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Crystallographic and Quasicrystallographic Lattices from the Finite Groups of Quaternions

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Quaternions are ordered quadruples of four numbers subject to specified rules of addition and multiplication, which can represent points in four-dimensional (4D) space and which form finite groups under multiplication isomorphic to polyhedral groups. Projection of the 8 quaternions of the dihedral group $\boldsymbol{D_{2h}}$, with only two-fold symmetry, into 3D space provides a basis for crystal lattices up to orthorhombic symmetry ($a \neq b \neq c$). Addition of three-fold symmetry to $\boldsymbol{D_{2h}}$ gives the tetrahedral group $\boldsymbol{T_d}$ with 24 quaternions, whose projection into 3D space provides a basis for more symmetrical crystal lattices including the cubic lattice ($a = b = c$). Addition of five fold symmetry to $\boldsymbol{T_d}$ gives the icosahedral group $\boldsymbol{I_h}$ with 120 quaternions, whose projection into 3D space introduces the $\sqrt{5}$ irrationality and thus cannot provide the basis for a 3D crystal lattice. However, this projection of $\boldsymbol{I_h}$ can provide a basis for a 6D lattice which can be divided into two orthogonal 3D subspaces, one representing rational coordinates and the other representing coordinates containing the $\sqrt{5}$ irrationality similar to some standard models for icosahedral quasicrystals.

INTRODUCTION

Shortly after the discovery of icosahedral quasicrystals in rapidly cooled Al/Mn alloys,[1] the description of quasicrystal structure with a long-range quasiperiodic translational order and lone-range orientation order began to receive considerable attention. In this connection, quasicrystals represent a new type of incommensurate crystal structure whose Fourier transform consists of a δ function as for periodic crystals but the point symmetries are incompatible with traditional crystallography. An important theoretical approach for the study of quasicrystal structure involves projection from a high-dimensional lattice into three dimensions to obtain the quasicrystal lattice.[2–6] The five-fold symmetry of icosahedral quasicrystals can be related to the five-fold symmetry of Penrose tiling.[7] In fact the theoretical Fourier transform of a Penrose tiling is found to resemble the experimentally observed diffractions of icosahedral quasicrystals.[8]

The use of Penrose tiling to describe quasicrystal structures as well as some of the other theoretical approaches starts with a six-dimensional (6D) space, which is divided into two orthogonal three-dimensional (3D) subspaces, namely the physical or parallel space $E_{\|}$ and the pseudo or perpendicular space $E_{\perp}$. The projection of a 6D cubic lattice onto the physical space, which is a 3D hyperplane in the 6D space, gives the typical 3D Penrose tiling consisting of prolate and oblate rhombohedra. The ratio between volumes of the two kinds of rhombohedra equals the golden ratio $\tau = \frac{1}{2}(1 + \sqrt{5})$.

A more recent approach to the study of icosahedral quasicrystals has been developed by Moody and Patera.[9] Their work makes use of the root lattice E_8, arising from Lie group theory,[10] and the icosian ring, found in the quaternions with coefficients in $\mathcal{Q}(\sqrt{5})$, to interpret the description of 3D quasicrystals in double dimension (6D). This paper uses the ideas of Moody and Patera[9] to show how quaternions can be used to represent both ordinary crystal lattices and the icosahedral quasicrystal lattice. In this connection classical quaternion theory[11] is examined in light of the symmetries of both crystallography and quasicrystallography.

FINITE GROUPS OF QUATERNIONS

A real quaternion is defined to be an ordered quadruple of four real numbers (w, x, y, z) subject to the following rules of addition and multiplication where $\boldsymbol{q} = (w, x, y, z)$ and $\boldsymbol{q}' = (w', x', y', z')$:

$$\boldsymbol{q} + \boldsymbol{q}' = (w+w', x+x', y+y', z+z') \tag{1a}$$

$$\begin{aligned}\boldsymbol{q}\boldsymbol{q}' = (&ww' - xx' - yy' - zz', wx' + xw' + yz' - zy', \\ &wy' - xz' + yw' + zx', wz' + xy' - yx' + zw') .\end{aligned} \tag{1b}$$

The quaternions thus form a ring which meets the mathematical requirements for a non-commutative field. The subring of the type $(w, 0, 0, 0)$ is isomorphic with the field of real numbers and the subring of the type $(w, x, 0, 0)$ (or, $(w, 0, y, 0)$ or $(w, 0, 0, z)$ is isomorphic with the complex numbers $a + bi$.

