Rudimentary quasicrystallography: The icosahedral and decagonal reciprocal lattices

Daniel S. Rokhsar and N. David Mermin
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501

David C. Wright
David Rittenhouse Laboratory, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6396
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We prove that there are precisely three distinct icosahedrally symmetric lattices in three dimensions that are integral linear combinations of six vectors. By lattice, we mean a set of vectors which is closed under addition and subtraction. These three lattices can be represented as projections of the six-dimensional simple, face-centered, and body-centered hypercubic lattices into three dimensions. We also show that there is only one distinct three-dimensional decagonal lattice that is integrally spanned by five vectors.

I. INTRODUCTION

Quasicrystals such as the icosahedral[1] and decagonal[2] phases of aluminum alloys cannot have the real-space symmetry of a Bravais lattice of translations, because their diffraction patterns have noncrystallographic point-group symmetries. One therefore cannot directly apply the conventional classification scheme for ordinary crystals, in terms of the real-space Bravais lattices and the further subclassification into space groups.

In Fourier space (k space), however, quasicrystals and ordinary crystals are less dissimilar. If a quasicrystal diffraction pattern contains spots corresponding to two wave vectors, one in general finds spots corresponding to the sum and difference of those wave vectors, unless such spots are forbidden by symmetry in a manner analogous to the vanishing of geometric structure factors in ordinary crystals. Quasicrystals, like ordinary crystals, can thus be indexed by a set of wave vectors that is closed under addition (sums *and* differences). For an ordinary crystal this set is just the reciprocal lattice, the set of wave vectors of plane waves with the periodicity of the direct lattice. For a quasicrystal this set still forms a lattice (in the sense that it is closed under addition),[3] but unlike an ordinary reciprocal lattice a quasicrystalline reciprocal lattice has no minimum distance between points, and the corresponding set of plane waves has no common real-space period. Although quasicrystalline wave vectors form a dense set in k space, a quasicrystalline diffraction pattern admits a countable indexing, unlike the diffraction pattern of an amorphous material.

The crystallographic classification of quasicrystals must therefore take place in reciprocal space. The first step is to determine the distinct reciprocal lattices (equivalent to specifying the real-space Bravais lattices when the point group is crystallographic). For each such reciprocal lattice, the second step is to enumerate the possible families of phase factors that can be associated with those wave vectors (equivalent in the crystallographic case to determining the space groups belonging to a given real-space Bravais lattice). In this paper we address the first half of the problem: the cataloging of the allowable icosahedral and decagonal reciprocal lattices. A second paper will discuss in detail the quasicrystallographic space groups.[4]

Although the literature contains conflicting assertions about the number of icosahedral lattices, particular attention has been paid to three of them.[5] These are constructed by viewing icosahedral lattices as projections of six-dimensional cubic Bravais lattices into three-dimensional space.[6] The three reciprocal lattices then appear as projections of the six-dimensional simple, face-centered, and body-centered cubic lattices.

We are unaware, however, of any argument that these are the only possibilities. One of the major aims of this paper is to provide the justification for this conclusion. Our proof requires not only considerations of icosahedral geometry, but also some basic number theoretic properties of the golden mean.

We also give the proof[7] that there are, in fact, only three cubic Bravais lattices in six dimensions, to make contact with the now conventional way of looking at icosahedral reciprocal lattices as projections. We stress, however, that our derivation of the three icosahedral reciprocal lattices is independent of the projection method, and entirely based in ordinary three-dimensional k space. In the case of structures with decagonal symmetry we show that there is only one possible reciprocal lattice.[8]

Our paper is organized as follows. In Sec. II we give a definition of reciprocal lattice which is broad enough to include sets of wave vectors with noncrystallographic symmetries and which reduces to the conventional one when the point group is crystallographic. Several further definitions are stated, and two useful lemmas are proved, one geometric and relevant to any reciprocal lattice, and the other number theoretic and only relevant to reciprocal lattices in which the golden mean plays a prominent role. In Secs. III and IV we use the results of Sec. II to determine the icosahedral and decagonal reciprocal lattices. In Appendix A we show that there are three cubic reciprocal lattices in three or more dimensions (except in four dimensions where there are just two). This discussion is not required for any of the earlier analysis, but is included to link our results to the projection method. In Appendix B we show that there is just one pentagonal reciprocal lattice, and note that it possesses an unusual symmetry.

Readers not interested in the details of our argument should simply read the definition of a reciprocal lattice at the beginning of Sec. II and note that the results of our analysis are as follows. When the point group is the 120-element icosahedral group with inversion, Y_h ($\overline{5}\,\overline{3}\,2/m$), there are just three distinct reciprocal lattices. The wave vectors in each can be expressed as linear combinations with integral coefficients of six "vertex vectors" of equal length along the six fivefold axes of Y_h. In the primitive icosahedral lattice all vectors with integral coefficients appear, in the body-centered icosahedral lattice all coefficients of a given vector have the same parity (i.e., either all even or all odd), and in the face-centered icosahedral lattice the sum of the coefficients of a given vector is even. Other possibilities that come to mind (e.g., all integral linear combinations of six independent "edge vectors" directed along six appropriately chosen twofold axes, or "face vectors" directed along threefold axes) are equivalent to one of these three. When the point group is one of the decagonal groups C_{10h} or D_{10h} ($10/m$ or $10/mmm$) there is only one distinct reciprocal lattice, consisting of all integral linear combinations of a vector along the tenfold axis and four vectors of equal length spaced 72° apart, in the plane perpendicular to the tenfold axis.

If one thinks of the wave vectors in k space as specifying k-space translations, then the icosahedral and decagonal reciprocal lattices are subgroups of the full three-dimensional Euclidean group. Yet one never encounters them in enumerations of those subgroups. The reason is that when there is a natural notion of continuity, the usual algebraic definition of a group is often augmented to define a *topological* group, by requiring the limit of any sequence of group operations (here k-space translations) to be also in the group. A noncrystallographic reciprocal lattice lacks this property; for example, an icosahedral such a lattice of wave-vectors forms a dense set in k space, so that its topological closure is the entire three-dimensional translation group.

The omission of these subgroups is in some ways peculiar. Had one applied the same requirement to algebraic studies of the real line, one would have ruled out the entire subject of quadratic number fields.[9] Nature has proven quite unambiguous in distinguishing between the very vivid quasicrystalline diffraction patterns based on dense but countable sets in k space, and the continuous diffraction patterns produced by structures with no positional symmetry whatever.

II. DEFINITIONS AND USEFUL GENERAL RESULTS

We call a set of vectors *integrally independent* if a linear combination with integral coefficients vanishes only when all the coefficients vanish. A given set $\mathbf{S}$ of vectors is said to be *generated* by vectors $\mathbf{v}^{(1)},\mathbf{v}^{(2)},\mathbf{v}^{(3)},\ldots,\mathbf{v}^{(n)}$ if every vector in $\mathbf{S}$ is an integral linear combination of the $\mathbf{v}^{(j)}$. The *rank*[10] of $\mathbf{S}$ is the number of integrally independent vectors in its generating set. Note that $\mathbf{S}$ need not necessarily contain *all* integral linear combinations of the generating set; if it does, $\mathbf{S}$ is said to be *primitively generated* by the generating set.

