Scale equivalence of quasicrystallographic space groups

Daniel S. Rokhsar
IBM Research Division, Thomas J. Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598

David C. Wright and N. David Mermin
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853-2501
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The space-group classification of ordered structures has been extended to quasicrystals by formulating the problem in wave-vector space. We list the space groups belonging to the icosahedral point groups Y and Y_h for the three icosahedral lattices of wave vectors, and show that taking into account the scaling properties of quasicrystal lattices is crucial for a correct enumeration.

I. INTRODUCTION

Two approaches have been used to extend the space-group classification to materials with noncrystallographic point groups. The first[1–4] views quasicrystals as physical space projections of higher-dimensional periodic structures. The classification is then based on the ordinary crystallographic space groups in the higher dimension. The second[5,6] is formulated in spaces with the physical dimensionality. The conventional concepts of crystallography are reformulated directly in terms of a lattice of wave vectors derived from a diffraction pattern, rather than constructed from a lattice of translations that describes real-space periodicity. Because there is no reason for such a k-space lattice to have a minimum distance between points, this approach is applicable to noncrystallographic as well as crystallographic point groups.

We have used the second approach to calculate the space groups belonging to the icosahedral point groups, Y and Y_h. The space groups we find agree with those computed by Janssen[1] from the higher-dimensional approach, with one important difference. The three-dimensional icosahedral lattices have nontrivial scale invariances which six-dimensional cubic lattices lack. As a result, certain distinct six-dimensional space groups characterize the same three-dimensional diffraction patterns.

(1) For the proper icosahedral point group Y, an analysis that ignores the scale invariances of the lattices associates with each of the three icosahedral lattices four distinct nonsymmorphic[7] groups, corresponding to four distinct types of five-fold screw axes. As a result of the scale invariance of the lattices, however, one finds that there is no way to distinguish among the four types. These groups are therefore not distinct, but map into each other under repeated scalings of the lattice.

(2) When the point group is the full icosahedral group Y_h, then for two of the three lattice types the analysis that ignores scale invariance yields either no nonsymmorphic (face-centered lattice) or a single nonsymmorphic (primitive lattice) space group. For the third lattice type (body-centered), however, such an analysis yields non-symmorphic space groups characterized by three apparently distinct types of glide planes. Once again, the three types are not, in fact, distinct, transforming into one another under a simple rescaling of the lattice.

We have noted elsewhere[5] a similar consequence of scale invariance for the enumeration of axial quasicrystallographic space groups in two and three dimensions. In space groups of odd rotational order N, it is possible for the point group operations to act on a $2N$-fold symmetric lattice in two distinct ways, depending on the orientation of the mirrors with respect to the primitive vectors: the mirrors can either lie along or between the vectors in a star that primitively generates the lattice. The only such crystallographic examples are the threefold point groups, in which the two kinds of action of the point group $3m$ on the lattice lead to the distinct space groups $p31m$ and $p3m1$. In the quasicrystallographic case, however, this dichotomy is only preserved when N is the power of an odd prime number. For other odd N (15,21,33,35, . . .) there exist alternative primitive vectors that differ by a scale change *and* a rotation by $2\pi/(2N)$, so that the two actions of the point group on the lattice cannot be distinguished. For such N, $pNm1$, and $pN1m$ reduce to a single space group, pNm.

II. REVIEW OF LATTICES AND SPACE GROUPS

Space groups are associated with a given point group, lattice, and action of the point group on the lattice. We briefly describe the lattices compatible with icosahedral symmetry (which are derived in Ref. 8) and the generalization of space groups to noncrystallographic systems (as formulated in Refs. 5 and 6).