The last three elements of a quaternion (w, x, y, z) can be regarded as the Cartesian coordinates of a 3D vector $\boldsymbol{v}$ so that equation (1b) becomes

$$\boldsymbol{qq'} = (w, \boldsymbol{v})(w', \boldsymbol{v'}) = (ww' - \boldsymbol{v} \cdot \boldsymbol{v'}, w\boldsymbol{v'} + w'\boldsymbol{v} + \boldsymbol{v} \times \boldsymbol{v'}) \tag{2}$$

where $\boldsymbol{v} \cdot \boldsymbol{v'}$ and $\boldsymbol{v} \times \boldsymbol{v'}$ are the standard dot and cross products, respectively. Furthermore, for quaternions of the type $(0, x, y, z)$, which are called the *imaginary prime* and correspond to 3D vectors, the multiplication process (Eq. (2)) with w and w' set to zero reduces to the standard vector cross product $\boldsymbol{v} \times \boldsymbol{v'}$ and is anticommutative, *i.e.* $\boldsymbol{v} \times \boldsymbol{v'} = -\boldsymbol{v} \times \boldsymbol{v}$. Anticommutative multiplication is also a property of Lie groups[10] and provides a link between quaternions, Lie groups, and vectors in 3D space.

The conjugate of a quaternion $\boldsymbol{q} = (w, x, y, z)$ is defined as $\overline{\boldsymbol{q}} = (w, -x, -y, -z)$. The product of a quaternion with its conjugate is a scalar positive number called its *norm* $|\boldsymbol{q}|$, *i.e.*

$$|\boldsymbol{q}| = \boldsymbol{q}\overline{\boldsymbol{q}} = \overline{\boldsymbol{q}}\boldsymbol{q} = (w, x, y, z)(w, -x, -y, -z) = (w^2 + x^2 + y^2 + z^2, 0, 0, 0) \tag{3}$$

Furthermore, since $|\boldsymbol{q}| \neq 0$ if $\boldsymbol{q} \neq 0$, the inverse of any quaternion $\boldsymbol{q}^{-1}$ can be defined by $\boldsymbol{q}^{-1} = \overline{\boldsymbol{q}}/|\boldsymbol{q}|$ so that $\boldsymbol{q}^{-1}\boldsymbol{q} = \boldsymbol{q}\boldsymbol{q}^{-1} = 1$ for all $\boldsymbol{q} \neq 0$. Thus every nonzero quaternion has a multiplicative inverse, namely its conjugate multiplied by the scalar inverse of its norm.

Quaternions with a norm of unity can be called *unit quaternions*. The unit quaternions form a multiplicative group, conveniently designated as Q. Consider a unit quaternion $\boldsymbol{p}$ of the type $\boldsymbol{p} = (\cos\alpha, \sin\alpha, 0, 0)$ and a general quaternion $\boldsymbol{q} = (w, x, y, z)$ representing a vector from the origin $(0, 0, 0, 0)$ to a point (w, x, y, z) in 4D space. The product $\boldsymbol{pq}$ is a double rotation of $\boldsymbol{q}$ by an angle α in the (w, x) plane and α in the (y, z) plane and the product $\boldsymbol{qp}^{-1}$ is a double rotation of $\boldsymbol{q}$ by an angle $-\alpha$ in the (w, x) plane and α in the (y, z) plane.[11,12] The so-called *inner automorphism* $\boldsymbol{pqp}^{-1}$ is then a single rotation of angle 2α in the (y, z) plane or about the (w, x) plane corresponding to a rotation in the imaginary prime of angle 2α about the x-axis. Similarly if the unit quaternion $\boldsymbol{p}$ has the form $(\cos\alpha, \boldsymbol{v}\sin\alpha)$ where $\mathbf{v}$ is any *unit* vector in the imaginary prime, the inner automorphism $\boldsymbol{pqp}^{-1}$ is also a rotation in the imaginary prime of angle 2α about the axis of the unit vector $\mathbf{v}$ corresponding to the most general rotation in the imaginary prime. This leads to a homomorphic mapping of the group Q on the 3D rotation group $\mathscr{R}_3$ with the element $(\cos\alpha, \boldsymbol{v}\sin\alpha)$ of Q corresponding to the rotation of angle 2α about the axis of the vector $\boldsymbol{v}$ in 3D space. This mapping is 2 : 1 with the structure $Q = C_2 \times \mathscr{R}_3$ with the kernel C_2 being the subgroup of Q consisting of the scalar elements ± 1. Every rotation in 3D space thus corresponds to two opposite elements $\pm\boldsymbol{p}$ of Q.

