Proc. Natl. Acad. Sci. USA
Vol. 96, pp. 3502–3506, March 1999
Physics

Screw rotations and glide mirrors: Crystallography in Fourier space

ANJA KÖNIG AND N. DAVID MERMIN

Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853-2501

Contributed by N. David Mermin, January 22, 1999

ABSTRACT The traditional crystallographic symmetry elements of screw axes and glide planes are subdivided into those that are removable and those that are essential. A simple real-space criterion, depending only on Bravais class, determines which types can be present in any space group. This terminological refinement is useful in expressing the complementary relation between the real-space and Fourier-space formulations of crystal symmetry, particularly in the case of the two nonsymmorphic space groups that have no systematic extinctions ($I2_12_12_1$ and $I2_13$). A simple analysis in Fourier space demonstrates the nonsymmorphicity of these two space groups, which finds its physical expression not in a characteristic absence of Bragg peaks, but in a characteristic presence of electronic level degeneracies.

This paper serves two related purposes. (*i*) We show how the geometric language of conventional crystallography can benefit from a subdivision of screw axes and glide planes into two varieties, which we call *essential* and *removable*, and we note the elementary geometric criterion that determines which varieties can be found in a given crystal structure. (*ii*) We discuss, in the comparatively new framework of Fourier space crystallography, the peculiar space group $I2_12_12_1$ (no. 24) and its cubic counterpart, $I2_13$ (no. 199). Alone among all the 157 nonsymmorphic three-dimensional space groups, these two have no systematic extinctions in their diffraction patterns: every wave vector in the face centered reciprocal lattice is associated with a Bragg peak of nonzero intensity.

The relation between these matters is this: while crystals characterized by space-groups $I2_12_12_1$ and $I2_13$ contain 2-fold screw axes (2_1 axes), those 2-fold rotations fail to satisfy the Fourier-space criterion for a screw. This clash of Fourier-space and conventional nomenclature occurs for none of the other space groups with n_j in their International space-group symbols. The reason is that the n_j axes appearing in all space-group symbols, with the sole exceptions of these two, are essential screw axes. The space groups $I2_12_12_1$ and $I2_13$ are unique among these nonsymmorphic space groups in having only removable screw axes, a feature the International nomenclature obscures. In the Fourier-space scheme, rotations with removable screw axes never are regarded as screws. Nomenclatural confusion can be avoided by using the terms screw rotation and glide mirror to characterize rotations with essential screw axes and mirrors with essential glide planes.

Below we define essential and removable screw axes and glide planes and give the simple connection between the Bravais class of a crystal and whether or not it can have them. We show how these elementary geometric criteria for the removability of screw axes and glide planes lead directly in Fourier space to the absence of the corresponding screw rotations and glide mirrors. We construct the space groups $I2_12_12_1$ and $I2_13$ directly in Fourier space, identifying the Fourier-space structure that makes them nonsymmorphic in spite of the absence of screw rotations.

The publication costs of this article were defrayed in part by page charge payment. This article must therefore be hereby marked "*advertisement*" in accordance with 18 U.S.C. §1734 solely to indicate this fact.

PNAS is available online at www.pnas.org.

Screws and Glides in Three-Dimensional Real Space

The traditional description of crystal symmetry as summarized in the *International Tables of Crystallography* (1) specifies two kinds of rotation axes and mirror planes. (*a*) Axes or planes for which the rotation or mirror is a symmetry of the crystal without an accompanying translation. We shall call such rotation axes or mirror planes *simple*. (*b*) Axes or planes for which the rotation or mirror is only a symmetry of the crystal when accompanied by a translation parallel to the axis or plane.[a] Such rotation axes or mirror planes are called *screw axes* or *glide planes*.

The space group of a crystal is said to be *symmorphic* if there is a single point through which the axis of every rotation and the plane of every mirror is simple; if there is no such point the space group is *nonsymmorphic*.

In terms of these two kinds of axes or planes, a given rotation (specified by the angle and direction, but not the location of its axis) or a given mirror (specified by the orientation but not the location of its plane) can come in three varieties: (*i*) a given rotation (mirror) has only simple axes (simple planes); (*ii*) a given rotation (mirror) has both simple and screw axes (simple and glide planes); and (*iii*) a given rotation [mirror] has only screw axes (glide planes).

