Scale Invariance and the Group Structure of Quasicrystals

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(Received 2 December 1985)

We define a set of generalized symmetries for quasicrystals and find that this leads naturally to the operators which generate scale transformations ("inflations"). Our methods are applied to 2D fivefold-symmetric patterns, but generalize to other point groups and dimensions.

PACS numbers: 61.10.Dp, 61.14.Dc

The unusual geometry of quasicrystals gives rise to symmetries which are not present in ordinary crystals. In particular, there is an arbitrariness in the choice of a basis for scattering space in the quasicrystal case which is not available for crystals. We shall call these "generalized symmetries" to distinguish them from the ordinary point-group symmetries. Understanding these operations is important since they should be as useful in the study of physical properties of quasicrystals, e.g., the electronic wave functions, as they were in one-dimensional Fibonacci lattices.[1] In this paper, we shall enumerate all possible transformations of a quasicrystal and its diffraction pattern which generate the generalized symmetries defined below. For crystals, this enumeration gives only the usual point-group operations, but for quasicrystals it leads to additional transformations, which in the cases we have considered correspond precisely to the scale transformations and reprojections which have been displayed previously by others.[2-4]

For the purposes of this paper, we define a "quasicrystal" as a crystal-like pattern with a point-group symmetry which is incompatible with translational symmetry.[5-8] While we illustrate our calculation for 2D patterns with fivefold symmetry, the methods are applicable to any translationally forbidden point-group symmetry. Our preliminary calculations for D_7 in 2D and for the icosahedral group in 3D convince us that the present method generates all interesting operations for translationally forbidden point groups.[9]

We begin by analyzing the scattering pattern from a quasicrystal with fivefold symmetry [Fig. 1(a)]. This pattern is similar to the Fourier transform $S(\mathbf{q})$ of a set of delta functions at the vertices of the solid pattern in Fig. 1(b). $S(\mathbf{q})$ is actually a dense collection of delta functions at the scattering wave vectors $\mathbf{q}$; only the major peaks are shown in the figure.[5,6,10-12] Each $\mathbf{q}$ can be labeled by an $\tilde{\mathbf{n}} \in Z^5$ (the set of all integer quintuples), where $\mathbf{q}(\tilde{\mathbf{n}}) = \sum_{J=0}^{4} \tilde{n}_J \mathbf{G}_J$ with $\{\mathbf{G}_J\}$ a set of fundamental vectors pointing to the vertices of a pentagon.[3,4,10] However, the $\mathbf{G}_J$'s are not all independent since $\sum_{J=0}^{4} \mathbf{G}_J = 0$, so we work instead with four basis vectors and label $\mathbf{q}$ by $\mathbf{n} \in Z^4$:

$$\mathbf{q}(\mathbf{n}) = \sum_{J=1}^{4} n_J \mathbf{G}_J. \tag{1}$$

The correspondence between the $\mathbf{q}$'s and the points of Z^4 is now one to one.[13] We shall often refer to Z^4 as the *indexing space*. Since the set $\{\mathbf{G}_J\}_{1 \le J \le 4}$ is linearly independent over the integers, the equality $\mathbf{q}(\mathbf{n}) + \mathbf{q}(\mathbf{m}) = \mathbf{q}(\mathbf{p})$ is true if and only if $\mathbf{n} + \mathbf{m} = \mathbf{p}$. Thus the group Z^4 (quadruples of integers with addition) is isomorphic as a group to the set $\{\mathbf{q}(\mathbf{n})\}$ with vector addition. In general, the dimension of the in-

