

# Symbolic symmetry verification for harmonic functions invariant under polyhedral symmetries

Yibin Zheng and Peter C. Doerschuk<sup>a)</sup>

School of Electrical Engineering, Purdue University, West Lafayette, Indiana 47907-1285

(Received 18 January 1995; accepted 3 May 1995)

Methods for using symbolic computation systems to verify polyhedral symmetries of harmonic functions on the sphere are presented. The particular case of icosahedral symmetry, which is important in the structure of small spherical viruses, fullerenes, and quasi-crystals, is examined in detail. Previous work by the authors, in which general expressions for polyhedral harmonics in terms of spherical harmonics were derived, is verified by checking the symmetry of all icosahedral harmonics up to order 44. © 1995 American Institute of Physics.

## INTRODUCTION

The availability of inexpensive and easy-to-use symbolic computation systems, such as Mathematica, allows the performance of exact computations too complicated to be done by hand. In this article we present novel methods and Mathematica software to verify the polyhedral symmetries (specifically, icosahedral symmetries) of harmonic functions on the sphere. Harmonic functions invariant under the symmetries of the icosahedral group are of special importance because the icosahedral group plays a prominent role in at least three problems: the structure of small spherical viruses,<sup>1</sup> fullerenes,<sup>2</sup> and quasi-crystals.<sup>3</sup> More generally, for any function which is expected to exhibit a rotational symmetry and which can be expressed as a linear combination of spherical harmonics, the methods we describe can be used to verify the presence of the symmetry.

## I. HARMONICS ON THE SPHERE

In mathematical physics problems where there are intrinsic symmetries, it is often convenient to introduce basis functions which possess such symmetries. For example, the electron density of a small spherical virus obeys icosahedral symmetry. If the electron density is expanded in terms of ordinary spherical harmonics, the expansion coefficients would have to obey complicated relationships in order to satisfy the icosahedral symmetry. In order to have both the icosahedral symmetry and weights that are not constrained, it is necessary to replace the spherical harmonics by a different set of functions, which we denote by  $T_{l,n}(\theta, \phi)$ . The two key properties of the  $T_{l,n}$ 's are that every weighted sum of  $T_{l,n}$ 's is a function that has icosahedral symmetry and every smooth icosahedrally symmetric function can be expanded as a weighted sum of  $T_{l,n}$ 's. The  $T_{l,n}$ 's are called

*icosahedral harmonics*. This terminology is somewhat different from that used for spherical harmonics, since only the lowest-order spherical harmonic actually has the symmetry of the sphere while every icosahedral harmonic has the symmetry of the icosahedron.

Each icosahedral harmonic is a linear combination of ordinary spherical harmonics, denoted by  $Y_{l,m}$ , of the same order:

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

In Ref. 4 the authors have derived explicit expressions for the  $b_{l,n,m}$ 's for all icosahedral harmonics, as well as the simpler *tetrahedral harmonics* and *octahedral harmonics*. Since the symmetries of the dodecahedron are the same as the symmetries of the icosahedron and likewise for the cube and the octahedron, these results cover all of the Platonic solids.

The first few (unnormalized) icosahedral harmonics are

$$T_{0,0}(\theta, \phi) = 1$$

$$T_{6,0}(\theta, \phi) = 3960P_{6,0}(\cos \theta) - P_{6,5}(\cos \theta)\cos 5\phi$$

$$T_{10,0}(\theta, \phi) = 896313600P_{10,0}(\cos \theta) \\ + 27360P_{10,5}(\cos \theta)\cos 5\phi \\ + P_{10,10}(\cos \theta)\cos 10\phi$$

$$T_{12,0}(\theta, \phi) = 14250297600P_{12,0}(\cos \theta) \\ - 55440P_{12,5}(\cos \theta)\cos 5\phi \\ + P_{12,10}(\cos \theta)\cos 10\phi$$

where  $P_{l,m}$  are associated Legendre functions. Except for  $T_{0,0}$ , the fact that these functions obey all of the 60 rotational symmetries in the icosahedral group is not evident.