Cases *ii* and *iii* provide grounds for an elementary but nontraditional distinction between two kinds of screw axes or mirror planes. We shall call the screw axes or mirror planes occurring in case *ii removable* because their rotations or mirrors can be made simple by a mere translation of the axis or plane. We call the screw axes and mirror planes occurring in case *iii essential* because there is no parallel axis or plane about which the rotation or mirror is simple.

In terms of this distinction, there are evidently two different ways in which the space group of a crystal can be nonsymmorphic: (*i*) the crystal has at least one essential screw axis or at least one essential glide plane and (*ii*) all screw axes and glide planes are removable, but there is no single origin about which all rotations and mirrors have simple axes and planes.

Somewhat surprisingly, among all the 230 space groups in three dimensions, there are only two instances of nonsymmorphic space groups of type *ii*: the nonsymmorphic space groups $I2_12_12_1$ (no. 24) and $I2_13$ (no. 199) have only removable screw axes, but there is no single origin through which every axis is simple. Every one of the remaining 155 nonsymmorphic space

[a]Translations parallel to the rotation axis or mirror plane are special because such translations are restricted to a small number of discrete values. In contrast, given an axis A for a rotation r and any translation $\mathbf{d}$ perpendicular to that axis, there is another axis A' parallel to A such that application of r about A' is the same as application of r about A followed by translation through $\mathbf{d}$; and given a mirror plane P and any translation $\mathbf{d}$ perpendicular to that plane, there is another mirror plane P' parallel to P such that mirroring in P' is the same as mirroring in P followed by a translation through $\mathbf{d}$.

groups has at least one essential screw axis or essential glide plane.

The 2_1 occurring in the space-group symbols $I2_13$ and $I2_12_12_1$ are unique among all such subscripted rotation axes in being associated with removable 2-fold screw axes. This deviant notation[b] is needed to distinguish $I2_13$ and $I2_12_12_1$ from the corresponding symmorphic space groups I23 and I222. The notation is potentially misleading, because every screw axis in the nonsymmorphic cases is removable, and the symmorphic cases also contain (removable) 2-fold screw axes.

There are elementary geometric criteria that determine when a simple rotation axis or simple mirror plane can or cannot be accompanied by parallel screw axes or glide planes, and when a screw axis or glide plane is removable. The criteria depend only on the Bravais lattice of translations that leave the crystal invariant[c]: (*a*) a simple rotation axis (simple mirror plane) has screw axes (glide planes) parallel to it if and only if there are vectors in the lattice of translations whose components parallel to the axis (plane) are not in the lattice; and (*b*) a screw axis (glide plane) is essential if and only if its associated nonlattice translation is not the component of a lattice vector parallel to the axis (plane). These criteria follow straightforwardly from two facts: (*i*) the nonlattice translation associated with a screw axis or glide plane is only specified to within an additive vector from the lattice of translations; and (*ii*) a change of origin can shift that nonlattice translation by an arbitrary translation perpendicular to the rotation axis or mirror plane.

Several elementary geometric facts about screw axes and glide planes follow directly from these criteria.

The simplest consequences are for 2- or 3-fold rotations. The only possible nonlattice translations (modulo the sublattice along the axis) for a 2- or 3-fold screw axis is a half or a third of a lattice vector that primitively generates that sublattice. But nonlattice projections of lattice vectors on the axis also must differ from a lattice vector on the axis by a half or a third of a primitive generating vector for the sublattice on the axis. Therefore, if there are any lattice vectors with nonlattice projections onto a 2- or 3-fold screw axis, then that screw axis is removable. Thus, for example, because all rhombohedral and cubic Bravais classes have lattice vectors whose projections on the 3-fold axes are not lattice vectors, no space groups in these Bravais classes can have essential 3-fold screw axes, but all have removable 3-fold screw axes. And because the body-centered orthorhombic lattice has nonlattice projections on its 2-fold axes, both of its space groups have removable 2-fold screw axes.

Because a 6-fold axis (present only in the hexagonal system) is also an axis of both 2- and 3-fold symmetry, all lattice vectors must project to lattice vectors on the axis.[d] Therefore 6-fold screw axes are always essential.

Because 4-fold axes are also axes of 2-fold symmetry, twice the projection of any lattice vector onto the axis is a lattice vector. As a result, if there are nonlattice projections onto a 4-fold axis (which happens in the centered cubic and tetragonal Bravais classes) these prohibit essential 4_2 axes and produce removable 4_2 axes. They are compatible with the existence of essential 4-fold screw axes, but these must always occur as coexisting parallel 4_1 and 4_3 axes.