By a *lattice,* we mean a set of vectors closed under addition and subtraction (an additive group). For a given point group, we define a *reciprocal lattice* in d dimensions to be a set $\mathbf{S}$ of wave vectors such that (1) $\mathbf{S}$ is lattice, (2) $\mathbf{S}$ is closed under all point group operations, and (3) the rank of S is the smallest rank greater than or equal to d compatible with the point-group symmetry. Two reciprocal lattices are equivalent if they differ only by a scale transformation and/or rotation. Condition (1) implies that the point group of a reciprocal lattice, the "Laue group" of the diffraction pattern, always contains the inversion operation.

The smallest rank referred to in (3) we call the *indexing dimension* of the point group. A *crystallographic* point group is one whose indexing dimension is equal to the spatial dimension d. As noted below, the indexing dimension of the icosahedral Laue group Y_h is six; for the decagonal Laue groups C_{10h} and D_{10h} it is five.

Stipulation (3) is included to ensure that our definition leads only to the fourteen three-dimensional Bravais lattices when the point groups are crystallographic. Without it an arbitrary set of vectors, when symmetrized under an arbitrary point group, would yield an admissible reciprocal lattice. Note that the diffraction patterns of incommensurate crystals with crystallographic point groups violate condition (3), and therefore require a less restrictive definition of reciprocal lattice. This is the feature of icosahedral and decagonal quasicrystals that distinguishes them from other incommensurate structures.

We conclude this section with two elementary lemmas, one geometric and one algebraic, that are important for the analysis of both icosahedral and decagonal reciprocal lattices.

A. A geometric lemma

Suppose $\mathbf{S}$ is a lattice generated by the D integrally independent vectors $\mathbf{b}^{(1)},\mathbf{b}^{(2)},\ldots,\mathbf{b}^{(D)}$, so that any vector $\mathbf{k}$ in $\mathbf{S}$ can be expressed as

$$\mathbf{k}=\sum_{i=1}^{D} n_i\mathbf{b}^{(i)} , \tag{2.1}$$

with integral n_i. Let $\mathbf{c}^{(1)},\mathbf{c}^{(2)},\ldots,\mathbf{c}^{(D)}$ be any other D integrally independent vectors in $\mathbf{S}$. We show that $\mathbf{S}$ can be rescaled so that it is generated by (the unrescaled) $\mathbf{c}^{(1)},\mathbf{c}^{(2)},\ldots,\mathbf{c}^{(D)}$. Thus *any set of D integrally independent vectors contained in a lattice of rank D can be taken as generating vectors for a scaled version of the lattice.*[11] (As with any generating set, the indexing need not necessarily be primitive.)

This result follows directly form the definition of integral independence. Since the $\mathbf{c}^{(i)}$ are in $\mathbf{S}$ they have the form

$$\mathbf{c}^{(i)}=\sum_{j=1}^{D} M_{ij}\mathbf{b}^{(j)} , \tag{2.2}$$

where M is a matrix of integers. The $\mathbf{c}^{(i)}$ are integrally independent, so $\sum_{i=1}^{D} r_i\mathbf{c}^{(i)}$ vanishes for rational numbers r_i

if and only if the r_i are all zero. Because the $\mathbf{b}^{(j)}$ are integrally independent, this condition implies that $\sum_{i=1}^{D} r_i M_{ij}$ vanishes for all j only if the r_i vanish, which is precisely the condition that the matrix M have an inverse. We use this inverse to expand the $\mathbf{b}^{(i)}$ in terms of the $\mathbf{c}^{(j)}$,

$$\mathbf{b}^{(i)} = \sum_{j=1}^{D} [M^{-1}]_{ij} \mathbf{c}^{(j)} . \tag{2.3}$$

The elements of M^{-1} are integers divided by the determinant of M, so the vectors $\mathbf{B}^{(i)} = \det(M)\mathbf{b}^{(i)}$ can be expressed as integral linear combinations of the $\mathbf{c}^{(i)}$. If $\mathbf{S}$ is scaled up by a factor of $\det(M)$, then any vector in the rescaled $\mathbf{S}$ will be an integral linear combination of the $\mathbf{B}^{(i)}$, and therefore an integral linear combination of the $\mathbf{c}^{(i)}$.

An alternative way to state this result (without invoking a rescaling) is that the vectors in a lattice of rank D can all be written as rational linear combinations of any set of D integrally independent vectors contained in the set. We make use of this alternative formulation in Sec. IV.

B. An algebraic lemma

Our second lemma depends on certain number-theoretic properties of the golden mean τ, which we take to be $\frac{1}{2}(1+\sqrt{5}) = 2\cos(36°) = 1.618\,03\ldots$. We introduce the following additional nomenclature:

A *golden integer* is a real number of the form $n + m\tau$, where n and m are integers. We will denote golden integers by Greek letters; the term "integer" will be reserved for integers in the usual sense. Because $\sqrt{5}$ is irrational, every golden integer is given by a unique n and m. Note that since $\tau^{-1} = \tau - 1$ and $\tau^2 = 1 + \tau$, the set of golden integers is (1) closed under multiplication, and (2) invariant under a scaling by τ; i.e., multiplying the set of golden integers by τ yields the golden integers.

The following lemma is of central importance for determining the icosahedral lattices: Given a subset $\mathbf{T}$ of the golden integers which is (a) closed under addition, and (b) closed under multiplication by τ, there is a particular golden integer β such that $\mathbf{T}$ consists of *all* points of the form $(n + m\tau)\beta$, where n and m run through all ordinary integers; i.e., $\mathbf{T}$ is merely a scaled version of the golden integers.[12]

To establish this result, we first define[9] a *conjugate* for $r + s\tau$, r and s rational, by

$$(r + s\tau)^{\star} \equiv r - s\tau^{-1} = r + s - s\tau , \tag{2.4}$$

and a *norm* $N(r + s\tau)$ by

$$N(r + s\tau) \equiv |(r + s\tau)(r + s\tau)^{\star}| = |r^2 + rs - s^2| . \tag{2.5}$$

(Conjugation changes the sign of $\sqrt{5}$, just as complex conjugation changes the sign of $\sqrt{-1}$.) It follows immediately that (a) the conjugate of a product is the product of the conjugates, so that the norm of a product is the product of the norms, and (b) the norm of $r + s\tau$ vanishes if and only if r and s are both zero (since a vanishing norm would require r/s to be irrational).

Armed with these definitions we proceed as follows: Let β be an element of $\mathbf{T}$ with minimum nonzero norm. Such a β exists since the norm of any nonzero golden integer is a positive integer (though it is not unique, since the norm of any integral power of τ is unity). Since $\mathbf{T}$ is closed under addition and multiplication by τ, it is closed under multiplication by arbitrary golden integers. In particular, since $\mathbf{T}$ contains β, it therefore contains all golden integral multiples of β. We now show that $\mathbf{T}$ contains nothing else: If α is in $\mathbf{T}$, then α/β must be a golden integer.

Consider α/β, rewritten as $\alpha\beta^{\star}/(\beta\beta^{\star})$. The numerator is a golden integer while the denominator is an (ordinary) integer, so α/β can be written as $r + s\tau$ for r,s rational. Let $\gamma = n + m\tau$ be a golden integral approximant to α/β, with n and m the integers closest to r and s, respectively. Then since $|r - n|$ and $|s - m|$ do not exceed one half, we have

$$N\left[\frac{\alpha}{\beta} - \gamma\right] = |(r-n)^2 + (r-n)(s-m) - (s-m)^2| < 1 , \tag{2.6}$$

and therefore

$$N(\alpha - \beta\gamma) = N(\beta) N\left[\frac{\alpha}{\beta} - \gamma\right] < N(\beta) . \tag{2.7}$$

Since all golden integral multiples of β are in $\mathbf{T}$, so is $\alpha - \beta\gamma$. Since by assumption β has the smallest nonzero norm of any member of $\mathbf{T}$, $\alpha - \beta\gamma$ must vanish, and thus α is a golden integral multiple of β.