Certain finite subgroups $\boldsymbol{G}$ of the unit quaternion group Q correspond to the symmetry point groups of polyhedra including the regular polyhedra.[11] However, because of the 2 : 1 nature of the mapping $Q = C_2 \times \mathscr{R}_3$ every finite subgroup G of $\mathscr{R}_3$ has an image in Q twice its order since every element p of $\mathscr{R}_3$ has two images $\pm\boldsymbol{p}$ in Q. Every finite subgroup $\boldsymbol{G}$ of Q is thus either 2 : 1 homomorphic or isomorphic to a finite subgroup G of $\mathscr{R}_3$ and in the latter case consists of only one of the two images in Q of every element of G so that the total image of G in Q has the form $C_2 \times G$ where $C_2 = \{\pm 1\}$. However, if G contains a 180° rotation, it cannot have an isomorphic image in Q for the two images in Q of the 180° rotation about a unit vector $\boldsymbol{v}$ are $(0, \pm\boldsymbol{v})$ and as the cube of each of these is the other, every subgroup of Q that contains either of them contains the other. Since the only finite subgroups of $\mathscr{R}_3$ containing *no* 180° rotations are C_n for odd values of n, all the finite groups G have a unique image in Q, namely its total image $\boldsymbol{G}$ with the mapping $\boldsymbol{G} \to G$ being 2 : 1 with kernel C_2.

The following finite point groups can be considered in this manner.

(1) The pure rotation groups $\boldsymbol{C_n}$: The quaternions $(\cos 2r\pi/n, \boldsymbol{v}\sin 2r\pi/n)$ form a cyclic group of order n, which is the image of the multiplicative group of the nth roots of unity in the isomorphism between the quaternions $(a, b\mathbf{v})$ and the complex numbers $a + ib$ which is the pure rotation group $\boldsymbol{C_n}$. For odd values of n this group consists of one of the two images of each element of the subgroup C_n of $\mathscr{R}_3$ with the same axis $\mathbf{v}$. However, for even values of n, it consists of both images of each element of $C_{n/2}$ of $\mathscr{R}_3$. The corresponding set of points are the vertices of a regular n-gon with one vertex at the point 1.

(2) The dihedral groups $\boldsymbol{D_{nh}}$: The image $\boldsymbol{D_{nh}}$ in Q of the dihedral subgroup D_{nh} of $\mathscr{R}_3$ is of order $4n$ and has a subgroup $\boldsymbol{C_{2n}}$ which is the image of the subgroup C_{2n} in D_{nh}. If the principal axis of $\boldsymbol{C_{2n}}$ is the z-axis, then the elements of $\boldsymbol{C_{2n}}$ have the form $(\cos r\pi/n, 0, 0, \sin r\pi/n)$ where $r = 0, \ldots, 2n - 1$. If the twofold axes of D_{nh} are $y = x \tan r\pi/n$, $z = 0$, then the remaining elements of $\boldsymbol{D_{nh}}$ have the form $(0, \cos r\pi/n, \sin r\pi/n, 0)$ so that the set of points of D_{nh} are the set of vertices of a prism where the two parallel faces are two regular $2n$-gons. Of particular importance is the image $\boldsymbol{D_{2h}}$ of the dihedral group D_{2h} consisting of the eight principal unit quaternions $(\pm 1, 0, 0, 0)$, $(0, \pm 1, 0, 0)$, $(0, 0, \pm 1, 0)$, and $(0, 0, 0, \pm 1)$; this group is sometimes known as the *quaternion group*.[13]