In the case of a mirror, all nonlattice projections of lattice translations into the plane of the mirror are the same, modulo the sublattice of translations in the plane of the mirror.[e] Simple mirrors must coexist with removable glide planes having such special nonlattice translations. Essential glide planes are those with nonlattice translations that are not of this special kind.

The View from Fourier Space

Fourier-space crystallography[f] starts with a point group whose operations act on the reciprocal lattice L of wave vectors. All point group operations act about the same origin, $\mathbf{k} = 0$. Under point group operations, density Fourier coefficients acquire a phase:

$$\rho(g\mathbf{k}) = e^{2\pi i\Phi_g(\mathbf{k})}\rho(\mathbf{k}). \qquad \textbf{[1]}$$

The *phase functions* Φ_g are linear[g] on L and satisfy, as a direct consequence of **1**, the *group compatibility condition*

$$\Phi_{gh}(\mathbf{k}) \equiv \Phi_g(h\mathbf{k}) + \Phi_h(\mathbf{k}). \qquad \textbf{[2]}$$

Two sets of phase functions related by

$$\Phi'_g(\mathbf{k}) \equiv \Phi_g(\mathbf{k}) + \chi(g\mathbf{k} - \mathbf{k}), \qquad \textbf{[3]}$$

where χ is linear on L, are said to be *gauge equivalent*. The function χ is called a gauge function and Φ' is said to differ from Φ by a *gauge transformation*. Such gauge equivalent phase functions can characterize densities that differ only by

$$\rho'(\mathbf{k}) = e^{2\pi i\chi(\mathbf{k})}\rho(\mathbf{k}). \qquad \textbf{[4]}$$

The significance of **4** with χ *linear* on L is that ρ' and ρ have identical positionally averaged real space autocorrelation functions. Symmetry types of densities therefore are characterized not by individual phase functions, but by gauge equivalence classes of phase functions. Note that it follows from **3** that the value of a phase function Φ_g at wave vectors $\mathbf{k}$ in the invariant subspace of the point group operation g (i.e., with $g\mathbf{k} = \mathbf{k}$) is the same throughout the entire gauge equivalence class. These gauge invariant values of phase functions play a central role in Fourier-space crystallography. Importantly, it follows from **1** that if $\Phi_g(\mathbf{k})$ is not zero (modulo 1) at a vector in the invariant subspace of g, then $\rho(\mathbf{k})$ must vanish—i.e., the Bragg peak associated with the reciprocal lattice vector $\mathbf{k}$ is extinguished.[h]

The above paragraph may be viewed as just a re-expression of well-known elementary facts about the symmetries of the real space density $\rho(\mathbf{r})$ in Fourier-space language. Thus for a point group operation g acting on a crystal in real space to leave the crystal invariant it must in general be accompanied by a translation $\mathbf{a}$ that depends on the origin about which g acts.

[b]It is cited in section 4.1 of volume A of the *International Tables of Crystallography* (1) as a violation of the "priority rule," which decrees that when a rotation has parallel 2 (simple) and 2_1 (screw) axes (i.e., when a screw axis is removable) it should be identified in the space-group symbol by a 2 without a subscript. The two space groups also are cited in section 3.5 of the *International Tables* as a second very special instance (the many examples of the first being provided by Friedel's law) of when a space group cannot be determined from the diffraction diagram. This feature of $I2_12_12_1$ and $I2_13$ seems first to have been noted independently by M. J. Buerger (2) and G. Zhdanov and V. Popelov (3).

[c]We know of no explicit statement of these simple rules in the crystallographic literature, perhaps because the distinction between essential and removable screw axes or glide planes has received so little attention.

[d]For a lattice vector that projected to a nonlattice vector on the axis would have to be both a third and a half of a primitive sublattice vector, modulo the sublattice on the axis, which is impossible.

[e]View the lattice as a family of lattice planes parallel to the mirror plane. The special translation is (any) one taking neighboring planes into one another.

[f]Formulated by Bienenstock and Ewald (4), refined and extended by Rokhsar, Wright, and Mermin (5), expounded in some detail by Rabson, Mermin, Rokhsar, and Wright (6) and Mermin (7), and given a rigorous and concise formulation by Dräger and Mermin (8). This paragraph states those definitions of Fourier-space crystallography that are essential for what follows.

[g]As a consequence of the requirement that point group operations preserve all positionally averaged real space density autocorrelation functions of all orders.

[h]Mermin (9) gives a concise discussion of how Fourier-space crystallography treats extinctions.