III. ICOSAHEDRAL RECIPROCAL LATTICES

We first note that the indexing dimension of the icosahedral group is six. Take an arbitrary vector in an icosahedral lattice, $\mathbf{S}$, and find a fivefold axis which is not orthogonal to it. Adding up the images of this vector under five successive fivefold rotations about the chosen axis yields a nonzero vector in $\mathbf{S}$ along this five-fold direction, and icosahedral symmetry requires vectors of the same length along the other fivefold axes. These six vectors are integrally independent, and the set of all integral linear combinations of them is an explicitly icosahedrally symmetric lattice. Thus the indexing dimension is six.

We choose a convenient coordinate system[13] by inscribing the icosahedron in a cube as shown in Fig. 1, orienting three orthogonal icosahedral twofold axes along the Cartesian axes $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$. We then show that one can choose an overall scale factor for an icosahedral reciprocal lattice such that (A) along the icosahedral twofold axes $\mathbf{S}$ contains precisely those vectors which are even golden integer multiples of the unit vectors along these axes (a golden integer is said to be *even* if it is twice a golden integer), and (B) a general vector in $\mathbf{S}$ can have only golden integral Cartesian coordinates. Finally, we show that vectors in $\mathbf{S}$ not on the Cartesian axes are further restricted by icosahedral symmetry, leading to just three distinct reciprocal lattices.

Consider a vector $\mathbf{w}$ in $\mathbf{S}$. If R is an icosahedral twofold rotation, then $R\mathbf{w}$ is in $\mathbf{S}$, and closure under addition

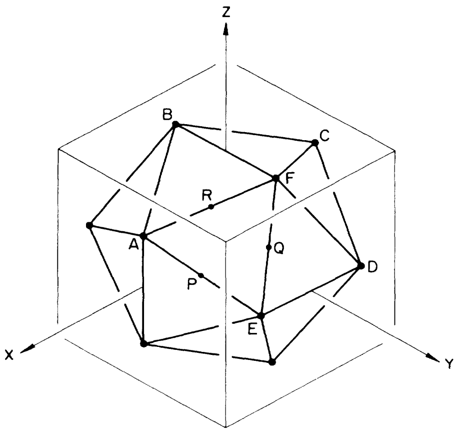

FIG. 1. An icosahedron with edges of length 2 inscribed in a cube, with the cubic axes $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ along mutually orthogonal twofold axes of Y_h. One easily verifies that the condition $BF=AF$ requires that the cube edge length is $2\tau=1+\sqrt{5}$. The points P, Q, and R have coordinates $\frac{1}{2}(1+\tau,\tau,1)$, $\frac{1}{2}(1,1+\tau,\tau)$, and $\frac{1}{2}(\tau,1,1+\tau)$, respectively. The coordinates of A, E, and F are $(\tau,0,1)$, $(1,\tau,0)$, and $(0,1,\tau)$, respectively.

requires that $\mathbf{w}+R\mathbf{w}$ is also in $\mathbf{S}$. This is simply the vector along the twofold direction whose length is twice the projection of $\mathbf{w}$ onto that axis. Thus twice the projection of any vector in $\mathbf{S}$ along a twofold axis is also contained in $\mathbf{S}$.

Consider now a vector $\mathbf{w}$ in $\mathbf{S}$ along the twofold $\hat{\mathbf{z}}$ axis. An icosahedral fivefold rotation about F (Fig. 1) takes $\mathbf{w}$ into $\frac{1}{2}|\mathbf{w}|(1,\tau-1,\tau)$, which must therefore be in the lattice, along with twice its projection onto the $\hat{\mathbf{z}}$ axis, $\tau\mathbf{w}$. By icosahedral symmetry, the sets of vectors lying along each of the fifteen twofold axes are identical in form, so *the sets of vectors along each twofold axis are closed under multiplication by* τ.

We first choose the scale of $\mathbf{S}$ so that it contains unit vectors along the twofold axes. $\mathbf{S}$ then contains not only $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$, but also τ times these three vectors. Since the indexing dimension of the icosahedral group is six, the geometric lemma of Sec. II tells us that the reciprocal lattice $\mathbf{S}$ can be rescaled so it is generated (not necessarily primitively) by the six integrally independent vectors $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, $\hat{\mathbf{z}}$, $\tau\hat{\mathbf{x}}$, $\tau\hat{\mathbf{y}}$, and $\tau\hat{\mathbf{z}}$.

The set $\mathbf{L}$ of lattice vectors lying along the twofold axis $\hat{\mathbf{z}}$ is then generated by $\hat{\mathbf{z}}$ and $\tau\hat{\mathbf{z}}$, so it contains only vectors of the form $\alpha\hat{\mathbf{z}}$, with α a golden integer. We have shown that $\mathbf{L}$ is closed under multiplication by τ; moreover, since $\mathbf{S}$ is closed under addition, so is $\mathbf{L}$. It then follows from the algebraic lemma of Sec. II that there exists a golden integer β such that $\mathbf{L}$ consists precisely of all vectors of the form $\beta\gamma\hat{\mathbf{z}}$, where γ runs through *all* golden integers.

Icosahedral symmetry requires the same structure along each of the icosahedral twofold axes, with the same scale factor β. It is convenient, as we shall see below, to choose a final scale for $\mathbf{S}$ so that $\beta=2$. Given this choice, the only vectors in $\mathbf{S}$ which lie along twofold axes are even golden integral multiples of unit vectors in these 15 twofold directions. This is result (A).

Closure under addition implies that all sums and differences of the vectors along twofold axes must also be present in $\mathbf{S}$. The sublattice of $\mathbf{S}$ consisting of just these vectors we call $\mathbf{S}_F$ (F for "face centered," as explained below). This set is explicitly icosahedrally symmetric, and is the first of the three icosahedral reciprocal lattices. We have just shown that $\mathbf{S}_F$ is *contained as a sublattice* in *any* icosahedral lattice. Note that $\mathbf{S}_F$ is invariant under multiplication by τ, a consequence of the invariance of the golden integers themselves under such a scale change.

We now consider whether an icosahedral reciprocal lattice $\mathbf{S}$ can contain additional vectors which are not in the sublattice $\mathbf{S}_F$. For any vector $\mathbf{w}$ in $\mathbf{S}$, recall that twice the projection of $\mathbf{w}$ along the twofold axes $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ must be in $\mathbf{S}$. However, we have picked the scale of $\mathbf{S}$ so that vectors along the twofold axes are even golden integral multiples of the unit vectors along the axes. Consequently the Cartesian coordinates of $\mathbf{w}$ itself must be golden integers. This is result (B): Any vector in $\mathbf{S}$ can be written as

$$(l+l'\tau)\hat{\mathbf{x}}+(m+m'\tau)\hat{\mathbf{y}}+(n+n'\tau)\hat{\mathbf{z}}\ . \tag{3.1}$$

with l, l', m, m', n, and n' integers.