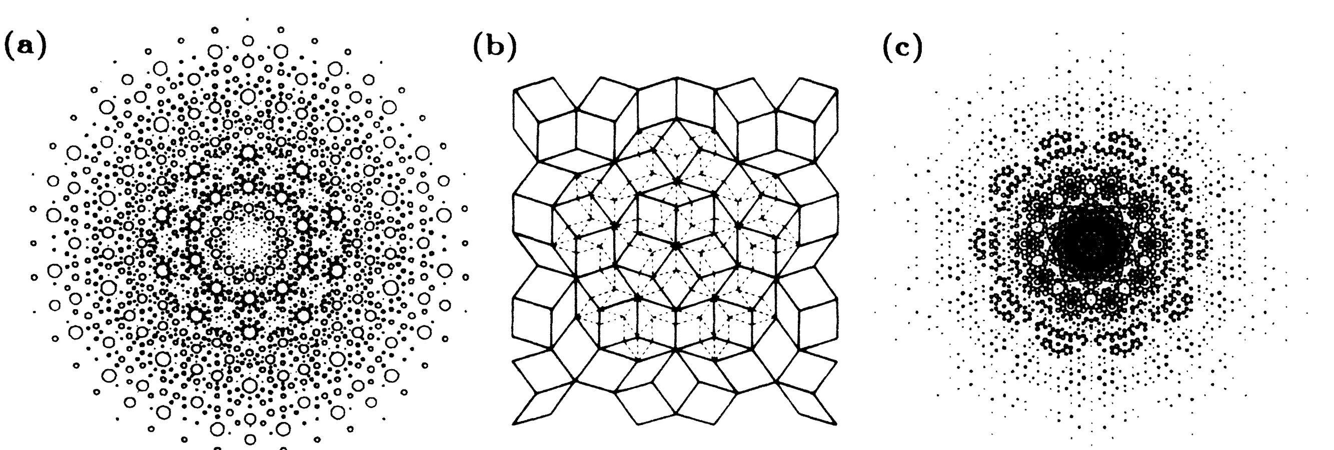

FIG. 1. (a) The scattering pattern from the vertices of the solid pattern in (b), with spot area proportional to $S(\mathbf{q})$; (b) a quasicrystal pattern (solid lines) and its image after transforming by δ (broken lines); (c) the plot of (a) after transformation by β.

dexing space can be taken to be the minimum number of rationally linearly independent vectors required to span q space. In 2D, the vectors representing the mth roots of unity form a basis for an m-fold symmetric pattern. From number theory we know that the number of rationally linearly independent mth roots of unity is equal to the Euler number of m, $E[m]$, which is the number of integers less than m which are relatively prime to m. It therefore follows that the indexing space has dimension $E[m]$.

The largest point group that leaves both Figs. 1(a) and 1(b) invariant is D_5, the dihedral group of order 5, which contains five rotations through integer multiples of $2\pi/5$ and five reflections, one across each image of the x axis. D_5 has two generators which we can choose to be τ_5, a rotation by $2\pi/5$, and σ, the reflection $x \to x$, $y \to -y$. Instead of transforming the $\mathbf{q}$'s directly, we operate on the points $\mathbf{n}$ of the indexing space Z^4 by $\tau_5(\mathbf{q}(\mathbf{n})) = \mathbf{q}(M(\tau_5)\mathbf{n})$, where $M(\tau_5)$ is the representation of τ_5 in Z^4, and similarly for σ. These operators are

$$M(\tau_5) = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{pmatrix}, \quad M(\sigma) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{2}$$

This is easily verified if one remembers that $\mathbf{G}_0 = -\sum_{j=1}^{4} \mathbf{G}_j$.

The indexing scheme (1) is clearly not unique, but depends on the basis $\{\mathbf{G}_j\}$ chosen for the scattering space. An acceptable basis must have the property that all integer linear combinations of the basis vectors span q space in a one-to-one manner. For a crystal, the basis vectors must therefore be chosen to be a subset of the shortest scattering vectors. However, quasicrystals have a dense set of scattering spots, so no such fundamental set of basis vectors is picked out, and the choice of an acceptable basis is somewhat arbitrary.

We can therefore ask what transformations of Z^4 induce acceptable basis transformations of q space. These transformations are symmetries in the sense that they leave the positions of the points in scattering space invariant, although they may permute the scattering intensities associated with those points. We therefore call them generalized symmetries, and label the set of such operations H. H would, for example, transform between indexing schemes which used different sets of fundamental scattering vectors to index a scattering pattern.

We shall now construct H. These transformations must generate one-to-one mappings of Z^4 onto itself, since both before and after the transformation, each point of Z^4 should be associated with a unique scattering vector. We also require that H preserve addition of the $\mathbf{q}$'s, i.e., that the sum of the images of two vectors under H gives the image of the sum of the two vectors, which restricts H to be linear. Thus H must be automorphisms of Z^4 (one to one and preserving of addition), and therefore be a subgroup of $\mathrm{GL}_4(Z)$, the 4×4 matrices with integer entries[14] and determinant ± 1.