<sup>a)</sup>Author to whom correspondence should be addressed: 1285 Electrical Engineering Building, Purdue University, West Lafayette, Indiana 47907-1285; e-mail: doerschu@ecn.purdue.edu.

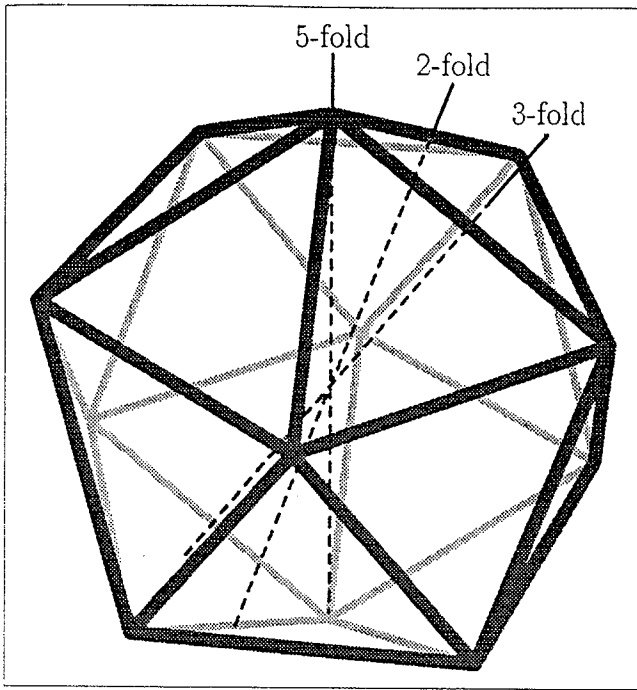


Figure 1. An icosahedron and three of its axes of rotational symmetry. One axis of each type of rotational symmetry—fivefold, threefold, and twofold—is shown. The icosahedron is constructed from 20 identical equilateral triangles. Fivefold axes pierce the surface of the icosahedron at vertices where five triangles meet, threefold axes pierce the surface in the center of triangles, and twofold axes pierce the surface at the midpoint of the edge shared by two adjacent triangles.

## II. METHOD

Our coordinate system is that used by Altman,<sup>5</sup> where the  $z$  axis passes through two opposite vertices and the  $xz$  plane includes one edge of the icosahedron. Figure 1 shows an icosahedron with three of its symmetry axes.

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

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

- (1) The rotational operation is more easily expressed in Cartesian coordinates than spherical coordinates (a linear transformation versus complicated angular relations).
- (2) Most symbolic computation systems, including Mathematica, have much better facilities for computing with polynomials than for computing with trigonometric functions. Specifically, the manipulation of polynomi-

als (collecting terms, expansion and factorization, etc.) is fairly mechanical and the behavior of the output is predictable while, on the other hand, the manipulation of trigonometric functions requires the use of possibly many trigonometric identities and the sequence of their application may greatly change the appearance of the output. For these reasons, symbolic computation software rarely arrives at the simplest form of a trigonometric expression without the intelligent interference of the user.

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

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

$$S = \begin{bmatrix} \cos \frac{2\pi}{5} & -\sin \frac{2\pi}{5} & 0 \\ \sin \frac{2\pi}{5} & \cos \frac{2\pi}{5} & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$U = \begin{bmatrix} \frac{1}{\sqrt{5}} & 0 & \frac{2}{\sqrt{5}} \\ 0 & 1 & 0 \\ -\frac{2}{\sqrt{5}} & 0 & \frac{1}{\sqrt{5}} \end{bmatrix},$$

$$P = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Table I tabulates the first 30 rotations of the icosahedral group in terms of  $S$  and  $T = USU^{-1}$ . The second 30 rotations are related to the first 30 rotations by  $R_{i+30} = PR_i$  for  $i = 0, 1, \dots, 29$ .

We illustrate the verification procedure by demonstrating that  $T_{6,0}(\theta, \phi)$  is invariant under the operation  $U$ . The demonstration requires the following steps:

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

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

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

$$P_{6,5}(\cos \theta) = -10395 \cos \theta \sin^5 \theta.$$

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

Table I. The first 30 icosahedral rotations in terms of  $S$  and  $T$ .