Since $\mathbf{S}$ is icosahedrally symmetric, the image of a general point (3.1) under a fivefold rotation about F (Fig. 1) yields

$$\tfrac{1}{2}(-l+n+l'-m')\hat{\mathbf{x}}+\tfrac{1}{2}(m-n+l'+n')\hat{\mathbf{y}}+\tfrac{1}{2}(-l-m+m'+n')\hat{\mathbf{z}} + \tfrac{1}{2}\tau(l-m-m'+n')\hat{\mathbf{x}}+\tfrac{1}{2}\tau(l+n+l'+m')\hat{\mathbf{y}}+\tfrac{1}{2}\tau(m+n-l'+n')\hat{\mathbf{z}}\ , \tag{3.2}$$

which must be in $\mathbf{S}$ and, by (B), must have golden integral coordinates. Substituting $l'=m+m_0$, $m'=n+n_0$, and $n'=l+l_0$ into (3.2), one finds that the components of the rotated vector differ from golden integers by $\frac{1}{2}(l_0+m_0)$, $\frac{1}{2}(m_0+n_0)$, and $\frac{1}{2}(n_0+l_0)$, so that l_0, m_0, and n_0 must have the same parity, i.e., $l-n'$, $m-l'$, and $n-m'$ must all have the same parity.[13]

Note that since $\mathbf{S}$ must contain $\mathbf{S}_F$, and $\mathbf{S}$ is closed under addition, the presence (or absence) of any vector (3.1) requires the presence (or absence) of all $\mathbf{S}_F$ translates of that vector. We call two vectors *equivalent* if they differ by an $\mathbf{S}_F$ lattice vector. It is then a consequence of the parity restriction that the only allowed vectors in $\mathbf{S}$ are those which are either in $\mathbf{S}_f$ [i.e., equivalent to (0,0,0)] or equivalent to one of the three vectors

$$(1,1,1),\ (\tau,\tau,\tau),\ \text{or}\ (\tau^2,\tau^2,\tau^2)=(1,1,1)+(\tau,\tau,\tau)\ . \tag{3.3}$$

To see this, note that any vector of the form (3.1) is equivalent to one of the 64 vectors of this form with l, l', m, m', n, and n' equal to 0 or 1, since $\mathbf{S}_F$ contains all even golden integral multiples of $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$. For given l m, and n the parity restriction allows only two choices for l', m', and n', reducing the 64 vectors to 16. Of these 16, four of them (the origin and the S_F vectors along the twofold axes, P, Q, and R in Fig. 1),

$$\begin{aligned}&(0,0,0),\ (1+\tau,\ \tau,\ 1),\\ &(1,\ 1+\tau,\ \tau),\ \text{and}\ (\tau,\ 1,\ 1+\tau)\ ,\end{aligned} \tag{3.4}$$

are already in $\mathbf{S}_F$, reducing the 16 to 12. These 12 are easily enumerated and found to be either the three vectors (3.3), or equivalent to one of these three through the $\mathbf{S}_F$ translation vectors (3.4).

To consider exhaustively all possible icosahedral lattices, we need therefore only consider all ways of appending to $\mathbf{S}_F$ its translations through some or all of the three vectors (3.3). (Constructing the other icosahedral lattices in this way is analogous to constructing a body-centered cubic lattice out of interpenetrating simple cubic lattices.[14])

If any two of the three vectors (3.3) are present in the lattice, their sums produce a vector equivalent to the third. Consequently, if any are present at all, it will be either all three or just a single one.

When scaled by τ, (1,1,1) becomes (τ,τ,τ); (τ,τ,τ) becomes (τ^2,τ^2,τ^2); and (τ^2,τ^2,τ^2) becomes (τ^3,τ^3,τ^3), which is equivalent to (1,1,1), since $\tau^3=1+2\tau$ differs from 1 by an even golden integer. As we have noted, the set $\mathbf{S}_F$ is invariant under scaling by τ. Consequently, the three ways of appending to $\mathbf{S}_F$ its translations through a single one of the three vectors (3.3) yield three lattices which differ from one another only by scale factors. We call this type of lattice $\mathbf{S}_P$ (for "primitive").

$\mathbf{S}_P$ is icosahedrally symmetric, since the twenty icosahedral images of (1,1,1) are all equivalent to (1,1,1). It is invariant under scaling by τ^3, since $\mathbf{S}_F$ is invariant under scaling by τ, and each of the three vectors (3.3) is equivalent to itself after multiplication by τ^3. $\mathbf{S}_P$ is not invariant under scaling by τ, and is therefore distinct from $\mathbf{S}_F$, which is.

The only remaining case consists of appending to $\mathbf{S}_F$ its translations through all three vectors (3.3). We call this lattice $\mathbf{S}_B$ (for "body centered"). $\mathbf{S}_B$ is invariant under scaling by τ, but it is distinct from $\mathbf{S}_F$, since $\mathbf{S}_F$ contains only vectors which are integral linear combinations of lattice vectors along twofold axes, while $\mathbf{S}_B$ contains vectors which are not of this form.

Our nomenclature for these three structures is based on viewing them as projections into three dimensions of the simple (primitive), face-centered, and body-centered six-dimensional cubic Bravais lattices (see Appendix A). To make this identification, note that the projected lattices are given as linear combinations of six vectors $\mathbf{V}^{(i)}$ of equal length along the six fivefold axes with indexing that is primitive (arbitrary six integers), face centered (six integers with an even sum), and body centered (six integers of the same parity). The resulting structures are independent of the sign given these six vectors, but for comparison with the structures we have just found, it is convenient to pick them symmetrically arranged about the (111) direction (Fig. 1):

$$\begin{aligned}&\mathbf{V}^{(0)}=(\tau,0,1),\ \ \mathbf{V}^{(1)}=(\tau,0,-1)\ ,\\ &\mathbf{V}^{(2)}=(1,\tau,0),\ \ \mathbf{V}^{(3)}=(-1,\tau,0)\ ,\\ &\mathbf{V}^{(4)}=(0,1,\tau),\ \ \mathbf{V}^{(5)}=(0,-1,\tau)\ .\end{aligned} \tag{3.5}$$

Since

$$\begin{aligned}&(2\tau,0,0)=\mathbf{V}^{(0)}+\mathbf{V}^{(1)},\ \ (0,0,2)=\mathbf{V}^{(0)}-\mathbf{V}^{(1)}\ ,\\ &(0,2\tau,0)=\mathbf{V}^{(2)}+\mathbf{V}^{(3)},\ \ (2,0,0)=\mathbf{V}^{(2)}-\mathbf{V}^{(3)}\ ,\\ &(0,0,2\tau)=\mathbf{V}^{(4)}+\mathbf{V}^{(5)},\ \ (0,2,0)=\mathbf{V}^{(4)}-\mathbf{V}^{(5)}\ ,\end{aligned} \tag{3.6}$$

the vectors with even golden integral Cartesian coordinates are just the points of the form

$$\sum_{i=0}^{5} n_i\mathbf{V}^{(i)}\ , \tag{3.7}$$

with n_0+n_1, n_2+n_3, and n_4+n_5 all even. To get $\mathbf{S}_F$ we add to this set of vectors its translations through the three additional nonzero vectors in (3.4),

$$\begin{aligned}&(1+\tau,\ \tau,\ 1)=\mathbf{V}^{(0)}+\mathbf{V}^{(2)}\ ,\\ &(1,\ 1+\tau,\ \tau)=\mathbf{V}^{(2)}+\mathbf{V}^{(4)}\ ,\\ &(\tau,\ 1,\ 1+\tau)=\mathbf{V}^{(4)}+\mathbf{V}^{(0)}\ .\end{aligned} \tag{3.8}$$

This reduces the constraints on the n_i to the single constraint that the sum of all six must be even. Thus $\mathbf{S}_F$ is generated by the vectors (3.5) with face-centered indexing.

