes may be constructed which have vanishing spherical moments over a range of ranks, i.e.

$$\sigma_{\ell m n'}^S = 0 \quad \text{for } 1 \leq \ell \leq \ell_{\text{max}}^S$$

Schemes of this kind often provide a good approximation for the isotropic average of an observable $Q$, using a sampling set $S$ of relatively small size. Their performance is particularly good if $Q$ is a smooth function of orientation $\Omega$. This is called Gaussian spherical quadrature since it describes a numerical approach to integration of a function over three-dimensional space that is analogous to Gaussian numerical integration on a line interval. The Wigner functions play the same role as orthogonal polynomials in the case of Gaussian line integration.

In general, sampling schemes with large values of $\ell_{\text{max}}^S$ provide a more accurate isotropic average than schemes with small values of $\ell_{\text{max}}^S$, but require a larger number of elements $N_S$ for their realization. The central problem in Gaussian spherical quadrature is to achieve large values of $\ell_{\text{max}}^S$ with as small $N_S$ as possible.

1.2. Two-angle Sampling and Regular Polyhedra

In many physical situations, the observable of interest $Q$ depends on only two of the three Euler angles defining the orientation in three-dimensional space. This situation arises, for example, in the ordinary NMR of static solids, where the rotational angle of the sample around the static magnetic field has no influence on NMR observables. This is also true for some classes of NMR experiments in rotating solids, as discussed in Reference [4].

Consider an experiment, or computational procedure, of this type, in which the observable of interest does not depend on the third Euler angle $\gamma$. In such cases, the only relevant spherical moments of an orientational sampling scheme have $m' = 0$. The known relationships between Wigner functions of the type $D_{m\ell}^0(\Omega)$ and the spherical harmonics $Y_{\ell m}(\theta, \phi)$ allows the relevant spherical moments to be written as follows:

$$\sigma_{\ell m 0}^S = \sqrt{\frac{4\pi}{2\ell + 1}} \sum_{j=1}^{N_S} w_j^S Y_{\ell m}^S(\beta_j^S, \alpha_j^S) \ast$$

where $\ast$ means complex conjugation. The problem of two-angle orientational sampling is therefore closely related to the problem of Gaussian quadrature on the surface of a sphere, using spherical harmonics as the orthogonal basis functions. The correspondence of the Euler angles $\{\alpha, \beta\}$ to the polar angles $\{\theta, \phi\}$ of a point on the surface of a sphere is as follows:

$$\alpha \leftrightarrow \phi$$

$$\beta \leftrightarrow \theta$$

For small values of $\ell_{\text{max}}^S$, efficient two-angle sampling schemes may be constructed from the vertices of the regular three-dimensional polyhedra. As discussed below, the point symmetry groups of such polyhedra ensure that many of the spherical moments $\sigma_{\ell m 0}^S$ vanish. For example, the 12 vertices of the icosahedron may be used to construct an orientational sampling set with $N_S = 12$, all $w_j^S = 1/12$, and spherical moments $\sigma_{\ell m 0}^S = 0$ for $1 \leq \ell \leq 5$. All spherical moments with odd values of $\ell$ vanish for this
set as well. These favourable properties are well-known in nuclear magnetic resonance and have led to numerous applications \([11,12]\).

It is not possible to construct sampling sets with \(\ell_{\text{max}}^S > 5\) from the vertices of the regular 3D polyhedra. However Lebedev and co-workers \([13–15]\) have constructed schemes with large values of \(\ell_{\text{max}}^S\) by using well-chosen orientational sampling points and non-uniform weights. Alternative methods are also available, which do not have such well-defined mathematical properties, but which perform well in many circumstances, for example the REPULSION approach of Bak and Nielsen, which uses numerical optimization under a repulsive electrostatic potential to distribute many points evenly on the surface of a 3D sphere \([3]\).

1.3. Three-Angle Sampling and Regular 4-Polytopes

There are numerous cases where the observable of interest depends on all three Euler angles defining the orientation \(\Omega\). Some examples from the field of solid-state nuclear magnetic resonance are discussed in Reference\([4,5]\). In such cases, it is important that the spherical moments \(\sigma_{\ell m m'}^S\) vanish for all \((2\ell + 1)^2\) combinations of \(m\) and \(m'\) within a given rank \(\ell\), and not just the special components with \(m' = 0\).

As described in Reference\([4]\), it is possible to construct three-angle orientational sampling sets with the appropriate properties by (i) taking a two-angle sampling set with the property \(\sigma_{\ell m 0}^S = 0\) for \(1 \leq \ell \leq \ell_{\text{max}}^S\), and (ii) repeating each sampling point while stepping the third angle through \((\ell_{\text{max}}^S + 1)\) regularly-spaced subdivisions of \(2\pi\). This generates a three-angle sampling set with the desired property \(\sigma_{\ell m m'}^S = 0\) for all \(\{m, m'\}\) and \(1 \leq \ell \leq \ell_{\text{max}}^S\). For example, an icosahedral two-angle set with \(N_S = 12\) may easily be extended to a three-angle set with \(N_S = 72\) and \(\ell_{\text{max}}^S = 5\). The Lebedev two-angle sets may be extended in analogous fashion. The problems with this approach are (i) it is not efficient, requiring large numbers of orientational samples for modest values of \(\ell_{\text{max}}^S\) and (ii) it does not treat the Euler angles \(\alpha\) and \(\gamma\) in the same way.

Since efficient two-angle sampling schemes may be derived from the vertices of regular polyhedra, which fall on a sphere in 3D space, it is natural to speculate that efficient three-angle sampling schemes may be derived from the vertices of regular solids in four dimensions, which fall on a sphere in 4D space. The regular 4D solids are known as regular 4-polytopes or regular polychora \([16]\) and have been studied extensively by mathematicians, in particular Coxeter \([17]\).

Suppose that a 4-polytope is constructed with the vertices lying on the surface of a 4D sphere with unit radius. Each vertex may be converted into a rotation operation in 3D space by identifying it as a unit vector of the following form:

\[
q = \begin{pmatrix}
\cos \frac{\xi}{2} \\
n_x \sin \frac{\xi}{2} \\
n_y \sin \frac{\xi}{2} \\
n_z \sin \frac{\xi}{2}
\end{pmatrix}
\] (7)

where \(\xi\) is the rotation angle and \(n = (n_x, n_y, n_z)\) is the unit rotation axis in 3-space, \(n \cdot n = 1\). Hence, uniformly distributed rotations in 3-space may be constructed from the vertices of regular 4-polytopes deducing the corresponding 3D rotation angles and rotation axes from Equation 7. There is one important complication: unit vectors of the form \(q\) and \(-q\) correspond to rotations differing by an angle of \(2\pi\), which have the same physical effect on ordinary 3D objects, or on quantum states with integer spin.
Hence, a 4-polytope which has the inversion amongst its symmetry operations gives rise to only half the number of physically distinct 3D rotations as its number of vertices. As discussed below, this property applies to all the regular 4-polytopes, with one exception.

Suppose now that a set of $N$ 3D rotations is constructed from the vertices of a regular 4-polytope, and that all of the sampling weights are uniform, $w_j^S = N^{-1}$, $j \in \{1, 2, \ldots, N\}$. Many of the spherical moments, defined in Equation 2, are expected to vanish, through symmetry. The question is: for which ranks $\ell$ do all spherical moments of the form $\sigma^S_{\ell m m'}$ vanish? Although this question has been answered in part using the theory of spherical designs [18], it is also possible to treat this problem by relatively simple group theoretical arguments that may be more accessible to non-mathematicians. However, the application of group theory to this problem is made more difficult by the fact that the symmetry operations of the regular 4-polytopes, and the character tables of the corresponding symmetry groups, are distributed over several sources [19–23]. In this article we collate the symmetry operations and their characters for the regular 4-polytopes in the $(2\ell + 1)^2$-dimensional representations spanned by the Wigner matrices $D^{(\ell)}(\Omega)$. We derive by group theory the vanishing spherical moments for 3D rotation sets derived from each of the regular 3D and 4D solids. Explicit tables of Euler angles are given, based on the vertices of the regular 4-polytopes. These results should be useful for workers in a wide range of physical sciences, especially magnetic resonance, where one such scheme is already in use [9,24].