We further demand that H preserve the original point-group symmetry of q space. This requires that the images under H of two scattering vectors which were related by a point-group operation in the original pattern should again be related by a point-group operation. Explicitly, if $\mathbf{q}_1 = d\mathbf{q}_2$ for some $d \in D_5$, then after transformation by $h \in H$, we must have $h\mathbf{q}_1 = d'h\mathbf{q}_2$, $d' \in D_5$, where d' may depend on d and h. This leads to the condition:

$$hdh^{-1} = d' \text{ or } hD_5h^{-1} = D_5. \tag{3}$$

The group H_N of all h's which satisfy this condition is called the *normalizer* of D_5 in $\mathrm{GL}_4(Z)$; it is the largest subgroup of $\mathrm{GL}_4(Z)$ which has D_5 as a normal subgroup.[13] We therefore require that $H \subseteq H_N$.

Depending on one's interests, it can be useful to constrain further the definition of a generalized symmetry operation. For example, we can require that $d = d'$. This requirement is appealing since it removes the possibility that H reorders the basis vectors. The resulting group, H_C, defined as the set of operations $h \in \mathrm{GL}_4(Z)$ satisfying $hdh^{-1} = d$, is called the *centralizer* of D_5 in $\mathrm{GL}_4(Z)$, or the largest subgroup of $\mathrm{GL}_4(Z)$ which commutes with D_5.

Since reflections do not commute with rotations, H_C does not even contain the full symmetry group D_5, and so we define a group H_P, the product of D_5 and H_C, by augmenting the generators of H_C by the generators of D_5. This condition is equivalent to requiring that d' in (3) be conjugate to d, so that H_P is defined by the elements $h \in \mathrm{GL}_4(Z)$ satisfying $hdh^{-1} = \tilde{d}d\tilde{d}^{-1}$ for all d and appropriate $\tilde{d} \in D_5$.

The four groups H_C, H_P, H_N, and $\mathrm{GL}_4(Z)$ satisfy $H_C \subseteq H_P \subseteq H_N \subseteq \mathrm{GL}_4(Z)$. The point group D_5 is contained in H_P, but not in H_C. Computing these groups is straightforward; we state the results below.

The centralizer H_C is generated by two elements δ and τ_2:

$$M(\delta) = \begin{pmatrix} -1 & 1 & 0 & -1 \\ 0 & 0 & 1 & -1 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & -1 \end{pmatrix},$$
$$M(\tau_2) = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{4}$$

The operation τ_2 is an inversion (rotation by π) and δ replaces the scattering basis vector $\mathbf{G}_J$ by $\mathbf{G}_{J-1}+\mathbf{G}_{J+1}$, which is a rescaling of $\mathbf{G}_J$.

Finally, we introduce two additional operators

$$M(\tau_{10})=\begin{pmatrix}0 & 1 & -1 & 0\\ 0 & 1 & 0 & -1\\ 0 & 1 & 0 & 0\\ -1 & 1 & 0 & 0\end{pmatrix},\quad M(\beta)=\begin{pmatrix}0&0&1&0\\1&0&0&0\\0&0&0&1\\0&1&0&0\end{pmatrix}. \tag{5}$$

H_P is obtained by adjoining the generators of D_5 given in Eq. (2) with the generators of H_C. We can take the generators of H_P to be τ_{10}, δ, and σ. The normalizer H_N requires the additional generator β, which replaces $\mathbf{G}_J$ by $\mathbf{G}_{\langle 2J\rangle}$, where the angular brackets mean modulo five. To summarize, the generators Gen(H) are $\mathrm{Gen}(D_5)=\{\tau_5,\sigma\}$, $\mathrm{Gen}(H_C)=\{\delta,\tau_2\}$, $\mathrm{Gen}(H_P)=\{\delta,\tau_{10},\sigma\}$, and $\mathrm{Gen}(H_N)=\{\delta,\beta,\tau_{10},\sigma\}$.