We can obtain $\mathbf{S}_P$ by adjoining to $\mathbf{S}_F$ its translation by the vector

$$(1,1,1)+(\tau,\tau,\tau)=\mathbf{V}^{(0)}+\mathbf{V}^{(2)}+\mathbf{V}^{(4)}\ . \tag{3.9}$$

This introduces all the n_i whose sum is odd and shows that $\mathbf{S}_P$ is generated by the vectors (3.5) with primitive indexing.

We can get $\mathbf{S}_B$ from $\mathbf{S}_P$ by adjoining to $\mathbf{S}_P$ its translation through the vector

$$(\tau,\tau,\tau)=\tfrac{1}{2}\sum_{i=0}^{5}\mathbf{V}^{(1)}\ , \tag{3.10}$$

which introduces half integral as well as integral coordinates. Thus $\mathbf{S}_B$, when scaled by a factor 2, is generated by the vectors (3.5) with body-centered indexing.

The three lattices can be primitively generated by the following vectors:

$$\begin{aligned}&\mathbf{S}_P\text{: }\ \mathbf{V}^{(0)},\ \mathbf{V}^{(1)},\ \mathbf{V}^{(2)},\ \mathbf{V}^{(3)},\ \mathbf{V}^{(4)},\ \text{and}\ \mathbf{V}^{(5)}\ ;\\ &S_B\text{: }\ \mathbf{V}^{(0)},\ \mathbf{V}^{(1)},\ \mathbf{V}^{(2)},\ \mathbf{V}^{(3)},\ \mathbf{V}^{(4)},\ \text{and}\ \tfrac{1}{2}(\mathbf{V}^{(0)}+\mathbf{V}^{(1)}+\mathbf{V}^{(2)}+\mathbf{V}^{(3)}+\mathbf{V}^{(4)}+\mathbf{V}^{(5)})\ ;\\ &S_F\text{: }\ (\mathbf{V}^{(0)}+\mathbf{V}^{(1)}),\ (\mathbf{V}^{(2)}+\mathbf{V}^{(3)}),\ (\mathbf{V}^{(3)}+\mathbf{V}^{(4)}),\ (\mathbf{V}^{(4)}+\mathbf{V}^{(5)}),\ \text{and}\ (\mathbf{V}^{(5)}-\mathbf{V}^{(0)})\ .\end{aligned} \tag{3.11}$$

IV. DECAGONAL RECIPROCAL LATTICES

T-phase structures have diffraction patterns[2] with one of the two decagonal Laue groups C_{10h} or D_{10h} ($10/m$ or $10/mmm$). The diffraction patterns also indicate real-space periodicity along the tenfold axis.

We first reduce the classification problem to that of classifying the two-dimensional reciprocal lattices with the decagonal symmetry groups C_{10} or D_{10} (10 or $10/mm$). Because the T phases are periodic along z, there are vectors in any three-dimensional decagonal reciprocal lattice with minimum nonzero z component. In terms of our definition of reciprocal lattices, if there were no minimum nonzero z component, then either the structure would be two-dimensional (all z components zero) or it would have to be quasiperiodic in the z direction. Either would violate provision (3) of our definition of a reciprocal lattice and, more importantly, would be inconsistent with observed T-phase diffraction patterns. We set the scale of the z axis so that the shortest nonzero z component of any vector in the lattice is unity.

Let $\mathbf{w}$ be any vector in the reciprocal lattice with unit z component, let M be a mirroring in the x-y plane, and let R be a 72° rotation about the z axis. The lattice must contain $\mathbf{w}-M\mathbf{w}$ which is just $2\hat{\mathbf{z}}$, it must contain $(1+R+R^2+R^3+R^4)\mathbf{w}$ which is just $5\hat{\mathbf{z}}$, and therefore it must contain $5\hat{\mathbf{z}}-2\hat{\mathbf{z}}-2\hat{\mathbf{z}}$ which is $\hat{\mathbf{z}}$ itself. The three-dimensional structure must therefore be a simple stacking of identical two-dimensional structures directly above each other.

We now show that there is just one planar reciprocal lattice $\mathbf{S}$ with decagonal C_{10} symmetry. Since the two-dimensional decagonal group D_{10} contains C_{10}, this is the unique planar decagonal lattice.

Let $\mathbf{b}^{(0)}$ be any vector in a planar decagonal lattice and let $\mathbf{b}^{(n)}$ be its rotations through $2\pi n/5$ about the tenfold axis (Fig. 2). Any four of these are integrally independent, and the set of all integral linear combinations of them is explicitly decagonally symmetric. Thus the indexing dimension of the two-dimensional decagonal group C_{10} is four and the indexing dimension of the three-dimensional decagonal groups is five.

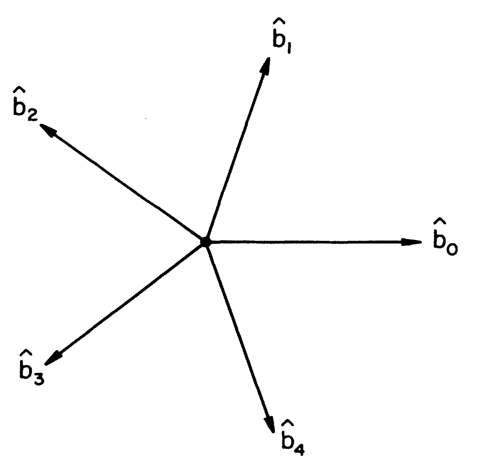

FIG. 2. Five pentagonal vectors in two dimensions.

By the geometric lemma of Sec. II we can rescale any planar decagonal reciprocal lattice $\mathbf{S}$ so that any vector $\mathbf{w}$ in $\mathbf{S}$ is an integral linear combination of these four vectors $\mathbf{b}^{(1)},\ldots,\mathbf{b}^{(4)}$. Choosing the overall scale so that the $\mathbf{b}^{(n)}$ are unit vectors, we then find that $\mathbf{w}\cdot\mathbf{w}$ is a golden integer, since $\mathbf{b}^{(n)}\cdot\mathbf{b}^{(n+1)}=\frac{1}{2}(\tau-1)$ and $\mathbf{b}^{(n)}\cdot\mathbf{b}^{(n+2)}=-\frac{1}{2}\tau$. We call $N(\mathbf{w}\cdot\mathbf{w})$ the *golden norm* of the vector $\mathbf{w}$, using the norm (2.5) defined in Sec. II.[15] Note that the golden norm of $\mathbf{w}$ vanishes only if $\mathbf{w}\cdot\mathbf{w}$ (and hence $\mathbf{w}$ itself) vanishes.