2. Group Theory and Symmetry Averaging

2.1. Groups, Representations and Characters

A minimal introduction to group theory is now given in order to establish the notation. For more details, consult the standard texts, for example [25–28].

An abstract group $\{G, \circ\}$ is a collection of elements $G$ for which a particular associative operation $\circ$ combines any two elements to give another element in the group. A valid group must include an identity element $E$ such that $G \circ E = G$, and all elements must have an inverse $G^{-1}$ such that $G \circ G^{-1} = E$. Any subset of a group which itself satisfies the group axioms above is called a subgroup.

Groups can be represented by matrices. An $n$-dimensional linear representation $\Gamma$ of a group $G$ assigns an invertible $n \times n$ (real or complex) matrix $M^\Gamma(G)$ to each group element $G$, so that the group operation $\circ$ corresponds to the operation of matrix multiplication:

$$M^\Gamma(G_1 \circ G_2) = M^\Gamma(G_1) \cdot M^\Gamma(G_2)$$

A representation is said to be irreducible if it is not possible to find a basis in which all the matrix representatives of the group elements have the same block diagonal form.

The explicit matrix representations $M^\Gamma(G)$ are dependent on the choice of the basis vectors. However, for a given representation $\Gamma$, the characters, defined as the traces of the matrix representations

$$\chi^\Gamma(G) = \text{Tr} \left\{ M^\Gamma(G) \right\}$$

(9)
are independent of the basis. Two group elements \( G \) and \( G' \) are said to belong to the same class \( C \) if they are related through a similarity transformation of the form \( G = AG'A^{-1} \) where \( A \) also belongs to the group \( \mathcal{G} \). All elements in the same class have the same character for all representations \( \Gamma \), i.e.

\[
\chi_\Gamma (G) = \chi_\Gamma (C) \quad \text{for all } G \in C
\]  

(10)

**2.2. Subgroup Averaging**

Suppose now that the group \( \mathcal{G} \) contains a finite subgroup \( \mathfrak{g} \) containing \( h(\mathfrak{g}) \) elements. A representation \( \Gamma \) of the group \( \mathcal{G} \) is also a representation of the subgroup \( \mathfrak{g} \). The finite group orthogonality theorem [28] implies that the number of independent linear combinations of basis vectors spanning the representation \( \Gamma \) which are invariant under all of the subgroup operations \( G \in \mathfrak{g} \) is given by

\[
a^\Gamma (\mathfrak{g}) = h(\mathfrak{g})^{-1} \sum_{G \in \mathfrak{g}} \chi_\Gamma (G) = h(\mathfrak{g})^{-1} \sum_C h_C (\mathfrak{g}) \chi_C^\Gamma
\]  

(11)

where \( h_C (\mathfrak{g}) \) is the number of elements of \( \mathfrak{g} \) that belong to the class \( C \). The last two formulations on the right-hand side of (11) are equivalent since all elements in the same class have the same character. This equation leads to the following property:

\[
\sum_C h_C (\mathfrak{g}) \chi_C^\Gamma = 0 \implies \sum_{G \in \mathfrak{g}} M_\Gamma (G) = 0
\]  

(12)

The sum of matrices in the representation \( \Gamma \) vanishes if the characters sum to zero over all classes of \( \mathfrak{g} \), taking into account the number of subgroup elements \( h_C (\mathfrak{g}) \) in each class.

**2.3. Average of a Function in \( n \)-dimensional Space**

Consider now the case where the group elements \( G \) are transformations acting on the points \( x = \{x_1, x_2 \ldots x_n\} \) of the \( n \)-dimensional real space \( \mathbb{R}^n \), i.e.

\[
Gx = x'
\]  

(13)

For each group element \( G \), there exists a corresponding operator \( \hat{G} \) acting on functions of the coordinate vectors \( f(x) \) to generate new functions \( f'(x) \), defined as follows:

\[
f'(x) = \hat{G}f(x) = f(G^{-1}x)
\]  

(14)

The definition above corresponds to an active transformation of the object \( f \) [28].

The average function over a finite subgroup \( \mathfrak{g} \) of \( \mathcal{G} \) is defined by

\[
\langle f \rangle_\mathfrak{g} = h(\mathfrak{g})^{-1} \sum_{G \in \mathfrak{g}} \hat{G}f
\]  

(15)

where the sum is taken over all \( h(\mathfrak{g}) \) elements \( G \in \mathfrak{g} \) and the same argument \( x \) is implied on both sides of the equation.
Now suppose we have a set of \( m \) functions \( f^\Gamma_1, \ldots, f^\Gamma_m \) forming a basis for an \( m \)-dimensional representation \( \Gamma \) of \( G \). Any operator \( \hat{G} \) is then represented by an \( m \times m \) matrix \( M^\Gamma(G) \) acting on the set of basis functions from the right \[29\]:

\[
\hat{G} f^\Gamma_i(x) = \sum_j f^\Gamma_j(x) M^\Gamma_{ji}(G)
\]

Equation 12 gives a sufficient condition for the average of each \( f^\Gamma_i \) function to vanish:

\[
\sum_C h_C(g) \chi^\Gamma_C = 0 \Rightarrow \langle f^\Gamma_i \rangle_g = 0
\]

2.4. Average of a Function Over the Polytope Vertices

The average value of a function \( f \) over a finite set \( P \) of \( N_0 \) points in the \( n \)-dimensional space is defined as follows:

\[
\langle f \rangle_P = N_0^{-1} \sum_v f(x_v)
\]

where \( x_v \) denote the coordinate vectors of the points for \( v \in \{1, 2, \ldots, N_0\} \). A group \( G \) of \( n \)-dimensional transformations is said to act transitively on the \( P \) when for any given pair of points \( x_v, x'_v \in P \) there is a transformation \( G \) which connects such points \( x'_v = G x_v \) \[25\].

The orbit stabilizer and Lagrange theorems for finite groups \[25\] relate the average of a function \( f \) over \( P \) to the average over any finite group \( g_P \) acting transitively on the set:

\[
N_0^{-1} \sum_v f(x_v) = h(g_P)^{-1} \sum_{G \in g_P} f(G^{-1} x_1) = h(g_P)^{-1} \sum_{G \in g_P} \hat{G} f(x_1)
\]

The right-hand side corresponds to Equation 15, evaluated at any point \( x_1 \) in the set. From Equation 17, the average vanishes if the function \( f \) is one of the basis functions of the representation \( \Gamma \), and the characters of the given finite group sum \( g_P \) to zero for that representation:

\[
\sum_C h_C(g_P) \chi^\Gamma_C = 0 \Rightarrow \langle f^\Gamma_i \rangle_P = 0
\]

Equation 20 is the central result of this section. The point symmetry group of an \( n \)-dimensional regular polytope is a finite group which acts transitively on the polytope vertices. It is a subgroup of the (infinite) orthogonal group \( O(n) \), which is the group of all the \( n \)-dimensional space transformations in with a single fixed point and which preserve distance between transformed points. Using Equation 20, the averaging properties of a function over the vertices of a polytope may be deduced from the characters of the symmetry elements and the classes of its symmetry point group. This result is now applied to the spherical moments of the regular solids.