The three distinct icosahedral lattices are integral linear combinations of wave vectors of the same length along each of the six icosahedral five-fold axes. The primitive icosahedral lattice P^* is given by *all* sets of integral coefficients, the body-centered lattice I^* is given by those sets of six integers which are either all odd or all even, and the face-centered lattice F^* is given by those sets of six integers whose sum is even. The asterisk is to emphasize that the lattices in question are k-space lattices, since in the conventional space group nomenclature the labels P, I, and F refer to real-space lattices. Thus if one wants to compare cubic and icosahedral space groups, one must compare I with F^* and F with I^*. The primitive icosahedral lattice is invariant under a scaling by τ^3, while both centered icosahedral lattices are invariant under a scaling by τ, where τ is the golden mean, $\frac{1}{2}(1+\sqrt{5})$.

Viewed in wave-vector space, the crystallographic classification by space groups is a classification of the distinct ways of assigning phases to the Fourier coefficients consistent with the point group, lattice, and action of the group on the lattice.[9] This formulation can be generalized immediately to noncrystallographic point groups and lattices.[5,6] The quasicrystallographic space groups belonging to a given point group, lattice, and action of the group on the lattice, are given by equivalence classes of *phase functions* relating the density Fourier coefficients at symmetry related points. The phase function $\Phi_g(k)$ is defined by

$$\rho(g\mathbf{k})=e^{2\pi i\Phi_g(\mathbf{k})}\rho(\mathbf{k}) , \qquad (2.1)$$

for all lattice vectors $\mathbf{k}$ with nonvanishing Fourier coefficients $\rho(\mathbf{k})$, where g is any operation in the point group G. The requirement that all macroscopic translationally invariant properties of a material be invariant under the operations of its point group G implies that each phase function is linear on the lattice (to within an arbitrary additive integer).[5,6]

Two sets of phase functions, Φ_g and Φ'_g are *gauge equivalent*[10] if they describe densities that are macroscopically indistinguishable (and which therefore differ only by a real-space displacement and/or a "phason"). The mathematical condition for the gauge equivalence of phase functions is that

$$\Phi'_g(\mathbf{k})-\Phi_g(\mathbf{k})\equiv\chi(g\mathbf{k})-\chi(\mathbf{k}) , \qquad (2.2)$$

where "$\equiv$" denotes equality to within an additive integer, and the function χ is also linear on the lattice (to within an additive integer) and independent of the group element g. The condition (2.2) relating two equivalent sets of phase functions is called a *gauge transformation.*[5,6] Note that if $\mathbf{k}$ is invariant under the action of a point-group operation g, then the value of $\Phi_g(\mathbf{k})$ is gauge invariant. This provides a test for the gauge equivalence of phase functions.

Two densities with the same macroscopic point group and lattice type belong to the same *space-group type* if it is possible to deform continuously one density into the other in such a way that (a) the macroscopic point-group symmetry and lattice type are preserved at all stages of the deformation and (b) the phase functions on the correspondingly deformed lattices all have the same values (to within gauge transformations). In the case of crystallographic space groups the fact that space-group classes must be invariant under such deformations is not always given explicit attention[11] since it merely ensures the obvious requirement that inessential differences in the lattice (e.g., hexagonal lattices with different c/a ratios, or cubic lattices with different overall scales) should not lead to different space-group assignments. If one limits attention to one "canonical" specimen of a lattice type, then space-group equivalence simply reduces to gauge equivalence of the phase functions on that lattice.

In the quasicrystallographic case, however, the equivalence of space groups is not this simple, because of the scale invariance of quasicrystallographic lattices. Two densities $\rho(\mathbf{r})$ and $\rho(\lambda\mathbf{r})$ that differ only by an overall scale factor, evidently belong to the same space-group type. In the crystallographic case this merely means that the phase functions $\Phi_g(\mathbf{k})$ and $\Phi_g(\mathbf{k}/\lambda)$ are essentially the same phase functions, characterizing the same space group on lattices differing by the scale factor λ. If, however, rescaling by λ leaves the lattice invariant, then $\Phi_g(\mathbf{k})$ and $\Phi_g(\mathbf{k}/\lambda)$ can also be regarded as two *different* phase functions defined on the *same* lattice. Since they still characterize densities differing only by a scale factor, they must still characterize the same space group. Since in general such phase functions are not gauge equivalent, we arrive at a second condition for the equivalence of space groups, *scale equivalence.*