The phase function $\Phi_g(\mathbf{k})$ is nothing more than $\mathbf{a}\cdot\mathbf{k}/2\pi$. The different phase functions in a gauge equivalence class simply correspond to the different values of **a** associated with different choices of real space origin. The power of the Fourier-space formulation is that nothing changes when the lattice of wave vectors is generalized from a three-dimensional reciprocal lattice to a rank-D Z-module of wave vectors consisting of the integral linear combinations of D three-dimensional wave-vectors that are linearly independent over the integers.[i] This more general case applies to an enormous variety of aperiodic crystals whose densities have neither translational nor rotational symmetry in real space, but whose density autocorrelation functions continue to possess rotational symmetries. The Fourier-space language is essential if one wishes to explore in a three-dimensional space the three-dimensional symmetries of aperiodic crystals. It also can be a useful and powerful tool for characterizing the more familiar symmetries of ordinary periodic crystals, as we illustrate below.

Because all point group operations act through the origin of Fourier space, the terms screw and glide cannot apply to a point group operation in combination with a real-space origin through which it acts; the terms give global characterizations of the point group operation itself. Whether a point group operation g is a screw or glide depends on the associated phase function Φ_g. A point group operation g is a *screw rotation* or a *glide mirror* if and only if the associated phase function Φ_g has a nonzero (modulo unity) value for some reciprocal lattice vector **k** in the invariant subspace of g. As noted above, such values are invariant under gauge transformations (**3**).

It is a basic theorem of Fourier-space crystallography that a phase function Φ_g can vanish on the invariant subspace of g, if and only if there is a gauge in which it vanishes everywhere.[j] In such a gauge **1** reduces to

$$\rho(g\mathbf{k}) = \rho(\mathbf{k}), \qquad [5]$$

and g is a simple rotation or simple mirror about the point $\mathbf{r} = 0$. Thus a Fourier-space screw rotation or glide mirror is one that in real space has only essential screw axes or essential glide planes. Removable real-space screw axes or glide planes are not associated with Fourier-space screw rotations or glide mirrors.

We noted above that essential 2- and 3-fold screw axes are incompatible with the existence of vectors in the real-space lattice of translations with nonlattice projections on the axis. It is instructive to examine how the existence of such vectors leads directly in Fourier space to the vanishing of the associated phase function on the axis. Note first that such vectors exist in the real-space lattice of translations if and only if they exist in the reciprocal lattice of wave vectors.[k] For let P project into the invariant subspace, and let **a** be a direct lattice vector with $P\mathbf{a}$ not in the direct lattice. Because $P\mathbf{a}$ is not a direct lattice vector there must be some vector of the reciprocal lattice **k** for which $(P\mathbf{a}, \mathbf{k})$ is not an integral multiple[l] of 2π. But because $(P\mathbf{a}, \mathbf{k}) = (\mathbf{a}, P\mathbf{k})$ it follows that $(\mathbf{a}, P\mathbf{k})$ is not an integral multiple of 2π, which means that $P\mathbf{k}$ is not in the reciprocal lattice.

So it is enough to understand why the existence of a reciprocal lattice vector whose projection on a 2- or 3-fold axis is not in the reciprocal lattice, should guarantee the vanishing of the phase function associated with that 2- or 3-fold rotation at wave vectors on the axis. This follows from the group compatibility condition (**2**), which, applied repeatedly to the identity $g^n = e$ requires for arbitrary **k** that

$$0 \equiv \Phi_e(\mathbf{k}) \equiv \Phi_{g^n}(\mathbf{k}) \equiv \Phi_g(\mathbf{k} + g\mathbf{k} + \cdots + g^{n-1}\mathbf{k}) = \Phi_g(nP\mathbf{k}), \qquad [6]$$

where P projects into the invariant subspace of g. Necessarily, $nP\mathbf{k}$ is a reciprocal lattice vector. Therefore when n is 2 or 3, if $P\mathbf{k}$ is not a reciprocal lattice vector, then $P\mathbf{k}$ must differ from an integral multiple of **b** by $\pm\mathbf{b}/n$, where **b** is a primitive vector for the (one-dimensional) reciprocal sublattice along the axis. Consequently $nP\mathbf{k}$ differs from an integral multiple of $n\mathbf{b}$ by $\pm\mathbf{b}$. But because $\Phi_g(n\mathbf{b}) \equiv 0$ as a special case of **6**, it follows from **6** and the linearity of Φ_g that $0 \equiv \Phi_g(nP\mathbf{k}) \equiv \pm\Phi_g(\mathbf{b})$.