3. Polyhedral Averaging in Three Dimensions

Three dimensional polytopes are known as polyhedra. In this section we discuss the averaging properties of the regular polyhedra with respect to spherical harmonics. Although this topic has been treated before in Reference[11], a recapitulation is useful for framing the discussion of four-dimensional symmetries. In addition, the treatment in Reference[11] did not exploit all the available symmetries, as discussed below.
3.1. Proper and Improper Rotations

The proper rotations in three dimensions may be defined in various ways. For example, the symbol $R_n(\xi)$ indicates a rotation through the angle $\xi$ about a unit rotation axis $n$ whose direction is defined by the polar angles $\{\theta, \phi\}$. The identity operation $R(0)$ does not need any specification of the rotation axis. Any rotation in 3D space may be decomposed into the product of three consecutive rotations around the cartesian reference axes, for example:

$$R_n(\xi) = R_z(\alpha)R_y(\beta)R_z(\gamma),$$

where the rotations are applied in sequence from right to left. For a given rotation $R$ the three Euler angles $\Omega_R = \{\alpha, \beta, \gamma\}$ and the set $\{\xi, \theta, \phi\}$ are related \[10\]. Specifically, the rotation angle $\xi$ is related to the Euler angles as follows:

$$\cos \frac{\xi}{2} = \cos \frac{\beta}{2} \cos \frac{\alpha + \gamma}{2}$$ \hspace{1cm} (21)

The improper rotations in three-dimensional space may be expressed in various ways. In this article, we use the set of improper rotations, denoted $\tilde{R}_n(\xi)$. Each improper rotation corresponds to a proper rotation $R_n(\xi)$ followed by an inversion through the reference frame origin (roto-inversion). By definition, the inversion operation corresponds to the improper rotation $\tilde{R}(0)$, where the rotation axis does not need to be specified in this case.

Two other improper rotations are often used in the literature: the reflection $\sigma_h$ in the plane $h$, and the roto-reflection $S_m$ which is a rotation through $2\pi/m$ followed by reflection in the plane perpendicular to the rotation axis. Reflections and roto-reflections correspond to improper rotations as follows:

$$\sigma_h = \tilde{R}_{n'}(\pi)$$ where $n'$ is perpendicular to the plane $h$, and $S_m = \tilde{R}_{n''}(\pi + 2\pi/m)$ where $n''$ is the rotation axis defined by $S_m$ for $m \geq 3$. Clearly $S_2 = \tilde{R}(0)$ and $S_1 = \tilde{R}_{n''}(\pi)$.

3.2. Representations and Characters of $O(3)$ Isometries

The set of $2\ell + 1$ spherical harmonics of rank-$\ell$ is defined as follows:

$$Y_{\ell m}(\Theta, \Phi) = \sqrt{\frac{2\ell + 1}{4\pi} \frac{(\ell - m)!}{(\ell + m)!}} P^m_\ell(\cos \Theta) e^{im\Phi}$$ \hspace{1cm} (22)

where $\ell$ and $m$ are integers with $|m| \leq \ell$ and $P^m_\ell$ is the associated Legendre polynomial \[10\]. This set of functions is a basis for the $(2\ell + 1)$-dimensional irreducible representation of the $O(3)$ group. The action of any $O(3)$ operation $G$ on these functions defines an operator $\hat{G}$ which is represented by a $(2\ell + 1) \times (2\ell + 1)$ matrix $M^\ell(G)$:

$$\hat{G}Y_{\ell m}(\Theta, \Phi) = \sum_{m'} Y_{\ell m'}(\Theta, \Phi)M^\ell_{m'm}(G)$$ \hspace{1cm} (23)

In the case of a proper rotation $R$, the matrix representative is given by the rank-$\ell$ Wigner matrix:

$$M^\ell(R) = D^\ell(\Omega_R)$$ \hspace{1cm} (24)

In the case of an improper rotation $\tilde{R}$, the sign of the matrix changes for odd rank $\ell$:

$$M^\ell(\tilde{R}) = (-1)^\ell D^\ell(\Omega_R)$$ \hspace{1cm} (25)
The character of a proper rotation for the rank-$\ell$ representation is equal to the trace of the corresponding Wigner matrix, $\chi^{(\ell)}_D$, which depends on the rotation angle $\xi$ only [10, pp. 99-100]:

$$\chi^{(\ell)} \left\{ R_n(\xi) \right\} = \chi^{(\ell)}_D (\xi) \tag{26}$$

where

$$\chi^{(\ell)}_D (\xi) = \frac{\sin \left\{ (2\ell + 1) \frac{\xi}{2} \right\}}{\sin \frac{\xi}{2}} \tag{27}$$

This evaluates to $\chi^{(\ell)}_D (\xi) = 2\ell + 1$ when the rotation angle $\xi$ is an integer multiple of $2\pi$.

The character of an improper rotation is the same as for the corresponding proper rotation, but with a change in sign for odd values of $\ell$:

$$\chi^{(\ell)} \left\{ \tilde{R}_n(\xi) \right\} = (-1)^{\ell} \chi^{(\ell)}_D (\xi) \tag{28}$$

### 3.3. Regular Convex Polyhedra

The five regular convex polyhedra have been known since the Greeks. Their names and properties are listed in Figure 1. This figure also provides the Schl"afli symbols [17] of the form $\{p, q\}$, where $p$ indicates the number of edges of the regular polygonal face, and $q$ is the number of faces meeting at one vertex. For example, the cube has Schl"afli symbol $\{4, 3\}$, while the regular octahedron has the Schl"afli symbol $\{3, 4\}$. Polyhedra with Schl"afli symbols $\{p, q\}$ and $\{q,p\}$ are geometrical reciprocals of each other and belong to the same symmetry group, since the reciprocation operation corresponds to the mutual exchange of faces and vertices. The five Platonic solids therefore belong to only three symmetry point groups: (i) $T_d$, represented by the tetrahedron; (ii) $O_h$, populated by the cube and the octahedron; and (iii) $I_h$, populated by the icosahedron and the dodecahedron. The symmetry point groups of the regular polyhedra are given explicitly in Table 1.

**Figure 1.** The 3D regular convex polyhedra organised according to their symmetry group. Here $N_0$ is the number of vertices, $N_1$ is the number of edges and $N_2$ is the number of faces constituting the solid.

<table>
<thead>
<tr>
<th>Symmetry group</th>
<th>$T_d$</th>
<th>$O_h$</th>
<th>$I_h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Tetrahedron</td>
<td>Octahedron</td>
<td>Cube</td>
</tr>
<tr>
<td>Schl&quot;afli symbol</td>
<td>${3,3}$</td>
<td>${3,4}$</td>
<td>${4,3}$</td>
</tr>
<tr>
<td>$N_0$</td>
<td>4</td>
<td>6</td>
<td>8</td>
</tr>
<tr>
<td>$N_1$</td>
<td>6</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>$N_2$</td>
<td>4</td>
<td>8</td>
<td>6</td>
</tr>
</tbody>
</table>
3.4. Spherical Moments of the Regular Polyhedra

The theorem in Equation 20 may be used with Table 1 and the characters given in Equations 26 and 28 to deduce the vanishing spherical moments of the regular polyhedra. In general, both improper and proper rotations must be taken into account. The treatment in Reference [11] uses only the proper rotations, and gives slightly different results for the groups $O_h$ and $I_h$ (see below).