Choosing D_5 as our fundamental symmetry group was somewhat arbitrary. We could have chosen D_{10} since the scattering pattern has tenfold symmetry, or we might have excluded reflections. An appealing feature of our procedure is that the nontrivial elements δ and β will result from any of these choices. Which symmetry group we start with can be chosen for calculational convenience.

Having constructed the symmetry operations δ and β, we can ask how they act on $S(\mathbf{q})$ and a real-space quasicrystal pattern. For our purposes, we consider a quasicrystal pattern, or "tiling," T as the set of points $T=\{\mathbf{p}(\mathbf{n}):\mathbf{n}\in\{N_P\}\}$ where $\mathbf{p}(\mathbf{n})=\sum_{J=1}^{4} n_J\tilde{\mathbf{G}}_J$ [cf. Eq. (1)] with $\tilde{\mathbf{G}}_J$ dual[4] to $\mathbf{G}_J$ and $\{N_P\}$ a subset of Z^4. The operator δ acting on $S(\mathbf{q})$ replaces the basis vector $\mathbf{G}_J$ by $\mathbf{G}_{\langle J-1\rangle}+\mathbf{G}_{\langle J+1\rangle}=r\mathbf{G}_J$, which rescales all the $\mathbf{q}$'s by a factor $r=2\cos(2\pi/5)=(\sqrt{5}-1)$. Transforming T by δ results[15] in

$$T'=M(\delta)T=\{\mathbf{p}(M(\delta)\mathbf{n}):\mathbf{n}\in N_P\}.$$

The new pattern, shown as dotted lines in Fig. 1(b), is similar to the original solid pattern but with a transformed length scale, and the vertices of the original pattern form a subset of the new vertices. Thus δ generates the inflation transformations described previously by many authors.

We say a lattice is scale invariant if a transformation which maps the vertices of the pattern to a subset of the original vertices is an automorphism of the indexing space, and therefore preserves the geometry of q space. (Notice that simple magnifying of a regular crystal lattice would not be an automorphism of indexing space.) Our definition of scale invariance is less restrictive than that derived by inflation rules, since we do not consider tile decorations and other properties special to the so-called "Penrose" patterns. We believe that our definition is a more general feature of quasilattices than inflation rules. Circumstantial evidence suggests that scale transformations which have the special properties of inflations occur only when the dimension of the index space is precisely twice the ordinary spatial dimension, e.g., in 2D patterns with point group D_m, when $E[m]=4$ ($m=5,8,10,12$), and for the icosahedral group.

The inflation symmetries for the reciprocal lattice are obtained solely from the dimensionality and point-group symmetry of the pattern. Incorporating the structure factor of a real crystal can lead to extinctions of $S(\mathbf{q})$ for subsets of the $\{\mathbf{q}\}$, which can lead to a higher degree of inflation symmetry than derived here.[2]

Having constructed all operators which obey our restrictions, we have shown that δ is the only generator of scale transformations for this pattern. In the cases we have looked at (D_5, D_7, D_8, and the icosahedral group) the generators in the centralizer which are not in the point group can be interpreted as scale transformations.

We now turn to the dramatic effect of transforming $S(\mathbf{q})$ in Fig. 1(a) and the solid pattern in Fig. 1(b) with the element β. The pattern $S'(\mathbf{q}(\mathbf{n}))=S(\mathbf{q}(M(\beta)\mathbf{n}))$ is plotted in Fig. 1(c). The scattering peak intensities have been systematically reordered. The image under β of the quasicrystal pattern is even more dramatic. Every point in the entire infinite pattern is mapped into a compact domain: the interior of two pentagons centered at the origin and rotated relative to each other by $2\pi/10$. We shall explain the action of β below, in terms of the projection method of generating quasicrystal patterns.[7,10,12,16]

Since we index all vectors in T and $S(\mathbf{q})$ by quadruples of integers, we can think of $S(\mathbf{q})$ and T as functions defined on a 4D lattice. We can then consider a figure such as Fig. 1(a) to be a projection of this 4D structure onto a particular 2D subspace, where the projection of each basis vector $\mathbf{e}_1,\ldots,\mathbf{e}_4\in R^4$ in the 4D space onto the 2D subspace is precisely $\mathbf{G}_1,\ldots,\mathbf{G}_4\in R^2$.