Fourier-Space Treatment of Space Groups Nos. 24 and 199

In conventional crystallographic language a space group is symmorphic if there is a single origin about which every point group operation is a symmetry of the crystal without an accompanying translation. In Fourier-space language this translates into the requirement that there should be a gauge in which every phase function vanishes (modulo unity). A necessary condition for a space group to be symmorphic is thus that the phase function for each point group operation vanishes on the invariant subspace of that operation. Is this also sufficient?

We show in the *Appendix* that if a phase function vanishes on its invariant subspace then there is a gauge in which it vanishes everywhere. But for a space group to be symmorphic, there must be at least one gauge in which every phase function vanishes everywhere. Space groups nos. 24 and 199 are the unique examples of space groups in which all phase functions vanish on their invariant subspaces but there is no gauge in which they all vanish everywhere. Nevertheless, their nonsymmorphicity is established by the existence of certain gauge invariant, nonvanishing linear combinations of phase functions.

We show below how this follows directly from the rules of Fourier space crystallography summarized above, but first we note that it is a result of general interest, rather than a mere isolated curiosity. Within any given arithmetic crystal class, the absence of a nonsymmorphic space group without extinctions is the necessary and sufficient condition for the space-group types of that class to be entirely determined by the values of their phase functions on the invariant subspaces of their associated point group elements. Clearly the condition is necessary: if an arithmetic crystal class contains a nonsymmorphic space group without extinctions then there are two space groups within that class (the second being the symmorphic one) whose phase functions vanish (and therefore agree) on the invariant subspaces of their point group operations. The space-group type in such an arithmetic crystal class is thus not determined by the phase functions on the invariant subspaces.

But the condition is also sufficient, for if $\Phi_g^{(1)}$ and $\Phi_g^{(2)}$ are two sets of phase functions associated with two different space-group types, then the differences $\Phi_g^{(1)} - \Phi_g^{(2)}$ also will satisfy the group compatibility condition (**2**), and are therefore themselves a set of phase functions for some space-group type. But if $\Phi_g^{(1)}$ and $\Phi_g^{(2)}$ agree on the invariant subspaces of their point-group operations, then their differences will vanish on all those invariant subspaces. Because $\Phi_g^{(1)}$ and $\Phi_g^{(2)}$ describe distinct space-group types they cannot be gauge equivalent, and therefore their differences cannot be gauge equivalent to a set of phase functions that are zero everywhere. Their differences are thus a set of phase functions describing a nonsymmorphic space group, in the same arithmetic crystal class, without extinctions.

[i]Now, however, functions linear on L can no longer be extended to functions linear on all of three-dimensional wave-vector space.

[j]The "if" part is obvious; the "only if" part has not been explicitly stated in the literature; we give a proof (valid for periodic or aperiodic crystals) in the *Appendix*.

[k]This fact also holds for 4- and 6-fold rotations and for mirrors.

[l]Because otherwise Pa would be in the reciprocal of the reciprocal lattice, which is the direct lattice.

We now show that the phase functions for space groups nos. 24 and 199 have this peculiar property:

(a) $I2_12_12_1$ (No. 24). The basis of the face-centered orthorhombic reciprocal lattice consists of the three vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ that can be expressed in terms of three mutually orthogonal vectors **a**, **b**, **c** of different lengths as:

$$\mathbf{b}_1 = \mathbf{b} + \mathbf{c},\ \mathbf{b}_2 = \mathbf{c} + \mathbf{a},\ \mathbf{b}_3 = \mathbf{a} + \mathbf{b}. \quad [7]$$

The possible phase functions are determined by requiring the group compatibility condition (**2**) to hold throughout the point group. To ensure this it suffices to impose **2** on the point group generating relations. The generators of $G = 222$ can be taken to be the two 2-fold rotations r_a and r_b about the axes **a** and **b**, with generating relations:

$$r_a^2 = e,\ r_b^2 = e,\ (r_a r_b)^2 = e. \quad [8]$$

Because $\Phi_e(\mathbf{k}) \equiv 0$, application of the group compatibility condition (**2**) to each of **8** gives

$$\Phi_{r_a}(r_a\mathbf{k} + \mathbf{k}) \equiv 0,\ \Phi_{r_b}(r_b\mathbf{k} + \mathbf{k}) \equiv 0,\ \Phi_{r_c}(r_c\mathbf{k} + \mathbf{k}) \equiv 0, \quad [9]$$

where we have used $r_c = r_a r_b$ to write **9** in a symmetric form.