As a first example, consider the tetrahedron. As shown in Table 1, the tetrahedron has three symmetry classes of proper rotations, with number of elements $(1, 8, 3)$ and rotation angles $(0, 2\pi/3, \pi)$ respectively. In addition, there are two symmetry classes of improper rotations, with number of elements $(6, 6)$ and rotation angles $(\pi/2, \pi)$ respectively. The sum of characters for rank $\ell = 2$ is therefore given by

$$\sum_C h_C (T_d) \chi_C^{(2)} = \chi_D^{(2)} (0) + 8\chi_D^{(2)} (2\pi/3) + 3\chi_D^{(2)} (\pi) + 6(-1)^2\chi_D^{(2)} (\pi/2) + 6(-1)^2\chi_D^{(2)} (\pi) = 0$$

This proves the well-known fact that a tetrahedron averages second-rank spherical harmonics to zero:

$$\sigma_{2m0}(T_d) = 0 \quad (30)$$

The point symmetry groups of the octahedron and icosahedron contain the inversion element. Each proper rotation is therefore accompanied by an improper rotation through the same angle, as shown in Table 1. It follows that all odd-rank spherical moments harmonics vanish when summed over the vertices of polyhedra with symmetries $O_h$ and $I_h$:

$$\sum_C h_C (O_h) \chi_C^{(\ell)} = \sum_C h_C (I_h) \chi_C^{(\ell)} = 0 \quad \text{(for odd } \ell) \quad (31)$$

and hence

$$\sigma_{\ell m0}(O_h) = \sigma_{\ell m0}(I_h) = 0 \quad \text{(for odd } \ell) \quad (32)$$

The treatment of Reference [11] does not predict this result, since only proper rotations were taken into account. The two analyses differ for rank $\ell = 9$ and all odd ranks $\ell \geq 13$.

Figure 2 summarizes the spherical rank profiles of the regular convex polyhedra up to rank $\ell = 30$. Note that even the most symmetrical polyhedra (the icosahedron and the dodecahedron) fail to average the rank $\ell = 6$ terms.

There are 4 regular non-convex polyhedra (star-polyhedra), which all fall in the group $I_h$ [17]. Four of them have the same vertices of the icosahedron while one has the same vertices as the dodecahedron. All have the same spherical moment characteristics as the icosahedron.
Table 1. The three symmetry point groups of the regular polyhedra. \( h \) is the number of symmetry elements in the group. The last column shows the number of elements in each class (in square parentheses), followed by a single symmetry element of the class, for a polyhedron in standard orientation. The symbol \( R_{(a,b,c)}(\xi) \) indicates a rotation through the angle \( \xi \) about the axis \((a, b, c)\). The symbol \( \tilde{R}_{(a,b,c)}(\xi) \) indicates the improper operation constructed by the proper rotation \( R_{(a,b,c)}(\xi) \) followed by the inversion operation. \( R(0) \) is the identity operation and \( \tilde{R}(0) \) is the inversion operation. The symbol \( \tau = 2 \cos(\pi/5) = (\sqrt{5} + 1)/2 \) indicates the golden ratio.

<table>
<thead>
<tr>
<th>Symmetry group</th>
<th>( h )</th>
<th>Symmetry operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_d )</td>
<td>24</td>
<td>[1] ( R(0); [8] R_{(1,1,1)}(2\pi/3); [3] R_{(1,0,0)}(\pi); [6] \tilde{R}<em>{(1,0,0)}(\pi/2); [6] \tilde{R}</em>{(1,1,0)}(\pi) )</td>
</tr>
<tr>
<td>( O_h )</td>
<td>48</td>
<td>[1] ( R(0); [8] R_{(1,1,1)}(2\pi/3); [3] R_{(1,0,0)}(\pi); [6] R_{(1,0,0)}(\pi/2); [6] R_{(1,1,0)}(\pi); [1] \tilde{R}(0); [8] \tilde{R}<em>{(1,1,1)}(2\pi/3); [3] \tilde{R}</em>{(1,0,0)}(\pi); [6] R_{(1,0,0)}(\pi/2); [6] \tilde{R}_{(1,1,0)}(\pi) )</td>
</tr>
<tr>
<td>( I_h )</td>
<td>120</td>
<td>[1] ( R(0); [12] R_{(1,0,0)}(2\pi/5); [12] R_{(1,0,0)}(4\pi/5); [20] R_{(2,0,0,0)}(\pi); [15] R_{(\tau,0,0,0)}(\pi); [1] \tilde{R}(0); [12] \tilde{R}<em>{(1,0,0)}(2\pi/5); [12] \tilde{R}</em>{(1,0,0)}(4\pi/5); [20] \tilde{R}<em>{(2,0,0,0)}(\pi); [15] \tilde{R}</em>{(\tau,0,0,0)}(\pi) )</td>
</tr>
</tbody>
</table>

4. Polytopic Averaging in Four Dimensions

In this section we derive the spherical averaging properties of the regular 4-polytopes. In the discussion below, we make extensive use of quaternions [29]. As shown in Equation 7, quaternions provide a correspondence between points on a unit sphere in four-dimensional space, and the group of three-dimensional rotations.

4.1. Quaternions

Four-dimensional real space is a vector space: any two vectors can be added or multiplied by a scalar to give another vector. Quaternions extend the vectorial structure of 4D real space by allowing the multiplication of two 4D vectors \( \mathbf{q}(1) \) and \( \mathbf{q}(2) \) according to

\[
\begin{pmatrix}
q_1(2) \\
q_2(2) \\
q_3(2) \\
q_4(2)
\end{pmatrix}
\ast
\begin{pmatrix}
q_1(1) \\
q_2(1) \\
q_3(1) \\
q_4(1)
\end{pmatrix}
=
\begin{pmatrix}
q_1(2)q_1(1) - q_2(2)q_2(1) - q_3(2)q_3(1) - q_4(2)q_4(1) \\
qu_1(2)q_2(1) + q_2(2)q_1(1) + q_3(2)q_4(1) - q_4(2)q_3(1) \\
qu_1(2)q_3(1) - q_2(2)q_4(1) + q_3(2)q_1(1) + q_4(2)q_2(1) \\
qu_1(2)q_4(1) + q_2(2)q_3(1) - q_3(2)q_2(1) + q_4(2)q_1(1)
\end{pmatrix}
\tag{33}
\]
Figure 2. Spherical rank profiles for the regular convex 3D polyhedra. Open circles indicate that all \((2\ell + 1)\) spherical moments \(\sigma^S_{\ell m}\) of integer rank \(\ell\) are zero for the set of orientations corresponding to the vertices of the corresponding polyhedron. Closed circles indicate that there is at least one non-zero spherical moment of rank \(\ell\).

The adjoint of a quaternion is denoted here \(q^\dagger\) and is defined as follows:

\[
q^\dagger = \begin{pmatrix}
q_1 \\
-q_2 \\
-q_3 \\
-q_4
\end{pmatrix}
\]
and it can be verified that \( \{ q(1) * q(2) \}^\dagger = q^\dagger(2) * q^\dagger(1) \).

The inverse \( q^{-1} \) is defined for any non zero quaternion \( q \) as the unique quaternion that satisfies:

\[
q * q^{-1} = q^{-1} * q = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]

(35)

It can be shown that \( q^{-1} = q^\dagger / ||q||^2 \) where \( ||q|| = \sqrt{\sum_i q_i^2} \).

### 4.2. Unit Quaternions and 3D Rotations

The set of 4D unit vectors, together with the quaternion multiplication operation \(*\), forms the group of unit quaternions \( \mathbb{Q} \). The adjoint of a unit quaternion is the same as its inverse: \( q^{-1} = q^\dagger \). From Equation 7, a unit quaternion and its inverse represent a pair of rotations through opposite angles about the same axis.