(3) The tetrahedral group $\boldsymbol{T_d}$: The image $\boldsymbol{T_d}$ in Q of the tetrahedral subgroup T_d of $\mathscr{R}_3$ is of order 24 and corresponds to the normal subgroup D_{2h} together with 16 other elements corresponding to the rotations of order 3 about the diagonals of the cube; the latter are thus of the form $\pm(\tfrac{1}{2}, \pm\tfrac{1}{2}\sqrt{3}\boldsymbol{v})$ where $\pm\mathbf{v}$ are the unit vectors $\sqrt{1/3}(\pm 1, \pm 1, \pm 1)$ along the diagonals of the cube. The elements of $\boldsymbol{T_d}$ other than those of its normal subgroup $\boldsymbol{D_{2h}}$ are the 16 quaternions $\tfrac{1}{2}(\pm 1, \pm 1, \pm 1, \pm 1)$ corresponding to the 16 vertices of the 4D analogue of a cube, namely the hypercube or tesseract. This set of quaternions $\mathscr{W}$ breaks up into two cosets of its normal subgroup $\boldsymbol{D_{2h}}$ of the form $\boldsymbol{tv}$ and $\boldsymbol{t}^2\boldsymbol{v}$ where $\boldsymbol{t} = (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$.

(4) The icosahedral group $\boldsymbol{I_h}$: The image $\boldsymbol{I_h}$ in Q of the icosahedral subgroup I_h of $\mathscr{R}_3$ has five-fold, three-fold, and two-fold axes in directions which

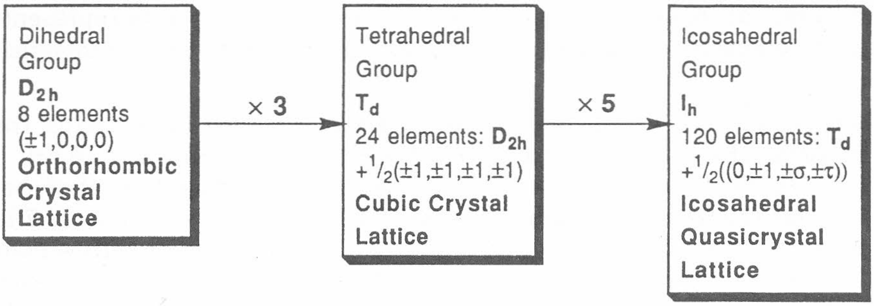

Figure 1. Crystal and quasicrystal lattices generated from the dihedral $\boldsymbol{D}_{2h}$, the tetrahedral $\boldsymbol{T}_d$, and the icosahedral $\boldsymbol{I}_h$ finite quaternion groups.

are derived by Du Val.[11] It contains the 24 elements of its tetrahedral subgroup $\boldsymbol{T}_d$ plus an additional 96 unit quaternions of the type $\frac{1}{2}((0, \pm 1, \pm\sigma, \pm\tau))$ where the double parentheses (()) denote all even permutations of the components, $\tau = \frac{1}{2}(1 + \sqrt{5})$, and $\sigma = \frac{1}{2}(1 - \sqrt{5})$ so that $\sigma + \tau = 1$ and $\sigma\tau = -1$. The 120 quaternions in $\boldsymbol{I}_h$ are sometimes called *icosians* because of their relationship to icosahedral symmetry.

The relationship between the dihedral group $\boldsymbol{D}_{2h}$, the tetrahedral group $\boldsymbol{T}_d$, and the icosahedral group $\boldsymbol{I}_h$ is considered in Figure 1. Note that ascent in symmetry from $\boldsymbol{D}_{2h}$ to $\boldsymbol{T}_d$ introduces three-fold symmetry and that ascent in symmetry from $\boldsymbol{T}_d$ to $\boldsymbol{I}_h$ introduces five-fold symmetry.