Because phase functions are linear on the reciprocal lattice, for the conditions (**9**) to hold for all **k** it suffices for them to hold for each of the reciprocal lattice primitive vector $\mathbf{b}_i$ given in **7**. Because $r\mathbf{k} + \mathbf{k}$ gives twice the projection of **k** onto the axis of a 2-fold rotation r, each of the three relations (**9**) gives just a single condition, when applied to each of the three primitive vectors in **7**.

$$\Phi_{r_a}(2\mathbf{a}) \equiv 0,\ \Phi_{r_b}(2\mathbf{b}) \equiv 0,\ \Phi_{r_c}(2\mathbf{c}) \equiv 0. \quad [10]$$

Because $2\mathbf{a}$, $2\mathbf{b}$, and $2\mathbf{c}$ are primitive generating vectors for the three sublattices on the three 2-fold axes, every phase function vanishes on the invariant subspace of its point-group operation—i.e., there are no extinctions.

The distinct gauge equivalence classes of phase functions are determined by the possible values for the two independent point-group generators r_a and r_b at the primitive reciprocal-lattice generating vectors $\mathbf{b}_i$. Expanding the third of the conditions (**10**) using $r_c = r_a r_b$ and the group compatibility condition (**2**) gives

$$-\Phi_{r_a}(2\mathbf{c}) + \Phi_{r_b}(2\mathbf{c}) \equiv 0. \quad [11]$$

Subtracting the first of the two relations of **10** from **11** and adding the second, converts it into a relation between primitive generating vectors:

$$\Phi_{r_b}(2\mathbf{b}_1) - \Phi_{r_a}(2\mathbf{b}_2) \equiv 0. \quad [12]$$

This allows for two classes of phase functions, satisfying

$$\Phi_{r_b}(\mathbf{b}_1) - \Phi_{r_a}(\mathbf{b}_2) \equiv 0 \text{ or } \tfrac{1}{2}. \quad [13]$$

Because **12** is a linear combination of relations derived from the (gauge invariant) group compatibility conditions (**2**), the combination of phases on the left side of **13** is gauge invariant (as can also be verified directly). The nonzero choice for this combination therefore gives a nonsymmorphic space group. Even though Φ_{r_a} and Φ_{r_b} both vanish on the invariant subspaces of their point-group operations, there is no gauge in which they both vanish everywhere.

The peculiar combination of phases appearing in **13** has no obvious geometric significance. Interestingly, however, it is precisely the combination of phases that determines that the electronic levels in the nonsymmorphic space group $I2_12_12_1$ have 2-fold degeneracies at the points ½($\pm\mathbf{a} \pm \mathbf{b} \pm \mathbf{c}$). This is shown in König and Mermin (10), which explains how the theory of electronic level degeneracies in crystals (the theory of space-group representations in the periodic case) is directly related to the phase functions of Fourier-space crystallography.

(b) $I2_13$ (No. 199). We can continue to take **7** to give the primitive generating vectors for the face-centered-cubic reciprocal lattice, with the understanding that the mutually orthogonal vectors **a**, **b**, and **c** now have equal lengths. The generators of the tetrahedral point group 23 can be taken to be the 2-fold rotation r_a about **a** and the 3-fold rotation r_3 that takes $\mathbf{a} \to \mathbf{b}$, $\mathbf{b} \to \mathbf{c}$, and $\mathbf{c} \to \mathbf{a}$. The generating relations can be take to be

$$r_a^2 = e,\ r_3^3 = e,\ (r_3 r_a)^3 = e. \quad [14]$$

As in the orthorhombic case, applying the group compatibility condition (**2**) to each of these gives the conditions

$$\Phi_{r_a}(r_a\mathbf{k} + \mathbf{k}) \equiv 0,\ \Phi_{r_3}(r_3^2\mathbf{k} + r_3\mathbf{k} + \mathbf{k}) \equiv 0,$$
$$\Phi_{r_{3'}}(r_{3'}^2\mathbf{k} + r_{3'}\mathbf{k} + \mathbf{k}) \equiv 0, \quad [15]$$

where $r_{3'} = r_3 r_a$, which takes $\mathbf{a} \to \mathbf{b}$, $\mathbf{b} \to -\mathbf{c}$, and $-\mathbf{c} \to \mathbf{a}$. Each part of **15** gives a single relation when applied to the $\mathbf{b}_i$:

$$\Phi_{r_a}(2\mathbf{a}) \equiv 0,\ \Phi_{r_3}(2\mathbf{a} + 2\mathbf{b} + 2\mathbf{c}) \equiv 0,\ \Phi_{r_3'}(2\mathbf{a} + 2\mathbf{b} - 2\mathbf{c}) \equiv 0. \quad [16]$$