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

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

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

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

• Apply the following transformation rules sequentially:

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

The result is that

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

(3) Expand the polynomial obtained in step 2 [Eq. (2)] and collect terms.

(4) If the polynomial obtained in step 3 is equal to that obtained in step 1 [Eq. (1)], then the symmetry is verified. In comparing the polynomials, it may be necessary to use the constraint that  $x$ ,  $y$ , and  $z$  lie on the surface of the unit sphere, i.e.,  $x^2 + y^2 + z^2 = 1$ . That is, if the difference of the polynomials is zero or if it contains a factor of  $x^2 + y^2 + z^2 - 1$ , then the two polynomials are equal on the surface of the unit sphere.

In the case of  $T_{6,0}$ , Eq. (2), after expansion, is exactly the same as Eq. (1).

Exactly the same idea can be applied to verify the invariance of a harmonic function under operations  $S$  and  $P$ . A set of transformation rules written in Mathematica scripts, which perform Steps 1–4, is given in the following section.

### III. MATHEMATICA PROGRAMS FOR VERIFYING ICOSAHEDRAL HARMONICS

(\*)

Verify the icosahedral symmetry of  $T[\theta, \phi]$ , a weighted sum of spherical harmonics. The coordinate system for the symmetries is the system defined in the text.

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

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

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

The result is that

\*)

<<Algebra 'Trigonometry'

(\* step 1: Transform the harmonics into polynomials in  
{Sin[phi], Cos[phi], Sin[theta], Cos[theta]};  
Note that ComplexToTrig or rule0 may not be necessary  
depending on how you write the spherical harmonics.  
Command:  
Expand[TrigReduce[ComplexToTrig[Simplify[T[theta,phi]]/.rule0]]].

\*)

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

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

\*)

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

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

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

(\* step 3: Now apply one of the transformations from which  
all of the transformations in the icosahedral group  
can be constructed;  
To verify symmetry under U, use rule4a;  
To verify symmetry under S, use rule4b;  
To verify symmetry under P, use rule4c.  
Command:  
Expand[%/rule4a].

\*)

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

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

\*)

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

#### IV. DISCUSSION

Using the methods described in this article, we have verified the symmetry properties of the icosahedral harmonics derived in Ref. 4 up to order  $l=44$ , including the so-called "second set" icosahedral harmonics  $T_{30,1}$ ,  $T_{36,1}$ ,  $T_{40,1}$  and  $T_{42,1}$  which have not appeared previously in the literature. The polynomials corresponding to these harmonics have a few hundred terms and it would be a daunting task to verify their symmetries exactly without the aid of a symbolic computing system. Computers have long been used to verify theorist's ideas numerically. However, it is only in recent years that inexpensive and easy-to-use computer systems have been available to aid in the *symbolic and exact* development of theory.

#### ACKNOWLEDGMENTS

We would like to thank Professor John E. Johnson (Department of Biological Sciences, Purdue University) for draw-

ing our attention to icosahedral harmonics and for his enthusiastic interest in the results. This work was supported by U.S. National Science Foundation Grant No. MIP-9110919, a Purdue Research Foundation Research Grant, and a Whirlpool Faculty Fellowship.

#### REFERENCES

1. L. Liljas, *Int. J. Biol. Macromol.* **13**, 273 (1991).
2. W. Kratschmer, L. D. Lamb, K. Fostiropoulos, and D. R. Huffman, *Nature (London)*, **347**, 354 (1990).
3. L. Elcoro, J. M. Perez-Mato, and G. Madariaga, *Acta Cryst., A* **50**, 182 (1994).
4. Y. Zheng and P. C. Doerschuk, Technical Report No. TR-EE-94-34, School of Electrical Engineering, Purdue University, October 1994 (unpublished).
5. S. L. Altmann, *Proceedings of the Cambridge Philosophical Society* **53**, 343 (1957).