The group of unit quaternions \( \mathbb{Q} \) is homomorphic with the group of proper three-dimensional rotations \( SO(3) \) [30]. The relationship between the product of quaternions and the product of proper 3D rotations is expressed by

\[
R \{ q(2) * q(1) \} = R \{ q(2) \} \circ R \{ q(1) \}
\]

(36)

where \( R(q) \) is the function which associates a unit quaternion \( q \) with the corresponding 3D rotation through Equation 7. Consider, for example, a rotation through the angle \( \xi(1) \) about the axis \( n(1) \), followed by a rotation through the angle \( \xi(2) \) about the axis \( n(2) \). The overall rotation angle \( \xi(2, 1) \) is given by

\[
\cos \frac{\xi(2, 1)}{2} = q_1(2, 1) = q_1(2)q_1(1) - q_2(2)q_2(1) - q_3(2)q_3(1) - q_4(2)q_4(1)
\]

\[
= \cos \frac{\xi(2)}{2} \cos \frac{\xi(1)}{2} - n(2) \cdot n(1) \times \sin \frac{\xi(2)}{2} \sin \frac{\xi(1)}{2}
\]

(37)

from Equation 7 and 33.

Using the notation \( D^\ell(q) \) to indicate the Wigner matrix of rank \( \ell \) evaluated for the 3D rotation corresponding to the unit quaternion \( q \), Equation 36 implies:

\[
D^\ell \{ q(2) * q(1) \} = D^\ell \{ q(2) \} \cdot D^\ell \{ q(1) \}
\]

(38)

The Wigner matrices of rank \( \ell \) form a \( 2\ell + 1 \)-dimensional representation of the unit quaternion group \( \mathbb{Q} \). In particular \( D^\ell(q^{-1}) = [D^\ell(q)]^{-1} \) and we can use the following properties for the Wigner matrix elements [10, pp.79-80]

\[
D^\ell_{mm'}(q^\dagger) = D^\ell_{mm'}(q^{-1}) = (-1)^{m-m'} D^\ell_{m'-m}(q)
\]

(39)

The explicit correspondence between the Euler angles and the unit quaternion components is as follows:

\[
\alpha + \gamma = 2 \arctan(q_1, q_4)
\]

\[
\beta = \arccos(1 - 2q_2^2 - 2q_3^2)
\]

\[
\alpha - \gamma = 2 \arctan(q_3, -q_2)
\]

(40)
where \( \arctan(x, y) \) is equal to \( \arctan(y/x) \), determining the quadrant from the sign of \( x \) and \( y \). In the special cases \( q_2 = q_3 = 0 \) or \( q_1 = q_4 = 0 \), only the combinations \( \alpha \pm \gamma \) are defined, as follows:

\[
\begin{align*}
\beta &= 0 \\
\alpha + \gamma &= 2 \arctan(q_1, q_4) \\
\beta &= \pi \\
\alpha - \gamma &= 2 \arctan(q_3, -q_2)
\end{align*}
\]

if \( q_2 = q_3 = 0 \)

\( q_1 = q_4 = 0 \)

(41)

4.3. Proper and Improper Rotations

Isometries in 4D space are classed as either *proper* (preserving the handedness of the four-dimensional axis system) or *improper* (changing the handedness of the axis system). The group of all isometries with one fixed point in four dimensions is called \( O(4) \). Any \( O(4) \) operation may be expressed in terms of two unit quaternions, denoted here \( q \) and \( r \) [19], as explained below. Proper operations will be denoted by \( R_{q,r} \) and improper operations by \( \tilde{R}_{q,r} \) respectively. The action of a proper rotation \( R_{q,r} \) on a point in 4D space \( q \) may be written as follows:

\[
q' = R_{q,r}q = q_l * q * q_r^{-1}
\]

(42)

The action of an improper rotation \( \tilde{R}_{q,r} \) is as follows:

\[
q' = \tilde{R}_{q,r}q = q_l * q^\dagger * q_r^{-1}
\]

(43)

The inverse operations are given by

\[
\{ R_{q,r} \}^{-1} = R_{q^{-1}, r^{-1}} \Leftrightarrow \{ R_{q,r} \}^{-1} q = q_l^{-1} * q * q_r
\]

(44)

\[
\{ \tilde{R}_{q,r} \}^{-1} = \tilde{R}_{q^{-1}, r^{-1}} \Leftrightarrow \{ \tilde{R}_{q,r} \}^{-1} q = q_r^{-1} * q^\dagger * q_l
\]

(45)

for proper and improper operations respectively.

4.4. Representation and Characters of \( O(4) \) Isometries

In this section we give the explicit matrix representations of the \( O(4) \) operators and their characters in the basis of the Wigner matrices. These results will then be used to establish the spherical averaging properties of the regular 4-polytopes.

According to Equations 14, 44, 38 and 39, a proper transformation in \( O(4) \) defines an operator \( \tilde{R}_{q,r} \) which acts as follows on the Wigner matrix elements evaluated at any unit quaternion \( q \):

\[
\tilde{R}_{q,r} D_{mm'}^{\ell} (q) = D_{mm'}^{\ell} (\{ R_{q,r} \}^{-1} q) = D_{mm'}^{\ell} (q_l^{-1} * q * q_r)
\]

\[
= \sum_{n,n'} D_{mn}^{\ell} (q_l^{-1}) D_{m'n'}^{\ell} (q) D_{n'm'}^{\ell} (q_r)
\]

\[
= \sum_{n,n'} (-1)^{m-n} D_{-m-n}^{\ell} (q_l) D_{n,n'}^{\ell} (q) D_{n'm'}^{\ell} (q_r)
\]

(46)

\[
= \sum_{n,n'} D_{n,n'}^{\ell} (q) \left[ (-1)^{m-n} D_{-m-n}^{\ell} (q_l) D_{n'm'}^{\ell} (q_r) \right]
\]
Similarly according to Equations 14, 45, 38 and 39 an improper transformation in \( O(4) \) defines an operator \( \hat{R}_{q_l,q_r} \), which acts as follows:

\[
\hat{R}_{q_l,q_r} \ D^\ell_{mm'}(q) = D^\ell_{mm'}\left( \left\{ \hat{R}_{q_l,q_r} \right\}^{-1} q \right) = D^\ell_{mm'}(q^{-1}_l * q^*_r * q_l)
\]

\[
= \sum_{n,n'} D^\ell_{m,n} (q^{-1}_r) \ D^\ell_{nn'} (q^*_l) \ D^\ell_{n'm'} (q_l)
\]

\[
= \sum_{n,n'} (-1)^{m-n} D^\ell_{-n,-m} (q_r) \ (-1)^{n-n'} D^\ell_{-n',-n} (q) \ D^\ell_{n'm'} (q_l)
\]

\[
= \sum_{n,n'} (-1)^{m+n'} D^\ell_{n-m} (q_r) \ (-1)^{n-n'} D^\ell_{nn'} (q) \ D^\ell_{n'm'} (q_l)
\]

\[
= \sum_{n,n'} D^\ell_{nn'} (q) (-1)^{m+n} \left[ (-1)^{m+n} D^\ell_{n,-m} (q_r) \ D^\ell_{n'm'} (q_l) \right]
\]

The action of any \( O(4) \) operation \( G \) on the \((2\ell + 1)^2\) Wigner functions \( D^\ell_{mm'}(q) \), evaluated for the rotation corresponding to the unit quaternion \( q \), defines an operator \( \hat{G} \) which may be represented as a \((2\ell + 1)^2 \times (2\ell + 1)^2\)-dimensional matrix \( M^\ell(G) \):

\[
\hat{G} \ D^\ell_{mm'}(q) = \sum_{n,n'} D^\ell_{nn'}(q) [M(G)]^\ell_{nn',mm'}
\]

This proves that the Wigner matrices are a basis for the representation of the group \( O(4) \). The matrix representations are given by

\[
[M(R_{q_l,q_r})]^\ell_{mm',mm'} = (-1)^{m-n} D^\ell_{n,-m} (q_l) \ D^\ell_{n'm'} (q_r)
\]

for a proper transformation \( R_{q_l,q_r} \) and

\[
\left[ M(\hat{R}_{q_l,q_r}) \right]^\ell_{nn',mm'} = (-1)^{m+n} D^\ell_{-n,m} (q_l) \ D^\ell_{n'-m} (q_r)
\]

for an improper transformation \( \hat{R}_{q_l,q_r} \). In both cases the Wigner matrix elements are evaluated for rotations corresponding to the left and right quaternions \( q_l \) and \( q_r \), as defined for the given \( O(4) \) operation.