Each of these relations sets a Φ_g equal to zero at a vector that primitively generates the invariant subspace of g, so there are no extinctions along the axes of r_a, r_3, or $r_{3'}$. There are therefore no extinctions at all, because the group compatibility condition (**2**) insures that if Φ_g vanishes on its invariant subspace, the same is true for all point group operations conjugate to g.[m] But because $r_3' = r_3 r_a$, under the group compatibility condition (**2**) the third relation in **16** expands to

$$\Phi_{r_3}(2\mathbf{a} - 2\mathbf{b} + 2\mathbf{c}) + \Phi_{r_a}(2\mathbf{a} + 2\mathbf{b} - 2\mathbf{c}) \equiv 0. \quad [17]$$

Subtracting the first relation of **16** from **17** and adding the second, converts **16** to

$$\Phi_{r_3}(4\mathbf{b}_2) + \Phi_{r_a}(2\mathbf{b}_3 - 2\mathbf{b}_2) \equiv 0. \quad [18]$$

This allows for two distinct gauge equivalence classes of phase functions, differing by the gauge invariant relations[n]

$$\Phi_{r_3}(2\mathbf{b}_2) + \Phi_{r_a}(\mathbf{b}_3 - \mathbf{b}_2) \equiv 0 \text{ or } \tfrac{1}{2}. \quad [19]$$

The way in which these two nonsymmorphic space groups without extinctions emerge from this analysis is so simple and natural, that what is surprising is not their existence, but the fact that in every one of the remaining cases, the vanishing of every phase function on its invariant subspace is incompatible with the existence of any nonzero gauge invariant linear combination of phase functions. It would be interesting to know whether such possibilities are more common in higher dimensional spaces.[o]

Appendix

The value of a phase function Φ_g is gauge invariant on the invariant subspace of g, so if there is a gauge in which Φ_g

[m]For it follows from Eq. **2** that $\Phi_{rgr^{-1}}(r\mathbf{k}) \equiv \Phi_r(g\mathbf{k}) + \Phi_g(\mathbf{k}) + \Phi_{r^{-1}}(r\mathbf{k})$ and that $0 \equiv \Phi_{r^{-1}}(r\mathbf{k}) + \Phi_r(\mathbf{k})$. Therefore, when $g\mathbf{k} = \mathbf{k}$, $\Phi_{rgr^{-1}}(r\mathbf{k}) \equiv \Phi_g(\mathbf{k})$.

[n]As in the orthorhombic case, the nonvanishing of this combination of phases is directly related to the existence of electronic level degeneracies, as shown in König and Mermin (10).

[o]No examples that are not trivially related to these two have yet turned up in any of the many investigations of space groups for aperiodic three-dimensional crystals.

vanishes, it must vanish on that invariant subspace. We prove here that this vanishing is also sufficient: if $\Phi_g(\mathbf{k}) \equiv 0$ whenever $g\mathbf{k} = \mathbf{k}$, then there is a gauge in which Φ_g vanishes for all $\mathbf{k}$.

We must show that if

$$\Phi_g(\mathbf{k}) \equiv 0 \text{ whenever } g\mathbf{k} = \mathbf{k}, \tag{20}$$

then there is a function χ linear on the lattice of wave-vectors L such that

$$\Phi_g(\mathbf{k}) + \chi(g\mathbf{k} - \mathbf{k}) \equiv 0. \tag{21}$$

Let L_g be the set of all vectors $\mathbf{q}$ of L that are of the form

$$\mathbf{q} = g\mathbf{k} - \mathbf{k} \tag{22}$$

for some vector $\mathbf{k}$ in L. Clearly L_g is a sublattice of L. Define χ on L_g by

$$\chi(\mathbf{q}) \equiv -\Phi_g(\mathbf{k}). \tag{23}$$

The definition is unique even if the correspondence (**22**) between $\mathbf{q}$ and $\mathbf{k}$ is not, because if