CRYSTALLOGRAPHIC AND QUASICRYSTALLOGRAPHIC LATTICES FROM FINITE QUATERNIONS GROUPS

A quaternion $\boldsymbol{q} = (w, x, y, z)$ can be considered as a point in 4D space as noted above. In addition such a quaternion can define the length and direction of a 4D vector from the origin (0, 0, 0, 0). A finite group G of quaternions with $|G|$ elements of the type $\boldsymbol{q} = (w, x, y, z)$ where w, x, y, and z are all rational numbers can be used to generate a 4D lattice consisting of all points of the type

$$\sum_{i=1}^{|G|} a_i \boldsymbol{q}_i \tag{4}$$

where each of the coefficients a_i can be any integer (positive or negative), and $\boldsymbol{q}_i$ is element i of the finite quaternion group $\boldsymbol{G}$. The standard 3D crystallographic lattices then correspond to projections of these 4D quaternionic lattices into the 3D imaginary prime where $w = 0$. The basis of such 3D crystallographic lattices consists of the projections of the 4D points represented by the $|G|$ elements of the finite quaternion group G into the 3D imaginary prime.

Let us first consider the generation of a 3D crystallographic lattice from the dihedral group D_{2h} which contains the 8 elements (±1, 0, 0, 0). (0, ±1, 0, 0), (0, 0, ±1, 0) and (0, 0, 0, ±1) as noted above. Projection of these 8 quaternions into the 3D imaginary prime where $w = 0$ gives a basis of 7 lattice points, namely the origin at (0, 0, 0) from the quaternionic lattice points (±1, 0, 0, 0) and the 6 points (±1, 0, 0), (0, ±1, 0), and (0, 0, ±1) at the centers of the faces of a cube (*i.e.* the vertices of a regular octahedron). Note that in this projection the two 4D quaternionic lattice points (±1, 0, 0, 0) become the single point (0, 0, 0) in its 3D image. The remainder of the infinite orthorhombic lattice can be generated from the 8 4D basis points of the D_{2h} dihedral quaternionic lattice or the 6 non-zero points of its projection into the 3D imaginary prime by taking all other possible combinations of positive and negative integers for the a_i coefficients (Eq. (4)). The dihedral group D_{2h} contains no symmetry elements which force the lattice distances a, b, and c in the x, y, and z directions, respectively, to be equivalent so that the orthorhombic crystal system is the highest symmetry crystal system that can be generated from the D_{2h} dihedral quaternion group. The less symmetrical monoclinic and triclinic systems can also be generated from the D_{2h} dihedral group if the x, y and z axes are no longer perpendicular.

A similar procedure can be used to generated the body-centered cubic lattice from the tetrahedral quaternionic group T_d. Again the basis of the 3D cubic lattice is obtained by projection of the 24 quaternions of T_d into the 3D imaginary prime where $w = 0$ as indicated in Table I. The remainder of the infinite cubic lattice can be generated from the 24 4D basis points of the T_d quaternionic lattice or the 14 non-zero points (*i.e.*, the 8 cube vertex points and the 6 cube face midpoints) of its projection in the the 3D imaginary prime taking all other possible combinations of positive and negative

TABLE I

The basis of the 3D cubic lattice as obtained by projection of the 4D quaternionic lattice from the tetrahedral quaternionic group T_d into the 3D imaginmary prime

Quaternionic Lattice Point Type	3D Lattice Basis Point Projection Type	Number of 3D Lattice Basis Points	Geometry of 3D Lattice Basis Points
(±1, 0, 0, 0)	(0,0,0)	1	Cube body center
(0, ±1, 0, 0) (0, 0, ±1, 0) (0, 0, 0, ±1)	(±1, 0, 0) (0, ±1, 0) (0, 0, ±1)	6	Cube face centres
½(±1, ±1, ±1, ±1)	½(±1, ±1, ±1)	8	Cube vertices

integers for the a_i coefficients (Eq. (4)). The three-fold symmetry of the T_d tetrahedral group forces the lattice distance a, b and c in the x, y, and z directions, respectively, to be equal so that the tetrahedral quaternionic group $\boldsymbol{T_d}$ generates the cubic crystal system.