Because every nonzero vector in $\mathbf{S}$ has a positive integer for its golden norm, there must be nonzero vectors in $\mathbf{S}$ of minimal golden norm. Choose one, call it $\mathbf{a}^{(0)}$, and let $\mathbf{a}^{(n)}$ be its images under rotations by $2\pi n/5$. Because $\mathbf{a}^{(1)},\ldots,\mathbf{a}^{(4)}$ are integrally independent, it follows from the geometric lemma of Sec. II (alternative formulation) that any vector $\mathbf{w}$ in $\mathbf{S}$ can be written (without a rescaling) as a *rational* linear combination of the $\mathbf{a}^{(i)}$:

$$\mathbf{w}=\sum_{i=1}^{4} w_i\mathbf{a}^{(i)} . \tag{4.1}$$

Because the reciprocal lattice $\mathbf{S}$ contains $\mathbf{a}^{(1)},\ldots,\mathbf{a}^{(4)}$, it contains all their *integral* linear combinations. We now show that $\mathbf{S}$ contains *only* these integral linear combinations: If $\mathbf{w}$ is any vector in $\mathbf{S}$, we can use closure under addition and the presence of all integral linear combinations of the $\mathbf{a}^{(i)}$ to find another lattice vector

$$\mathbf{u}=\sum_{i=1}^{4} u_i\mathbf{a}^{(i)} , \tag{4.2}$$

where the u_i differ from the corresponding w_i by integers, and with each of the $|u_i|<1$. For each nonintegral w_i there will be two possible choices for each u_i in the interval $-1<u_i<1$. We choose those u_i that yield the smallest possible value for the quantity

$$D=\max(0,u_1,\ldots,u_4)-\min(0,u_1,\ldots,u_4) , \tag{4.3}$$

so that the u_i and zero are contained in the smallest possible interval. Note hat if a, b, c, and d are the intervals between these five points when the u_i are arranged in ascending order (Fig. 3), then this choice insures that

$$0\le a,b,c,d\le 1-(a+b+c+d) . \tag{4.4}$$

(If this inequality were not satisfied, we could make a different choice of the u_i to replace one of the intervals a,b,c,d with the interval $[1-(a+b+c+d)]$, thereby diminishing D.)

We now show that with this choice for the u_i, the vector $\mathbf{u}$ has a golden norm less than the golden norm of $\mathbf{a}^{(0)}$.

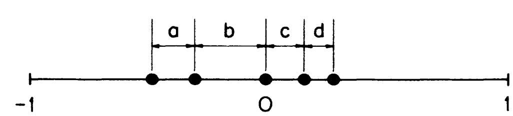

FIG. 3. The rational numbers u_0 ($\equiv 0$), $u_1,\ldots,u_4$ and the distances a, b, c, and d. For any assignment of the five u_i to the five points, the sums r and t [Eqs. (4.6) and (4.7)] are bounded by $D_{\max}$ [Eq. (4.10)].

Since $\mathbf{a}^{(0)}$ has the smallest nonzero golden norm any vector in $\mathbf{S}$ can have, $\mathbf{u}$ will then have to be zero, requiring $\mathbf{w}$ to be an *integral* linear combination of the $\mathbf{a}^{(i)}$.

To evaluate the golden norm of u, note that

$$\mathbf{u}\cdot\mathbf{u}=(r+s\tau)\mathbf{a}^{(0)}\cdot\mathbf{a}^{(0)} , \tag{4.5}$$

with

$$r=\tfrac{1}{2}[u_1^2+(u_1-u_2)^2+(u_2-u_3)^2+(u_3-u_4)^2+u_4^2] \tag{4.6}$$

and

$$s=t-r , \quad t=\tfrac{1}{2}[u_2^2+(u_2-u_4)^2+(u_4-u_1)^2+(u_1-u_3)^2+u_3^2] . \tag{4.7}$$

Since the norm of a product is the product of the norms,

$$N(\mathbf{u}\cdot\mathbf{u})=N(r+s\tau)N(\mathbf{a}^{(0)}\cdot\mathbf{a}^{(0)}) , \tag{4.8}$$

and since $\mathbf{a}^{(0)}$ has minimal golden vector norm, to show that $\mathbf{u}$ must vanish it is enough to show that $N(r+s\tau)<1$. We first separately bound r and t by unity, and then show that this yields the required bound on $N(r+s\tau)$.

Define u_0 to be zero, and define $D_{(ij)}$ to be square of the distance between points u_i and u_j, for $0\le i,j\le 4$. Equations (4.6) and (4.7) assert that

$$r=\tfrac{1}{2}[D_{(01)}+D_{(12)}+D_{(23)}+D_{(34)}+D_{(40)}] ,$$
$$t=\tfrac{1}{2}[D_{(02)}+D_{(24)}+D_{(41)}+D_{(13)}+D_{(30)}] . \tag{4.9}$$

Thus r is computed by making a round trip visit to each of the five points $u_0,\ldots,u_4$ in the order 0,1,2,3,4,0 and adding up half the squares of the lengths of each step; the visit yielding t is in the order 0,2,4,1,3,0. We show that r and t are both less than unity by showing that half the sum of the squares of the steps is less than unity for *any* such round trip visit.

Any round trip can be taken to start on the extreme left. There are then $\tfrac{1}{2}4!=12$ distinct sums, since traversing the same circuit in opposite senses yields the same sum. It is easy to show that the circuit giving the maximum sum of D's is the one that starts at the left, goes three steps to the right, back one, back another one, three more to the right, and four to the left. The sum of D's for this circuit is

$$D_{\max}=\tfrac{1}{2}[(a+b+c)^2+c^2+b^2+(b+c+d)^2+(a+b+c+d)^2] \tag{4.10}$$

(see Fig. 3). One establishes that this $D_{\max}$ exceeds any of the others by explicitly enumerating the other 11 circuits and noting that in each case the resulting sum is trivially less than $D_{\max}$, as a consequence of the non-negativity of a, b, c, and d. Since r and t correspond to particular round trips, we have established that, for a given set of u_i's (i.e., a given set of intervals a, b, c, and d), r and t are both bounded by $D_{\max}$.

We next show that $D_{\max}$ is bounded by unity for any a, b, c, and d satisfying (4.4). Setting $x=a+d$ and $y=b+c$, we write (4.10) as

$$D_{\max}=x^2+2xy+2y^2-(ad+bc) . \tag{4.11}$$

Since $ad+bc$ is non-negative we get an upper bound to $D_{\max}$ by discarding this term. With the aid of the inequality (4.4), however, we easily show that $x^2+2xy+2y^2$ is less than unity:

From (4.4) we see that a, b, c, and d are bounded above by $1-x-y$; hence x and y are bounded above by $2-2x-2y$. Consequently x and y are subject to the constraints

$$0\le x\le \tfrac{2}{3}(1-y) \text{ and } 0\le y\le \tfrac{2}{3}(1-x) . \tag{4.12}$$

For given x the quantity $x^2+2xy+2y^2$ is an increasing function of y for positive y, and is therefore bounded above by its value at the maximum y allowed by (4.12). This gives

$$D_{\max}\le \tfrac{1}{9}(5x^2-4x+8) . \tag{4.13}$$

But (4.12) confines x to the interval $0\le x\le \frac{2}{3}$, within which the polynomial (4.13) is bounded by $\frac{8}{9}$. Hence

$$0\le r,t\le D_{\max}\le \tfrac{8}{9}<1 . \tag{4.14}$$

Note, finally, that in terms of r and t the norm $N(r+s\tau)$ can be written as $|r^2+rs-s^2|=|3rt-r^2-t^2|$. Since $0\le r,t<1$, this is easily seen to be less than unity.