Two phase functions are said to belong to the same *quasicrystallographic space-group type* (or, more colloquially, the same space group) if they are gauge and/or scale equivalent.[12]

III. SCALE EQUIVALENCE OF SPACE GROUPS IN THE ICOSAHEDRAL CASE

Before demonstrating the scale equivalence of the icosahedral space groups, we briefly review how space groups are determined.[5,6,9] Because phase functions are linear, it is enough to specify their values at a set of primitive basis vectors $\{\mathbf{b}^{(\alpha)}\}$ for the lattice in question. As a simple consequence of its definition (2.1), the phase function satisfies the group combination rule

$$\Phi_{gh}(\mathbf{k})\equiv\Phi_g(h\mathbf{k})+\Phi_h(\mathbf{k}) , \qquad (3.1)$$

or, because the phase function is linear,

$$\Phi_{gh}(\mathbf{b}^{(\mu)})\equiv\sum_\alpha\Phi_g(\mathbf{b}^{(\alpha)})[h]^{\alpha\mu}+\Phi_h(\mathbf{b}^{(\mu)}) , \qquad (3.2)$$

where g and h are elements of the point group G and $[h]^{\alpha\mu}$ is the representation of h in the basis of $\mathbf{b}^{(\alpha)}$'s. The point group can be specified by a set of generators, and a set of generating relations which they obey. Since any element g in the group can be expressed as a product of the generators, Eq. (3.1) allows the phase function Φ_g for any g in the point group to be constructed from the phase functions of the generators.

To determine the phase functions of the generators, the group combination rule is applied to the generating relations. This produces a set of simultaneous linear equations, and the various solutions to these equations specify the possible values of the phase functions.

A. The proper icosahedral group

The 60-element proper icosahedral group, Y (532), is generated by two elements, t and u, satisfying the relations

$$t^5=u^2=(ut)^3=e , \qquad (3.3)$$

where e is the identity operation. If the lattice is P^*, we can choose the basis vectors $\mathbf{b}^{(\alpha)}$ to be the six unit vectors

$\mathbf{v}^{(0)}, \mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(5)}$ that lie along the fivefold axes of the icosahedron, with $\mathbf{v}^{(1)}$ through $\mathbf{v}^{(5)}$ related by fivefold rotations about $\mathbf{v}^{(0)}$ with positive projections onto $\mathbf{v}^{(0)}$. The spaces left invariant by rotations in the icosahedral case are dense one-dimensional sets of points that are spanned by two vectors of incommensurate lengths. The generator t can be taken to be the fivefold rotation that leaves the vectors $\mathbf{v}^{(0)}$ and $\mathbf{v}^{(1)}+\mathbf{v}^{(2)}+\cdots+\mathbf{v}^{(5)}$ invariant, and u can be taken to be the twofold rotation that leaves $\mathbf{v}^{(0)}+\mathbf{v}^{(1)}$ and $\mathbf{v}^{(2)}+\mathbf{v}^{(5)}$ invariant.

Since the phase function associated with the identity e vanishes, the generating relations (3.3) lead to a set of equations modulo one for $\Phi_t(\mathbf{b}^{(\alpha)})$ and $\Phi_u(\mathbf{b}^{(\alpha)})$. To solve these equations, we add an arbitrary integer to each, converting them to ordinary equalities. The solutions can be characterized in a gauge-invariant way by considering the values of the phase functions $\Phi_g(\mathbf{k})$ at wave vectors invariant under g [cf. (2.2)]. For the case of the primitive lattice P^*, since $\mathbf{b}^{(0)}$ and $\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\cdots+\mathbf{b}^{(5)}$ span the invariant space of t, the value of $\Phi_t(\mathbf{k})$ for any wave vector in the invariant space can be found by linear combinations of the values at these two wave vectors. After a calculation we find