An analogous procedure for the generation of a 3D crystallographic lattice from the icosahedral quaternionic group $\boldsymbol{I_h}$ (the icosians) is not possible since among the 120 quaternions in $\boldsymbol{I_h}$ the 96 quaternions of the type ½((0, ±1, ±σ, ±τ) contain the $\sqrt{5}$ irrationality. Projection of these 96 irrational quaternions into the 3D imaginary prime would give lattice point images of two types containing this $\sqrt{5}$ irrationality, namely (±σ, ±τ, ±1) and (0, ±σ, ±τ) and all of their even permutations corresponding to a total of 24 + 12 = 36 lattice points. The persistent occurrence of this $\sqrt{5}$ irrationality is the reason why regular icosahedra cannot be packed into three-dimensional space so that icosahedral symmetry is not one of the crystallographic symmetries.

Figure 1 indicates clearly the effect of ascent in symmetry in the finite 4D quaternion groups on the type of lattice generated by their corresponding projections into the 3D imaginary prime. The 3D lattice obtained from the dihedral quaternion group $\boldsymbol{D_{2h}}$ does not have symmetry-imposed equality in the three crystallographic directions and thus requires no symmetry higher than orthorhombic. Introduction of 3-fold symmetry in going from $\boldsymbol{D_{2h}}$ to $\boldsymbol{T_d}$ imposes equality in the three crystallographic directions and can lead to the maximum cubic crystallographic symmetry. Subsequent addition of 5-fold symmetry in going from $\boldsymbol{T_d}$ to $\boldsymbol{I_h}$ introduces the $\sqrt{5}$ irrationality thereby making a true crystallographic lattice no longer possible. This results in icosahedral quasicrystals described by a 6D lattice, which can represent rational and irrational components of the type $a + a'\sqrt{5}$ in the three directions.

Quasicrystals may thus be regarded as a special type of incommensurate system, which may be described by space groups of dimension larger than three in a similar way to modulated crystal phases and incommensurate composite structures.[14] In the case of icosahedral quasi-crystals the above model based on the icosahedral quaternion group $\boldsymbol{I_h}$ fits well into the idea of 6D space groups. Each of the three standard coordinates, namely x, y, and z, corresponds to two coordinates in 6D space, namelly a rational and an irrational coordinate corresponding to the rational and irrational portions of variables of the form $a + a'\sqrt{5}$ where a and a' are integers. Projection of the lattice points of this 6D space of icosahedral symmetry into conventional 3D space leads to the isocahedral quasicrystal lattice.

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SAŽETAK

Kristalografske i kvazikristalografske rešetke dobijene uz pomoć konačnih grupa kvaterniona

R. Bruce King

Kvaternioni su uređene četvorke brojeva za koje vrijede posebna pravila zbrajanja i množenja i koje se mogu predstaviti točkama u 4-dimenzijskom (4D) prostoru. Kvaternioni grade konačne multiplikativne grupe izomorfne poliedarskim grupama. Projekcija osam kvaterniona diedarske grupe $\boldsymbol{D_{2h}}$ za 3D prostor osigurava bazu za kristalne rešetke sve do ortorombske simetrije ($a \neq b \neq c$). Dodavanjem osi simetrije trećeg reda grupi $\boldsymbol{D_{2h}}$ dobiva se tetraedarska grupa $\boldsymbol{T_d}$ sa 24 kvaterniona, čijim se projiciranjem u 3D prostor dobiva baza za kristalne rešetke više simetrije, uključivo i kubične rešetke ($a = b = c$). Dodavanjem grupi $\boldsymbol{T_d}$ osi petog reda dobiva se ikosaedarska grupa I_h sa 120 kvaterniona, čija projekcija na 3D prostor uvodi iracionalni faktor $\sqrt{5}$ pa se ne dobiva baza za 3D rešetke. Ipak, projekcija $\boldsymbol{I_h}$ osigurava bazu za 6D rešetku koja se dade podijeliti na dva međusobno okomita 3D potprostora, od kojih jedan sadržava racionalne koordinate, a drugi koordinate s faktorom $\sqrt{5}$, kao u nekim standardnim modelima za ikosaedarske kvazikristale.