The character of a general 4D rotations in the rank-\( \ell \) representation is obtained by summing the matrix representations given by Equations 49 and 50 over the indices \( m = n \) and \( m' = n' \). For proper rotations this leads to the following result:

\[
\chi^{(\ell)} (R_{q_l,q_r}) = \chi^{(\ell)}_D (\xi_l) \chi^{(\ell)}_D (\xi_r)
\]

where \( \xi_l \) and \( \xi_r \) are the rotation angles for the pair of 3D rotations corresponding to the left and right quaternions. For improper rotations, on the other hand, we get

\[
\chi^{(\ell)} (\hat{R}_{q_l,q_r}) = \chi^{(\ell)}_D (\xi_{l,r})
\]

where \( \xi_{l,r} \) is the rotational angle associated with the quaternion product \( q(l,r) = q_l * q_r \).
4.5. Regular Convex 4-Polytopes

The six regular convex polytopes are summarized in Figure 3. Each of them is represented by a Schlafli symbol of the form \{p, q, r\} in which p and q determine the Schlafli symbol \{p, q\} for the 3-dimensional polyhedron that forms the boundary of the figure and r is the number of polyhedra meeting at one edge [17].

Polytopes with Schlafli symbols \{p, q, r\} and \{r, q, p\} are reciprocals of each other and belong to the same symmetry group. The six regular convex 4-polytopes therefore belong to only four symmetry groups. These are (i) the group \(A_4\) (isomorphic to the permutation group of 5 elements, \(S_5\)), populated by the 5-cell (hypertetrahedron); (ii) the group \(B_4\), populated by the mutually reciprocal 8-cell (hypercube) and 16-cell (hyperoctahedron); (iii) the group \(F_4\), populated by the 24-cell; and (iv) the group \(H_4\), populated by the mutually reciprocal 120-cell (hyperdodecahedron) and 600-cell (hypericosahedron).

**Figure 3.** A list of the 4D regular convex polytopes organized according to their symmetry group. Here \(N_0\) is the number of vertices, \(N_1\) is the number of edges, \(N_2\) is the number of faces and \(N_3\) is the number of three dimensional cells. The two dimensional graphs indicate the vertex connections.

<table>
<thead>
<tr>
<th>Symmetry group</th>
<th>(A_4)</th>
<th>(B_4)</th>
<th>(F_4)</th>
<th>(H_4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>5-cell</td>
<td>16-cell</td>
<td>8-cell</td>
<td>24-cell</td>
</tr>
<tr>
<td>Schlafli symbol</td>
<td>Hyper-tetrahedron</td>
<td>Hyper-octahedron</td>
<td>Hyper-cube</td>
<td>Hyper-icosahedron</td>
</tr>
<tr>
<td>Graph representation</td>
<td><img src="image.png" alt="Graph" /></td>
<td><img src="image.png" alt="Graph" /></td>
<td><img src="image.png" alt="Graph" /></td>
<td><img src="image.png" alt="Graph" /></td>
</tr>
<tr>
<td>(N_0)</td>
<td>5</td>
<td>8</td>
<td>16</td>
<td>24</td>
</tr>
<tr>
<td>(N_1)</td>
<td>10</td>
<td>24</td>
<td>32</td>
<td>96</td>
</tr>
<tr>
<td>(N_2)</td>
<td>10</td>
<td>32</td>
<td>24</td>
<td>96</td>
</tr>
<tr>
<td>(N_3)</td>
<td>5</td>
<td>16</td>
<td>8</td>
<td>24</td>
</tr>
</tbody>
</table>

Table 2 reports the four symmetry groups of the six regular polytopes and their symmetry elements, given in the quaternion form. The numbers of operations in each class are provided, together with one representative operation, using the notation \(R_{q_1, q_2}\) for proper transformations and \(\tilde{R}_{q_1, q_2}\) for improper transformations. In the case of the group \(H_4\), the symmetry classes and representative operations are given directly in quaternion form in Reference[23]. For the other groups, the information given in the literature [20–22] is not directly suitable for this type of analysis. In these cases, the quaternion form of the representative operations and the class structure were obtained by using the information provided in Reference[19] with the help of the symbolic software platform Mathematica [31].
Table 2. The four symmetry groups of the 4D regular polytopes. \( h \) denotes the total number of symmetry elements. The last column shows the number of elements in each class (in square parentheses), followed by a single symmetry element of the class, for a polytope in standard orientation. The symmetry elements are denoted \( R_{q_i,q_j} \) for a proper rotation and \( \tilde{R}_{q_i,q_j} \) for an improper rotation, see Equations 42 and 43. The quaternions \( \{q_1, q_2 \ldots q_{15}\} \) are given explicitly in the last section.