$$\Phi_t(\mathbf{b}^{(0)}) \equiv \frac{C}{5}, \quad \Phi_t(\mathbf{b}^{(1)}+\mathbf{b}^{(2)}+\cdots+\mathbf{b}^{(5)}) \equiv 0 , \tag{3.4}$$

where C is one of the arbitrary integers, and the choices $C=0,1,2,3,4$ give five distinct solutions. It follows from the group combination rule (3.1) that the phase functions associated with group elements in the same conjugacy class differ by at most a gauge function, so that (3.4) (with properly transformed $\mathbf{b}^{(\alpha)}$'s) holds for any fivefold rotation. The phase functions for the twofold and threefold rotations are found to vanish (mod 1) on their invariant spaces.

Up to this point, the problem is formally identical to determining the space groups of a crystal in six dimensions, with a lattice spanned by six basis vectors and a point group that permutes these basis vectors in the same way that the icosahedral group permutes the $\mathbf{b}^{(\alpha)}$'s. In the six-dimensional crystallographic case, (3.4) indicates the presence of five distinct space groups: a symmorphic one (corresponding to $C=0$), and four distinct nonsymmorphic ones (corresponding to $C=1,2,3,4$) with the fivefold screw operations[13] 5_1, 5_2, 5_3, and 5_4, respectively. This, in fact, is the point of view taken by Janssen.[1]

In the three-dimensional icosahedral case, however, the four nonsymmorphic groups are actually identical, as a consequence of the invariance of the P^* lattice under scaling[8] by τ^3. The scale invariance means that an equally good basis for the lattice is given by the vectors[14]

$$\mathbf{b}'^{(\alpha)} = \tau^3 \mathbf{b}^{(\alpha)} = \sum_{\beta=0}^{5} \mathbf{b}^{(\beta)} S_{P^*}^{\beta\alpha} ,$$

$$S_{P^*} = \begin{pmatrix} 2 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 1 & -1 & -1 & 1 \\ 1 & 1 & 2 & 1 & -1 & -1 \\ 1 & -1 & 1 & 2 & 1 & -1 \\ 1 & -1 & -1 & 1 & 2 & 1 \\ 1 & 1 & -1 & -1 & 1 & 2 \end{pmatrix} . \tag{3.5}$$

By using (3.4) and (3.5), and the linearity of the phase function, one easily verifies that

$$\Phi_t(\mathbf{b}'^{(0)}) \equiv \sum_{\beta=0}^{5} \Phi_t(\mathbf{b}^{(\beta)}) S_{P^*}^{\beta 0} \equiv \frac{2C}{5} \tag{3.6}$$

while $\Phi_t(\mathbf{b}'^{(1)}+\mathbf{b}'^{(2)}+\cdots \mathbf{b}'^{(5)})$ remains 0 (mod 1). Comparing (3.6) with (3.4), we see that the value of C characterizing the phase function depends on which set of basis vectors one chooses to work with. Under successive scalings by τ^3,

$$C = 1 \rightarrow 2 \rightarrow 4 \rightarrow 3 \rightarrow 1 . \tag{3.7}$$

Therefore all four of the nonsymmorphic groups of the six-dimensional crystal are indistinguishable in three dimensions and there is only one nonsymmorphic space group.

One can similarly verify that the F^* and I^* lattices also have a single nonsymmorphic space group with point group Y. For the purpose of computing the space groups associated with these lattices, it is convenient to represent each type of lattice as a set of *all* integral linear combinations of six integrally independent primitive basis vectors, $\mathbf{b}^{(0)}, \ldots, \mathbf{b}^{(5)}$. The primitive basis sets for the three icosahedral lattices can be taken to be

$$P^*: \quad \mathbf{b}^{(\alpha)} = \mathbf{v}^{(\alpha)}, \quad \alpha = 0,1,\ldots,5$$

$$F^*: \quad \mathbf{b}^{(0)} = 2\mathbf{v}^{(0)}, \quad \mathbf{b}^{(n)} = \mathbf{v}^{(0)} + \mathbf{v}^{(n)} , \quad n = 1,2,\ldots,5 , \tag{3.8}$$

$$I^*: \quad \mathbf{b}^{(0)} = \mathbf{v}^{(0)} + \mathbf{v}^{(1)} + \cdots + \mathbf{v}^{(5)}, \quad \mathbf{b}^{(n)} = 2\mathbf{v}^{(n)} , \quad n = 1,2,\ldots,5 .$$