We define the vector "conjugate" to $\mathbf{q}(\mathbf{n})$ by

$$\bar{\mathbf{q}}(\mathbf{q})=\sum_{J=1}^{4} n_J\mathbf{G}_{\langle 2J\rangle}.$$

From Eqs. (1) and (5), we see that $\bar{\mathbf{q}}(\mathbf{q})=q(M(\beta)\mathbf{n})$. The direct sum $q\oplus\bar{\mathbf{q}}$ forms coordinates for the 4D space R^4, with basis vectors $\mathbf{e}_J=\mathbf{G}_J\oplus\mathbf{G}_{\langle 2J\rangle}$. Figure 1(b) represents the projection of the 4D pattern onto the 2D subspace $\mathbf{q}\oplus 0$, whereas transforming the pattern by β reprojects it into the conjugate space $0\oplus\bar{\mathbf{q}}$. A complete description of the scattering from a quasiperiodic pattern requires both coordinates $\mathbf{q}$ and $\bar{\mathbf{q}}$, so that results from scattering experiments should be plotted[10] both as $S(\mathbf{q}(\mathbf{n}))$ and $S(\bar{\mathbf{q}}(\mathbf{q}))$. We can similarly define a conjugate space $\bar{\mathbf{p}}(\mathbf{n})$ for T using the same procedure with $\mathbf{q}$ replaced by $\mathbf{p}$ and $\mathbf{G}_J$ by $\tilde{\mathbf{G}}_J$. (The coordinates $\mathbf{p}$ and $\bar{\mathbf{p}}$ were called $\mathbf{x}_{\parallel}$ and $\mathbf{x}_{\perp}$ in Ref. 10 and $\mathbf{u}$ and $\mathbf{v}$ in Ref. 4.)

In the conventional projection method of producing quasicrystal patterns, a point of the 5D cubic lattice is projected into $\mathbf{p}$ space only if its projection into the space perpendicular to $\mathbf{p}$ falls into a compact "acceptance" region. Our coordinate $\bar{\mathbf{p}}$ corresponds to a 2D subspace of the perpendicular space. Since the operation β reprojects the points of the quasicrystal pattern into the perpendicular subspace, β maps the entire quasicrystal pattern into a compact domain determined by the projection of the 5D acceptance region into the 2D subspace $\bar{\mathbf{p}}$. We note that in many cases it is convenient to project from a space whose dimension is larger than the minimal dimension of the indexing space. To generate Penrose patterns by projection from a 4D lattice, we must project from a noncubic lattice.

Plotted as a function of $\bar{\mathbf{q}}(\mathbf{q})$, $S(\mathbf{q})$ is *continuous.*[17] (This will not be true if the vertices have nonzero structure factors.) This suggests that any experiment which is sensitive to the lattice structure in reciprocal space should have data plotted as a function of both $\mathbf{q}$ and $\bar{\mathbf{q}}$. Gaps in the phonon spectra and eigenstates of Schrödinger operators should also be viewed as functions of these two pairs of 2D coordinates.

Our symmetry arguments outlined above can be generalized to other point groups and dimensions. For 3D icosahedral patterns, the point group D_5 is replaced by I, the icosahedral group, and $\mathrm{GL}_4(Z)$ is replaced by $\mathrm{GL}_6(Z)$. A matrix similar to δ has been previously displayed for the icosahedral tilings by Elser[2] and by Katz and Duneau.[18]

The extension to the point groups D_m in two dimensions will be similar: D_m will replace D_5 and $\mathrm{GL}_4(Z)$ will be replaced by $\mathrm{GL}_{E[m]}(Z)$. For $m=7$, we find two generators of scale transformations.

We are particularly indebted to Ted Chinburg of the University of Pennsylvania Mathematics Department for teaching us much of what we needed to know. We also acknowledge useful discussions with Robert Amman, Veit Elser, Seung-hwan Kim, and Joshua Socolar. This research was supported by the National Science Foundation under Contract No. DMR-8216718 at the Laboratory for the Research in the Structure of matter at the University of Pennsylvania and by National Science Foundation Contract No. DMR-8414640.

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