We have therefore established that the vector $\mathbf{u}$ must be zero. Since any lattice vector $\mathbf{w}$ differs from $\mathbf{u}$ by an integral linear combinations of the $\mathbf{a}^{(i)}$'s, we have shown that any planar decagonal reciprocal lattice can be written as the set of all integral linear combinations of $\mathbf{a}^{(1)},\ldots,\mathbf{a}^{(4)}$.[16]

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APPENDIX A: CUBIC LATTICES IN d DIMENSIONS

In three dimensions there are just three cubic Bravais lattices: simple cubic (all integral Cartesian coordinates), face-centered cubic (all integral coordinates whose sum is even), and body-centered cubic (all integral coordinates of the same parity). In five or more dimensions there are also three cubic Bravais lattices, specified by precisely the same restrictions on the coordinates. In two dimensions there is only one, and in four dimensions only two. In view of the close connection between icosahedral reciprocal lattices and cubic Bravais lattices in six dimensions it seems worth deriving this here.[7]

The argument is similar to, but considerably simpler than that we have given in the icosahedral case. Cubic symmetry requires that if $(x_1, \ldots, x_d)$ is in **T**, then so are the vectors with any permutation of these coordinates, as well as the vectors $(\pm x_1, \ldots, \pm x_d)$. Consequently if x_i is any coordinate of any vector in **S**, then there are vectors along the axes with coordinates $2x_i$. If we pick the scale so that the shortest nonzero vectors along the axes have length 2, then the general vector must have integral coordinates, and we are left with the question of how to decorate the simple cubic unit cell $0 \le x_i < 2$ with vectors whose components are all 0 or 1.

Permutation symmetry requires that if any vector with a given number of 1's is in the set then so are all the others of that type. We first note that the minimum number of 1's any nonzero vector in the decoration can have is either 2 or d (a single 1 is not allowed, since the shortest vector along any axis has length 2). If the minimum number were greater than 2 and less than d then we could reach a contradiction: The decoration would contain a vector with the minimum number of 1's whose first four components were $(1,1,1,0,\ldots)$. Permutation symmetry would then require vectors with first four components $(0,1,1,1,\ldots)$ and $(1,0,1,1,\ldots)$ (the remaining components, if any, being the same for all three). The sum of these three vectors modulo 2, however, must also be in the decoration. But, this sum is just $(0,0,1,0,\ldots)$, again with the same unspecified components, which would have two fewer 1's than the minimum number.

The d-dimensional simple cubic lattice results if the decoration is the trivial $(0,0,\ldots,0)$. If the minimum number of 1's is d, then the decoration consists entirely of $(0,0,\ldots,0)$ and $(1,1,\ldots,1)$, and we have the d-dimensional body-centered cubic lattice. If the minimum number of 1's is two, the decoration must contain all vectors with even numbers of 1's, since these can all be constructed from sums of $(1,1,0,\ldots,0)$ with its permutations. No vectors with an odd number of 1's can be present, since we would then be able to get down to a single 1 by linear combinations modulo 2. Consequently, the decoration is unique, the lattice consists of all vectors the sum of whose coordinates is even, and we have the d-dimensional face-centered cubic lattice.

In five or more dimensions it is easy to show that these three cases give distinct lattices by making a table of the numbers of nearest neighbors, next-nearest neighbors, etc., of the origin, and noting that the tables are distinct. This argument fails to distinguish the four-dimensional lattices with face-centered and body-centered indexing, and they are, in fact, easily shown to be the same:

The following four vectors,

$$\hat{e}^{(1)} \equiv (1,1,0,0),\quad \hat{e}^{(2)} \equiv (1,-1,0,0)\,,$$
$$\hat{e}^{(3)} \equiv (0,0,1,1),\quad \hat{e}^{(4)} \equiv (0,0,1,-1)\,, \tag{A1}$$

primitively generate a simple cubic lattice, since $\hat{e}^{(i)} \cdot \hat{e}^{(j)} = 2\delta_{ij}$. That lattice consists of all vectors (l,m,l',m') with $l+m$ and $l'+m'$ both even. A body-centered cubic lattice is formed by appending to this structure its translation through

$$\tfrac{1}{2}(\hat{e}^{(1)}+\hat{e}^{(2)}+\hat{e}^{(3)}+\hat{e}^{(4)}) = (1,0,1,0)\,.$$

The translated set contains all vectors with $l+m$ and $l'+m'$ both odd, and therefore the full body-centered cubic structure consists of all vectors with $l+m+l'+m'$ even. However, this is just a face-centered cubic lattice.

Finally, for completeness, we note a simple way to see the connection between the three six-dimensional cubic Bravais lattices and the three icosahedral lattices. Let $\hat{v}^{(0)}$ be a unit vector along an icosahedral fivefold axis (F in Fig. 1), and let $\hat{v}^{(1)}, \ldots, \hat{v}^{(5)}$ be the five unit vectors along the other fivefold axes (A, B, C, D, and E in Fig. 1) with positive projections on $\hat{v}^{(0)}$. Consider the following six six-dimensional vectors:

$$\frac{\sqrt{2}}{2}(\hat{v}^{(0)},-\hat{v}^{(0)}),\quad \frac{\sqrt{2}}{2}(\hat{v}^{(1)},\hat{v}^{(1)})\,,$$
$$\frac{\sqrt{2}}{2}(\hat{v}^{(2)},\hat{v}^{(3)}),\quad \frac{\sqrt{2}}{2}(\hat{v}^{(3)},\hat{v}^{(5)})\,, \tag{A2}$$
$$\frac{\sqrt{2}}{2}(\hat{v}^{(4)},\hat{v}^{(2)}),\quad \frac{\sqrt{2}}{2}(\hat{v}^{(5)},\hat{v}^{(4)})\,.$$

Since $\hat{v}^{(i)} \cdot \hat{v}^{(j)} = -\hat{v}^{(i)} \cdot \hat{v}^{(j+1)}$, where i and j are $1,\ldots,5$ (we identify $\hat{v}^{(6)}$ with $\hat{v}^{(1)}$), it follows that the vectors (A2) are an orthonormal basis in six dimensions. The three-dimensional projection consisting of keeping only the first three components gives the six icosahedral vertex vectors.

The golden norm of an icosahedral reciprocal lattice vector **k** has an important relation to such projections. Let $\mathbf{k}_\perp$ be the orthogonal projection of the six-vector that projects to **k**. The magnitude of $\mathbf{k}_\perp$ is related to the intensity of the Bragg peak at the reciprocal lattice vector **k**.[6] Cahn *et al.*[13] have given a simple expression for this quantity, which assumes a very natural form when expressed in terms of the golden norm:

$$\mathbf{k}_\perp^2 = (\mathbf{k}^2)^\star = \frac{N(\mathbf{k}^2)}{\mathbf{k}^2}\,. \tag{A3}$$

APPENDIX B: PENTAGONAL RECIPROCAL LATTICES

We show here that there is just one distinct reciprocal lattice with pentagonal (but not decagonal) symmetry. The pentagonal reciprocal lattice is closely related to the decagonal, as rhombohedral is to hexagonal. It lacks a mirror plane normal to the fivefold axis (since such a symmetry in combination with the inversion would require the axis to be tenfold). Although no currently known quasicrystal has pentagonal symmetry, we note its properties here because they emerge as a corollary of the analysis in Sec. IV.

As in the decagonal case, we first note that there are vectors with minimum nonzero component (which we take to have unit length) along the fivefold axis $\hat{\mathbf{z}}$. Because, however, the pentagonal lattice **S** lacks a mirror plane perpendicular to $\hat{\mathbf{z}}$, we can only conclude that **S** contains $5\hat{\mathbf{z}}$.