The fivefold rotation t leaves $\mathbf{b}^{(0)}$ invariant for the F^* and I^* lattices, and one finds that the phase functions on the invariant space of t are again given by (3.4) for the new $\mathbf{b}^{(\alpha)}$'s. Both the F^* and I^* lattices are invariant under scaling[8] by τ. In the bases (3.8), scaling by τ of the F^* and I^* lattices is given by the matrices

$$S_{F^*} = \begin{pmatrix} -2 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 \end{pmatrix} ,$$

$$S_{I^*} = \begin{pmatrix} 3 & 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & 0 & -1 & -1 \\ -1 & -1 & 0 & 0 & 0 & -1 \\ -1 & -1 & -1 & 0 & 0 & 0 \\ -1 & 0 & -1 & -1 & 0 & 0 \end{pmatrix} . \tag{3.9}$$

By calculating the values of the phase function for the scaled lattice, one again finds that the four nonsymmorphic space groups are equivalent. (The phase functions for the twofold and threefold rotations are again integral on their invariant spaces.)

B. The full icosahedral group

The full 120-element icosahedral group Y_h ($\bar{5}\,\bar{3}m$) results from adjoining the inversion i to Y. There are again nonsymmorphic space groups, which contain glide planes, whose equivalence can again be overlooked if scale invariance is not taken into account. Y_h can be generated by two elements, u and $\bar{t}=ti$ (so that $i=\bar{t}^5$), with the generating relations

$$u^2=(\bar{t})^{10}=(u\bar{t}^6)^3=e,\quad u\bar{t}^5=\bar{t}^5u\ . \tag{3.10}$$

Applying the group combination law (3.1) to these relations and solving the resulting equations for the phase functions of the generators, one finds no space groups containing screw axes for any of the lattices, and for the F^* lattice one finds no nonsymmorphic space groups at all.

For the P^* and I^* lattices, the only operation with nonintegral phase functions on its invariant space is the mirror $m=iu$ perpendicular to the axis of the twofold rotation u (and its conjugates). A reflection leaves a plane invariant, and in the icosahedral case, the wave vectors lying in that plane are generated by four integrally independent vectors. For the P^* case, a set of primitive generating vectors for the invariant space of the mirror perpendicular to the axis of the twofold rotation u are $\mathbf{e}^{(1)}=\mathbf{b}^{(0)}-\mathbf{b}^{(1)}$, $\mathbf{e}^{(2)}=\mathbf{b}^{(2)}-\mathbf{b}^{(5)}$, $\mathbf{e}^{(3)}=\mathbf{b}^{(3)}$, and $\mathbf{e}^{(4)}=\mathbf{b}^{(4)}$, where the $\mathbf{b}^{(\alpha)}$'s are the P^* basis vectors. As before, the gauge-invariant part of the phase function is determined by the value of the phase function at these wave vectors. One finds

$$\Phi_m(\mathbf{e}^{(1)})\equiv\Phi_m(\mathbf{e}^{(2)})\equiv 0,\quad \Phi_m(\mathbf{e}^{(3)})\equiv\Phi_m(\mathbf{e}^{(4)})\equiv\frac{C}{2}\ , \tag{3.11}$$

where the distinct space groups are given by $C=0,1$. Thus the P^* lattice has a single nonsymmorphic group containing a glide plane.