$$\mathbf{q} = g\mathbf{k}' - \mathbf{k}' \tag{24}$$

with $\mathbf{k}' \neq \mathbf{k}$, then

$$g(\mathbf{k} - \mathbf{k}') = \mathbf{k} - \mathbf{k}'. \tag{25}$$

Therefore, $\mathbf{k} - \mathbf{k}'$ is in the invariant subspace of g where Φ_g vanishes. Because Φ_g is linear on L,

$$\Phi_g(\mathbf{k}) \equiv \Phi_g(\mathbf{k}'). \tag{26}$$

This leads to **21** holding for all $\mathbf{k}$ in L. Because χ is linear on L_g as a consequence of the linearity of $\mathbf{k} \to g\mathbf{k} - \mathbf{k}$ and the linearity of Φ_g, it only remains to show that χ can be extended from L_g to a function linear on the whole lattice L. This follows from the fact that any function linear on a submodule of a Z-module can be extended to a function linear on the entire Z-module. (We state this in the language of Z-modules—linear vector spaces over the integers—to establish that the proof applies even in the aperiodic case, where the rank of L exceeds the dimension of physical space.)

Let $\mathbf{b}_1, \ldots, \mathbf{b}_n$ be a basis for a rank n module L. Because L_g is a submodule, it also has a basis $\mathbf{c}_1, \ldots, \mathbf{c}_m$ and a rank $m \leq n$, (see for example theorem 7.8 of Hartley and Hawkes, ref. 11). Because $\mathbf{b}_1, \ldots, \mathbf{b}_n$ is a basis for the whole module we have

$$\begin{aligned} \mathbf{c}_1 &= \alpha_{11}\mathbf{b}_1 + \cdots + \alpha_{1n}\mathbf{b}_n \\ &\vdots \\ \mathbf{c}_m &= \alpha_{m1}\mathbf{b}_1 + \cdots + \alpha_{mn}\mathbf{b}_n \end{aligned}, \tag{27}$$

where α is an $m \times n$ matrix of integers.

Because both the $\mathbf{c}$ and the $\mathbf{b}$ are linearly independent over the rationals, it follows that the m n-dimensional row vectors of α are linearly independent over the rationals. Because the column rank of any matrix over a field is equal to its row rank, it follows that the n m-dimensional column vectors of α span a space of dimension m.

To extend the function χ linear on L_g to one linear on all of L, it suffices to specify values $\chi(\mathbf{b}_1), \ldots, \chi(\mathbf{b}_n)$ satisfying

$$\begin{aligned} \chi(\mathbf{c}_1) &= \alpha_{11}\chi(\mathbf{b}_1) + \cdots + \alpha_{1n}\chi(\mathbf{b}_n) \\ &\vdots \\ \chi(\mathbf{c}_m) &= \alpha_{m1}\chi(\mathbf{b}_1) + \cdots + \alpha_{mn}\chi(\mathbf{b}_n) \end{aligned}. \tag{28}$$

The existence of the $\chi(\mathbf{b}_i)$ is ensured by the fact that the n m-dimensional column vectors of α span an m-dimensional space over the rationals.

This work was supported by the National Science Foundation Grant DMR9531430.

1. Hahn, T., ed. (1995) *International Tables for Crystallography* (Kluwer, Dordrecht The Netherlands), Vol. A, 4th Ed.
2. Buerger, M. J. (1942) *X-Ray Crystallography* (Wiley, New York).
3. Zhdanov, G. & Popelov, V. (1945), *Zh. Eksp. Teor. Fiz.* **12,** 709–720.
4. Bienenstock, A. & Ewald, P. P. (1962) *Acta Crystallogr.* **15,** 1253–1261.
5. Rokhsar, D. S., Wright, D. C. & Mermin, N. D. (1988) *Phys. Rev. B* **37,** 8145–8149.
6. Rabson, D. A., Mermin, N. D., Rokhsar, D. S. & Wright, D. C. (1991) *Rev. Mod. Phys.* **63,** 699–733.
7. Mermin, N. D. (1992) *Rev. Mod. Phys.* **64,** 3–49.
8. Dräger, J. & Mermin, N. D. (1996) *Phys. Rev. Lett.* **76,** 1489–1492.
9. Mermin, N. D. (1995) *Phys. Stat. Sol.* **151,** 275–279.
10. König, A. & Mermin, N. D. (1997) *Phys. Rev. B* **56,** 13607–13610.
11. Hartley, B. & Hawkes, T. O. (1970) *Rings, Modules, and Linear Algebra* (Chapman and Hall, London).