<table>
<thead>
<tr>
<th>Symmetry group</th>
<th>( h )</th>
<th>Symmetry operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_4 )</td>
<td>120</td>
<td>[1] ( R_{q_1,q_1} ); [15] ( R_{q_3,q_3} ); [20] ( R_{q_8,q_8} ); [24] ( R_{q_{11},q_{12}} ); [10] ( \tilde{R}<em>{q_4,q_4} ); [30] ( \tilde{R}</em>{q_5,q_5} ); [20] ( \tilde{R}<em>{q_9,q</em>{10}} )</td>
</tr>
<tr>
<td>( B_4 )</td>
<td>384</td>
<td>[1] ( R_{q_1,q_1} ); [1] ( R_{q_1,-q_1} ); [6] ( R_{q_2,q_2} ); [12] ( R_{q_2,q_1} ) [12] ( R_{q_2,q_3} ); [24] ( R_{q_4,q_4} ); [12] ( R_{q_6,q_6} ); [12] ( R_{q_6,-q_6} ); [32] ( R_{q_7,q_7} ); [32] ( R_{q_7,-q_7} ); [48] ( R_{q_6,q_4} ); [48] ( R_{q_6,q_7} ); [32] ( R_{q_7,q_7} ); [32] ( R_{q_7,-q_7} )</td>
</tr>
<tr>
<td>( F_4 )</td>
<td>1152</td>
<td>[1] ( R_{q_1,q_1} ); [1] ( R_{q_1,-q_1} ); [12] ( R_{q_2,q_2} ); [18] ( R_{q_2,-q_2} ); [96] ( R_{q_2,q_7} ); [72] ( R_{q_4,q_4} ); [144] ( R_{q_6,q_6} ); [36] ( R_{q_6,-q_6} ); [16] ( R_{q_7,q_7} ); [16] ( R_{q_7,-q_7} ); [32] ( R_{q_7,q_7} ); [32] ( R_{q_7,-q_7} ); [12] ( \tilde{R}<em>{q_1,q_1} ); [72] ( \tilde{R}</em>{q_2,q_2} ); [12] ( \tilde{R}<em>{q_2,q_7} ); [96] ( \tilde{R}</em>{q_2,q_4} ); [12] ( \tilde{R}<em>{q_4,-q_4} ); [72] ( \tilde{R}</em>{q_6,q_6} ); [96] ( \tilde{R}<em>{q_6,q_5} ); [96] ( \tilde{R}</em>{q_6,-q_5} ); [96] ( \tilde{R}_{q_7,q_7} )</td>
</tr>
<tr>
<td>( H_4 )</td>
<td>14400</td>
<td>[1] ( R_{q_1,q_1} ); [1] ( R_{q_1,-q_1} ); [60] ( R_{q_1,q_3} ); [40] ( R_{q_1,q_{13}} ); [40] ( R_{q_1,-q_{13}} ); [24] ( R_{q_1,q_{14}} ); [24] ( R_{q_1,-q_{14}} ); [24] ( R_{q_1,q_{15}} ); [24] ( R_{q_1,-q_{15}} ); [450] ( R_{q_3,q_3} ); [1200] ( R_{q_3,q_{13}} ); [720] ( R_{q_3,q_{14}} ); [720] ( R_{q_3,q_{15}} ); [400] ( R_{q_{13},q_3} ); [400] ( R_{q_{13},q_{13}} ); [480] ( R_{q_{13},q_{14}} ); [480] ( R_{q_{13},q_{15}} ); [480] ( R_{q_{13},-q_{15}} ); [144] ( R_{q_{14},q_{14}} ); [144] ( R_{q_{14},-q_{14}} ); [288] ( R_{q_{14},q_{15}} ); [288] ( R_{q_{14},-q_{15}} ); [144] ( R_{q_{15},q_{15}} ); [144] ( R_{q_{15},-q_{15}} ); [60] ( \tilde{R}<em>{q_1,q_1} ); [60] ( \tilde{R}</em>{q_1,q_{13}} ); [1800] ( \tilde{R}<em>{q_3,q_3} ); [1200] ( \tilde{R}</em>{q_3,q_{13}} ); [1200] ( \tilde{R}<em>{q_3,-q</em>{13}} ); [720] ( \tilde{R}<em>{q</em>{14},q_1} ); [720] ( \tilde{R}<em>{q</em>{14},q_{13}} ); [720] ( \tilde{R}<em>{q</em>{14},q_{15}} ); [720] ( \tilde{R}<em>{q</em>{14},-q_{15}} )</td>
</tr>
</tbody>
</table>

\( q_1 = (1, 0, 0, 0) \); \( q_2 = (0, 0, 0, 1) \); \( q_3 = (0, 1, 0, 0) \);
\( q_4 = (0, 0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}) \); \( q_5 = (\frac{1}{\sqrt{2}}, 0, 0, \frac{1}{\sqrt{2}}) \); \( q_6 = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0, 0) \);
\( q_7 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \); \( q_8 = (\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \); \( q_9 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}) \);
\( q_{10} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \); \( q_{11} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0) \); \( q_{12} = (\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 0) \);
\( q_{13} = (\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}) \); \( q_{14} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}) \); \( q_{15} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0) \);

4.6. Spherical Moments of the Regular 4-Polytopes

The spherical averaging properties of the regular 4-polytopes may be deduced by using Equation 20 together with the sets of symmetry operations (Table 2), and the characters of the 4D rotations, given in Equations 51 and 52.

As an example, consider the 5-cell, which has symmetry group \( A_4 \). From Table 2, there are seven symmetry classes. The four classes of proper operations have \( (1, 15, 20, 24) \) elements respectively. The
rotational angles \((\xi_l, \xi_r)\) to be used in Equation 51 are obtained from Equation 7 and have the following values: \(((0, 0), (\pi, \pi), (2\pi/3, 2\pi/3), (2\pi/5, 6\pi/5))\). The remaining three classes of improper operations have \((10, 30, 20)\) elements respectively. The rotational angles \(\xi_{l,r}\) to be used in Equation 52 are obtained from Equations 7 and 37 and are as follows: \((2\pi, \pi, 2\pi/3)\). The sum of characters for rank \(\ell = 1\) is therefore given by

\[
\sum_{c} h_c(T_d)\chi^{(1)}_c = \chi^{(1)}_D(0)\chi^{(1)}_D(0) + 15\chi^{(1)}_D(\pi)\chi^{(1)}_D(\pi) + 20\chi^{(1)}_D(2\pi/3)\chi^{(1)}_D(2\pi/3) + 24\chi^{(1)}_D(2\pi/5)\chi^{(1)}_D(6\pi/5) + 10\chi^{(1)}_D(2\pi) + 30\chi^{(1)}_D(\pi) + 20\chi^{(1)}_D(2\pi/3) = 0
\]

(53)

This proves that all first-rank spherical moments of a 5-cell are equal to zero:

\[
\sigma_{1mm'(A_4)} = 0
\]

(54)

The spherical rank profiles of the other regular polytopes may be obtained in this way for any \(\ell\): Figure 4 summarizes the results up to rank \(\ell = 30\). As in the 3D case, even the 600-cell and 120-cell, which have the highest symmetry, fail to average out the rank-6 Wigner matrices.

This figure is slightly misleading since only integer ranks \(\ell\) are shown. Since the groups \(B_4, F_4\) and \(H_4\) possess an inversion operation, \(R_{q1,-q1}\) with \(q1 = (1, 0, 0, 0)\), all spherical moments of half-integer rank vanish for these groups. The group \(A_4\), on the other hand, lacks the inversion, so the spherical moments of half-integer rank do not vanish in this case. The fact that \(A_4\) and \(B_4\) appear to have the same rank profiles in Figure 4 is therefore due to the omission of half-integer ranks. Most applications of orientational averaging only require integer ranks, in which case the properties shown in Figure 4 are appropriate.

There are 10 regular non-convex polytopes (star-polytopes) in four dimensions, which all fall in the group \(H_4\) [17]. Nine of them have the same vertices as the 600-cell, while one has the same vertices as the 120-cell. All have the same spherical moment characteristics as the 600-cell.

Under the reviewing of this paper, an anonymous referee pointed out that the pattern of empty and filled circles in Figure 4 may also be derived using the theory of spherical designs [18]. In general, 4D spherical harmonics of degree \(k\) generate a \((k + 1)^2\)-dimensional representation of the group \(O(4)\) [18]. Such a representation is equivalent to the \((2\ell + 1)^2\)-dimensional representation constructed in Equation 48, with \(k = 2\ell\). A spherical \(t\)-design in 4 dimensions is defined as a subset of the hypersphere for which all the 4D spherical harmonics of degrees 1 to \(t\) average to 0 [18]. In other words, all the spherical moments of rank 1 to \(\ell = t/2\) vanish. In Reference [18] the largest values \(t\) of the spherical design have been derived to be 2 for the 5-cell, 3 for the 8-cell, 5 for the 24-cell, and 11 for the 600-cell, which correspond to \(\ell = 1, 1, 2, 5\) in Figure 4.

The anonymous referee also pointed out that invariant theory may be used to prove that non-zero spherical moments in the \(H_4\) column in Figure 4 may appear at \(\ell\) values corresponding to any sum of 6’s, 10’s and 15’s and for all \(\ell \geq 30\).
Figure 4. Spherical rank profiles of the regular convex 4-polytopes. Open circles indicate that all $(2\ell+1)^2$ spherical moments $\sigma_{\ell m n}^S$ of integer rank $\ell$ are zero for the set of orientations derived from the vertices of the corresponding polytope. Closed circles indicate that there is at least one non-zero spherical moment of rank $\ell$.