In the case of the I^* lattice we again consider a mirror perpendicular to the axis of the twofold rotation u, with an invariant space spanned by $\mathbf{e}^{(1)}=\mathbf{b}^{(0)}-\mathbf{b}^{(1)}-\mathbf{b}^{(2)}$, $\mathbf{e}^{(2)}=\mathbf{b}^{(2)}-\mathbf{b}^{(5)}$, $\mathbf{e}^{(3)}=\mathbf{b}^{(3)}$, and $\mathbf{e}^{(4)}=\mathbf{b}^{(4)}$, where the $\mathbf{b}^{(\alpha)}$'s are the I^* basis vectors listed in (3.8). One finds

$$\begin{aligned}\Phi_m(\mathbf{e}^{(1)})&\equiv\frac{C_1}{2},\quad \Phi_m(\mathbf{e}^{(2)})\equiv 0\ ,\\ \Phi_m(\mathbf{e}^{(3)})&\equiv\Phi_m(\mathbf{e}^{(4)})\equiv\frac{C_2}{2}\ ,\end{aligned} \tag{3.12}$$

where C_1 and C_2 are integers that arise in solving the equations modulo 1, and can each take on the values 0 or 1.

If scale invariance is overlooked, (3.12) leads to three distinct nonsymmorphic space groups corresponding to $(C_1,C_2)=(1,0)$, (0,1), and (1,1). Comparing the values of $\Phi_m(\mathbf{e}^{(\alpha)})$ with $\Phi_m(\tau\mathbf{e}^{(\alpha)})$, $\Phi_m(\tau^2\mathbf{e}^{(\alpha)})$, and $\Phi_m(\tau^3\mathbf{e}^{(\alpha)})$, one finds, however, that under successive scalings of the

TABLE I. The three-dimensional icosahedral space groups. This table lists the icosahedral space groups for the two icosahedral point groups Y (532) and Y_h ($\bar{5}\,\bar{3}m$). The symbols P^*, F^*, and I^* refer to the primitive, face-centered, and body-centered lattices, where the star indicates that the lattices are in wave-vector space. The notation $2/q$ indicates the presence of (quasi-) glide planes perpendicular to the twofold axes. Here ϕ_g is the (gauge-dependent) vector of values $\Phi_g(\mathbf{b}^{(\alpha)})$, $\alpha=0,\ldots,5$, for the primitive basis vectors given in (3.8). The extinctions listed in the final column are also in terms of the vectors in (3.8). The complete collection of extinct points contains those listed in the table and those obtainable from the ones in the table by point-group operations. For the space group $I^*\bar{5}\,\bar{3}(2/q)$, the value of the phase function ϕ_u for basis stars that are scaled by τ or τ^2 from the basis star used in the table are given by $\phi_u\cdot S_{I^*}$ and $\phi_u\cdot S_{I^*}^2$, where S_{I^*} is given in (3.9). The indices of the extinct points relative to those bases are the same as those given in the table, except that the condition "h odd" is replaced by "$h+l+m$ odd" or "$l+m$ odd" (cf. Sec. IV).

Point group	Space group	Phase functions of generators	Indices of extinct points
532	P^*532	$\phi_u=\phi_t=0$	
	P^*5_132	$\phi_u=(00\frac{4}{5}\,\frac{4}{5}0\frac{1}{5})$, $\phi_t=(\frac{1}{5}00\,000)$	$(hkk\ kkk)$, $h\neq 5n$
	F^*532	$\phi_u=\phi_t=0$	
	F^*5_132	$\phi_u=(\frac{1}{5}0\frac{1}{5}\,\frac{1}{5}00)$, $\phi_t=(\frac{1}{5}00\,000)$	$(hkk\ kkk)$, $h\neq 5n$
	I^*532	$\phi_u=\phi_t=0$	
	I^*5_132	$\phi_u=(\frac{4}{5}0\frac{3}{5}\,\frac{3}{5}0\frac{2}{5})$, $\phi_t=(\frac{1}{5}00\,000)$	$(hkk\ kkk)$, $h\neq 5n$
$\bar{5}\,\bar{3}\frac{2}{m}$ ($\bar{5}\,\bar{3}m$)	$P^*\bar{5}\,\bar{3}\frac{2}{m}$	$\phi_u=\phi_{\bar{t}}=0$	
	$P^*\bar{5}\,\bar{3}\frac{2}{q}$	$\phi_u=(000\,\frac{1}{2}\,\frac{1}{2}0)$, $\phi_{\bar{t}}=0$	$(h\bar{h}k\ lm\bar{k})$, $l+m$ odd
	$F^*\bar{5}\,\bar{3}\frac{2}{m}$	$\phi_u=\phi_{\bar{t}}=0$	
	$I^*\bar{5}\,\bar{3}\frac{2}{m}$	$\phi_u=\phi_{\bar{t}}=0$	
	$I^*\bar{5}\,\bar{3}\frac{2}{q}$	$\phi_u=(0\frac{1}{2}0\,000)$, $\phi_{\bar{t}}=0$	$(h,\bar{h},\bar{h}+k,l,m,\bar{k})$, h odd