Note next that the set $\mathbf{S}_0$ of vectors in **S** with vanishing z component is a two-dimensional reciprocal lattice with fivefold symmetry to which the analysis of Sec. IV directly applies: To within an overall scale factor $\mathbf{S}_0$ is just the set of all integral linear combinations of four unit vectors $\mathbf{b}^{(1)}, \ldots, \mathbf{b}^{(4)}$ spaced 72° apart (Fig. 2).

Because $\mathbf{S}$ is a lattice, successive layers—i.e., the sets of vectors with z components $1,2,\ldots$—must be simply displacements of $\mathbf{S}_0$ by successive integral multiples of a vector $\hat{\mathbf{z}}+\mathbf{a}$, where $\mathbf{a}$ is a vector in the x-y plane. The vector $\mathbf{a}$ cannot be in $\mathbf{S}_0$ (or successive layers would be identical, and we would have mirror symmetry) but $5\mathbf{a}$ must be in $\mathbf{S}_0$ (since $5\hat{\mathbf{z}}$ is in S). The vector $\mathbf{a}$ is therefore a linear combination of $\mathbf{b}^{(1)}, \ldots, \mathbf{b}^{(4)}$ with one-fifth integral coefficients. Because $\mathbf{a}$ is only determined up to a vector in $\mathbf{S}_0$ we can take those coefficients to be 0, $\pm\frac{1}{5}$, or $\pm\frac{2}{5}$.

One easily verifies that the requirement that each layer be invariant under a fivefold rotation about $\hat{\mathbf{z}}$ further restricts the possible choices of those coefficients to the following two (always to within an additive vector in $\mathbf{S}_0$):

$$\mathbf{a}=\tfrac{1}{5}(-\mathbf{b}^{(1)}-2\mathbf{b}^{(2)}+2\mathbf{b}^{(3)}+\mathbf{b}^{(4)})$$

or (B1)

$$\mathbf{a}'=\tfrac{1}{5}(-2\mathbf{b}^{(1)}+\mathbf{b}^{(2)}-\mathbf{b}^{(3)}+2\mathbf{b}^{(4)})$$

or their negatives. The negatives give structures that differ only by a rotation by 36°, so there might appear to be two distinct stackings of $\mathbf{S}_0$. A simple computation shows, however, that $\mathbf{a}'=\tau\mathbf{a}$ to within an additive vector in $\mathbf{S}_0$. Since $\mathbf{S}_0$ itself is invariant under a rescaling by τ, $\mathbf{a}$ and $\mathbf{a}'$ determine structures that differ only by a horizontal rescaling. There is therefore just a single pentagonal reciprocal lattice, determined by the vector $\mathbf{a}$.

Note that if one scales $\mathbf{a}$ by τ^2 the resulting vector turns out to be equivalent to $-\mathbf{a}$, so a horizontal rescaling of $\mathbf{S}$ by τ^2 is equivalent to a 36° rotation. Thus the product of a rotation which is not in the point group of $\mathbf{S}$ with a horizontal rescaling by τ^2 leaves $\mathbf{S}$ invariant. This is a novel symmetry, not found in crystallographic lattices. It resembles glide and screw operations (which, of course, are never symmetries of lattices), except that the rotation is here combined with a rescaling rather than a translation.

A pentagonal reciprocal lattice can be primitively generated by the symmetric set of vectors $\hat{\mathbf{z}}+\mathbf{c}^{(i)}$, $i=0,\ldots,4$, where the five $\mathbf{c}^{(i)}$ are spaced 72° apart in the x-y plane.

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[1]D. S. Shechtman, I. Blech, D. Gratias, and J. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).

[2]L. Bendersky, Phys. Rev. Lett. **55**, 1461 (1985). (The decagonal phases are also called "*T* phases".) For recent work on quasicrystals, see the proceedings of the Les Houches meeting in J. Phys. (Paris) Colloq. **47**, C3 (1986), especially the review articles of Shechtman and Bendersky.

[3]Note that closure under sums and differences is used to define a Bravais lattice in footnote 7 on p. 70 of N. W. Ashcroft and N. D. Mermin, *Solid State Physics,* (Saunders College, Philadelphia, 1976).

[4]D. Rokhsar, D. Wright, and N. D. Mermin (unpublished); see also T. Janssen, Acta Cryst. A **42**, 261 (1986). Space groups are also discussed in P. Bak, Phys. Rev. **32**, 5764 (1985); S. Alexander, J. Phys. (Paris) **47**, C3-143 (1986); and D. Frenkel, C. Henley, and E. Siggia, Phys. Rev. B **34**, 3649 (1986).

[5]P. Bak, Phys. Rev. B **32**, 5764, (1985) describes two lattices spanned by six vectors, but does not claim to be exhaustive; P. A. Kalugin, A. Yu Kitaev, and L. S. Levitov, J. Phys. Lett. **46**, L-601 (1985) say that there are five lattices; S. Alexander, J. Phys. (Paris) **47**, C3-143 (1986) says there are two lattices spanned by six vectors (and two spanned by more than six); J. Cahn, D. Shechtman, and D. Gratias, J. Mater. Res. **1**, 13 (1986) discuss only the three derived here but say there are five, citing Kalugin *et al.*; T. Janssen, Acta. Cryst. A **42**, 261 (1986) correctly says there are three spanned by six vectors but offers no proof.

[6]P. Kramer and R. Neri, Acta Cryst. A **40**, 580 (1984); V. Elser, *ibid.* **42**, 36 (1986); Phys. Rev. B **32**, 4891 (1985); P. A. Kalugin, A. Kitaev, and L. Levitov, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 119 (1985) [JETP Lett. **41**, 702 (1985)]; J. Phys. Lett. **46**, L-601 (1985); M. Duneau and A. Katz, Phys. Rev. Lett. **54**, 2688 (1985); J. Phys. (Paris) Colloq. **47**, C3-103 (1986).

[7]This result does not seem to have found its way into the physics literature. Our proof is based on R. L. E. Schwartzenberger, *N-Dimensional Crystallography* (Pitman, London, 1980).

[8]S. Alexander, J. Phys. (Paris) Colloq. **47**, C3-143 (1986); T. Janssen, Acta Cryst. A **42**, 261 (1986). Both state that there is only one decagonal reciprocal lattice, but neither offers a proof.

[9]For an introduction to this subject, as well as a wealth of information about the golden mean, we refer the interested reader to the charming monograph *Quadratic Number Fields in the Golden Section Unit* by F. W. Dodd (Polygonal, Washington, N.J., 1983).

[10]This terminology is that of Ref. 8.

[11]For an ordinary vector space over the real numbers, this is just the statement that any linearly independent set can serve as a basis. Because we allow only integral linear combinations of the generating vectors, the chage of basis will in general require a rescaling.

[12]Students of ring theory will recognize the argument that follows as the theorem that a nontrivial ideal of a Euclidean domain is always a principal ideal. The proof given below however, assumes no acquaintance with the theory of rings.

[13]J. Cahn, D. Shechtman, and D. Gratias, J. Mater. Res. **1**, 13 (1986) use this coordinate system to index quasicrystal diffraction patterns and note useful parity constraints.

[14]The more precise analogy is to the construction of simple and body-centered cubic lattices out of interpenetrating face-centered cubic lattices.

[15]The golden norm also has useful properties in the icosahedral case, as noted in Appendix A.

[16]Lest the reader view the preceding analysis as a lengthy journey to an obvious conclusion, we note that when generalized from 10-fold to n-fold symmetry, the conclusion is false for all but a finite set of n (N. D. Mermin, D. Rokhsar, and D. Wright, unpublished).