<table>
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<th>Symmetry group</th>
<th>$R_4$</th>
<th>$B_4$</th>
<th>$F_4$</th>
<th>$H_4$</th>
<th>O(4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>5-cell</td>
<td>16-cell</td>
<td>8-cell</td>
<td>24-cell</td>
<td>600-cell</td>
</tr>
<tr>
<td># Vertices</td>
<td>5</td>
<td>8</td>
<td>16</td>
<td>24</td>
<td>120</td>
</tr>
<tr>
<td>Graph representation</td>
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<td><img src="image" alt="16-cell" /></td>
<td><img src="image" alt="8-cell" /></td>
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<tr>
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<td><img src="image" alt="2" /></td>
<td><img src="image" alt="3" /></td>
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</table>

5. Euler Angles

In order to facilitate exploitation of these results, we provide explicit tables of Euler angles derived from the vertices of the regular 4-polytopes. The $z - y - z$ convention for the Euler angles is used throughout. All Euler angle sets are derived from 4-polytopes in their standard orientations, as defined
in Table 3. Ambiguities of the form given in Equation 41 were always resolved by choosing solutions with $\gamma = 0$. All angles are reduced to the interval $0$ to $2\pi$ by a modulo-$2\pi$ operation.

**Table 3.** The coordinates of the six convex regular 4-polytopes vertices in standard orientation, as reported in Reference [19]. The double round parentheses ($()$) indicate that all even permutations of the quartet are taken. The symbols $\tau$ and $\eta$ take the values $\tau = 2 \cos(\pi/5) = (\sqrt{5} + 1)/2$ and $\eta = \sqrt{5}/4$. The 600 vertices of the hyperdodecahedron are obtained by multiplying the quaternion $(2^{-1/2}, 2^{-1/2}, 0, 0)$ with all possible quaternion products of the 5 vertices of the hypertetrahedron $S$ and the 120 vertices of the hypericosahedron $I$. All the polytopes are centred at the origin of the coordinate system, with the vertices lying on the hypersphere of radius 1.

<table>
<thead>
<tr>
<th>Name</th>
<th>Vertex Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-cell or hypertetrahedron</td>
<td>$S = {(1, 0, 0, 0), (-1/4, \eta, \eta, \eta), (-1/4, -\eta, -\eta, \eta), \ldots}$</td>
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<tr>
<td>16-cell or hyperoctahedron</td>
<td>$V = ((\pm 1, 0, 0, 0))$</td>
</tr>
<tr>
<td>8-cell or hypercube</td>
<td>$W = ((\pm 1/2, \pm 1/2, \pm 1/2, \pm 1/2))$</td>
</tr>
<tr>
<td>24-cell</td>
<td>$T = V \cup W$</td>
</tr>
<tr>
<td>600-cell or hypericosahedron</td>
<td>$I = T \cup \frac{1}{2}((\pm \tau, \pm 1, \pm \tau^{-1}, 0))$</td>
</tr>
<tr>
<td>120-cell or hyperdodecahedron</td>
<td>$J = (2^{-1/2}, 2^{-1/2}, 0, 0) \ast S \ast I$</td>
</tr>
</tbody>
</table>

Different Euler angle sets with the same spherical averaging properties may be constructed by applying an equal but arbitrary 4D isometry to all the quaternions underlying the set.

The set of Euler angles corresponding to the 5 vertices of the 5-cell is provided in Table 4. As shown in Figure 4, all first-rank spherical moments vanish for this set of Euler angles. Since the 5-cell lacks an inversion operation, the number of orientations is the same as the number of vertices in this case.

The sets of Euler angles corresponding to the 8 vertices of the 16-cell, and the 16 vertices of the 8-cell are provided in Table 5 and 6. As shown in Figure 4, all first-rank spherical moments vanish for these sets of Euler angles. The symmetry groups of both polytopes include an inversion operation, so the number of distinguishable orientations is therefore one-half the number of the vertices. Clearly the four rotations specified in Table 5 comprise the most economical way to set all first-rank spherical moments to zero.

The set of 12 Euler angles corresponding to the 24 vertices of the 24-cell is provided in Table 7. As shown in Figure 4, all first and second-rank spherical moments vanish for this Euler angle set.

The sets of 60 and 300 Euler angles corresponding to the vertices of the 600-cell and the 120-cell are provided in Table 8 and 9. Figure 4 shows that all spherical moments up to and including rank 5 vanish for these Euler angle sets. The most economical way of annihilating spherical ranks up to and including rank 5 is therefore the 60-angle set in Table 8. This rotation set was previously described in Reference [24], where it was presented without any supporting theory.
Table 4. The set of Euler angles (in degrees) corresponding to the 5 vertices $S$ of the 5-cell whose cartesian coordinates are given in Table 3.

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Table 5. The set of Euler angles (in degrees) corresponding to the 8 vertices $V$ of the 16-cell whose cartesian coordinates are given in Table 3. The 8 vertices are reduced to 4 sets of Euler angles because each quaternion pair \{q, $-q$\} corresponds to the same geometrical 3D rotation.

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Table 6. The set of Euler angles (in degrees) corresponding to the 16 vertices $W$ of the 8-cell whose cartesian coordinates are given in Table 3. The 16 vertices are reduced to 8 sets of Euler angles because each quaternion pair \{q, $-q$\} corresponds to the same geometrical 3D rotation.

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Table 7. The set of Euler angles (in degrees) corresponding to the 24 vertices $T$ of the 24-cell whose cartesian coordinates are given in Table 3. The 24 vertices are reduced to 12 sets of Euler angles because each quaternion pair $\{q, -q\}$ corresponds to the same geometrical 3D rotation.

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It is worth pointing out that the 3D rotations discussed above for the 24-cell and the 600-cell have more intuitive descriptions. The set of Euler angles obtained from the vertices of the 24-cell generates exactly the 12 rotational symmetries of the tetrahedron, compare Table 7 with the last column for the group $T_d$ in Table 1. Similarly the set of Euler angles obtained from the vertices of the 600-cell generates exactly the 60 rotational symmetries of the icosahedron, compare Table 8 with the last column for the group $I_h$ in Table 1. The 24 rotational symmetries of the cube ($O_h$ group) do not correspond to any regular 4-polytope. In fact they are not well distributed in the sense of particle repulsion over the hypersphere in 4D as the other polytopic cases. Regarding this last point, it has been rigorously proven that that some of the regular 4-polytopes (the 5-cell, the 16-cell and the 600-cell) minimize a full class of repulsive potentials over the 4D sphere [32].
Table 8. The set of Euler angles (in degrees) corresponding to the 120 vertices $I$ of the 600-cell whose cartesian coordinates are given in Table 3. The 120 vertices are reduced to 60 sets of Euler angles because each quaternion pair $\{q, -q\}$ corresponds to the same geometrical 3D rotation.

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Table 9. The set of Euler angles (in degrees) corresponding to the 600 vertices $J$ of the 120-cell whose cartesian coordinates are given in Table 3. The 600 vertices are reduced to 300 sets of Euler angles because each quaternion pair $\{q, -q\}$ corresponds to the same geometrical 3D rotation.

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6. Conclusions

We expect that these sets of rotations will be useful for the computation of orientational averages in a range of physical sciences, and in experimental procedures such as spherical tensor analysis in nuclear magnetic resonance [7–9]. In addition, we anticipate that where necessary, finer sampling of orientational space may be implemented by interpolating between the vertices of the polytopes, or by four-dimensional tiling and honeycomb schemes, such as those described by Coxeter [17].

Finally, we note that highly-symmetric four-dimensional figures have been found by using a computational procedure [33] which is closely related to the REPULSION algorithm on the surface of a sphere [3]. Such methods could be adapted to generate much larger sets of evenly spaced three-dimensional rotations than those described here.

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References


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