lattice by τ

$$(C_1,C_2)=(1,0)\rightarrow(1,1)\rightarrow(0,1)\rightarrow(1,0)\ . \qquad (3.13)$$

Thus the three nonsymmorphic space groups are scale equivalent, and there is only one nonsymmorphic group with lattice I^*.

Our results for the icosahedral space groups are summarized in Table I.

IV. EXTINCTIONS IN THE SCATTERING PATTERN

We conclude by describing the extinctions in scattering patterns that occur when the space group is nonsymmorphic. An immediate consequence of the definition (2.1) of the phase function is that the Fourier amplitude $\rho(\mathbf{k})$ of any wave vector that is invariant under the point group operation g must vanish unless $\Phi_g(\mathbf{k})$ is an integer. Since nonintegral phase functions on the invariant space of an operation are the signatures of a nonsymmorphic space group, such extinctions occur only for the nonsymmorphic groups, and form a pattern characteristic of each space group. The indices of these extinct points for the icosahedral space groups are given in the last column of Table I.

Note that complications can arise from scale equivalence that are not present in the crystallographic case since the indices assigned to extinct points may be different for scale equivalent but gauge inequivalent space groups. In particular, for the space group $I^*\bar{5}\,\bar{3}(2/q)$, the indices of the extinct points depend on the star of basis vectors used for the indexing. A different set of indices results from a basis star scaled from the original star by τ, and a third set results from a star scaled by τ^2. A pattern of extinctions in an observed diffraction pattern that can be indexed in any one of these three ways is a signature of this space group, since either of the other indexing schemes would result simply by choosing a rescaled basis. This complication does not arise for the space groups associated with the point group 532, because the indexing of extinct points does not depend on the scale of the basis.

While currently all observed icosahedral quasicrystals appear to have symmorphic groups, there are indications of nonsymmorphic space groups in decagonal[6,15,16] and octagonal[6] quasicrystals.

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[7]A space group is said to be *nonsymmorphic* if it contains screw or glide operations (see Ref. 13).

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[10]This is the same as the definition of "equivalence" in Ref. 5. The refinement in terminology is required since here we also need the notion of "scale equivalence."

[11]But see, N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, New York, 1976), footnote 10, page 115.

[12]In Ref. 6 we give a general formulation of the consequences of the scale invariance of quasicrystallographic lattices for the classification of space groups by introducing the *extended holohedral group* of the lattice as the set of point-group operations, scalings, and scalings in conjunction with point operations not necessarily in the point group, that leave the lattice invariant.

[13]A *screw operation* from our point of view is a rotation associated with a phase function which has a (gauge-invariant) nonintegral value on wave vectors along the line left invariant by the rotation. Similarly, a *glide operation* is a reflection associated with a phase function which has nonintegral values for wave vectors in the invariant plane of the mirror. Because these operations are characterized in terms of phase functions rather than real-space translations, these definitions are equally valid for crystallographic or noncrystallographic point groups.

[14]That both the primed and unprimed sets of **b**'s form equally good bases is easily seen by noting that the transformation matrix S and its inverse [which is given by changing the sign of the diagonal entries in (3.5)] both have integral entries, so that either basis set can be written as integral linear combinations of the other.

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