# The space groups of axial crystals and quasicrystals

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We compute all the three-dimensional quasicrystallographic space groups with $n$-fold axial point groups and standard lattices by a method that treats crystals and quasicrystals on an equal footing. We do not rely on projecting higher-dimensional crystallographic space groups, our results are valid for arbitrary $n$, and our analysis is elementary. We regard space groups as a scheme for classifying diffraction patterns to be carried out in three-dimensional reciprocal space. The familiar three-dimensional crystallographic space groups with axial point groups emerge simply and directly as special cases of the general $n$-fold three-dimensional quasicrystallographic treatment with $n=3$, 4, and 6. We give a general discussion of extinctions in quasicrystals and give a simple (three-dimensional) geometrical specification of the extinctions for each axial space group. The paper is intended both for people trying to systematize quasicrystal diffraction patterns and for people interested in a simple alternative approach to the computation of crystallographic or quasicrystallographic space groups.

## CONTENTS



## I. INTRODUCTION

*We shall have mercifully little to say about the 230 space groups, except to point out that the number is larger than one might have guessed.*

Ashcroft and Mermin, 1976 (p. 125)

The well-known classification by Fedorov, Schönflies, and Barlow of the 230 crystallographic space groups in three dimensions applies to periodic arrangements of ob-

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jects, all alike in shape and orientation. Generally (and certainly before tunneling microscopy), direct imaging of atomic positions has been difficult, and crystallographers have used diffraction to deduce structure. The perfect translational order of a crystal implies δ-function Bragg peaks in the diffraction pattern, while the requirement of discreteness—atoms or arrangements of atoms take up space, so there must be a minimum distance between them—restricts the possible symmetry axes of a crystal, and hence of the diffraction pattern, to 2-, 3-, 4-, and 6-fold. The discovery in 1984 of icosahedral quasicrystals (Schechtman, Blech, Gratias, and Cahn, 1984), materials with forbidden rotational symmetry whose diffraction patterns nevertheless demonstrate long-range positional order, has motivated a reassessment of conventional crystallography.

The standard approach to extending crystallography to quasicrystals has relied on viewing quasicrystals as real-space projections of crystals in a higher number of dimensions; the number of dimensions required to describe a quasicrystal of arbitrary symmetry can be arbitrarily large. As a consequence, space-group computations following this approach have been limited to a six-dimensional projection yielding the icosahedral space groups (Levitov and Rhyner, 1988)[1] and to space groups with 5-, 8-, 10-, and 12-fold rotational axes, which are the only axial space groups obtained from five-dimensional projection (Gähler, 1988, 1990).

Rokhsar, Wright, and Mermin (1988a, henceforth RWM) have provided an alternative (but equivalent) formulation in a space with the physical number of dimensions, based on Bienenstock's and Ewald's reworking of ordinary crystallography (1962) in reciprocal space. Since reciprocal-space structure is generally more accessible to experiment than real space (or "real" hyperdimensional space!), we find this approach more natural. Using the reciprocal-space formulation, we derive here all the axial space groups[2] on standard lattices[3] in a unified and elementary scheme—not limited to the 5-, 8-, 10-, and 12-fold cases—in which crystals are merely particular members of general families.

We shall begin with a lattice which is not a crystallographic lattice in a higher dimensional real space, but a lattice in three-dimensional reciprocal space, determined by a simple generalization of the crystallographic rule giving the reciprocal lattice in terms of the wave vectors in the diffraction pattern. There is also a point group that permutes lattice vectors and is a suitable subgroup of the full set of symmetries of the diffraction pattern. Operations in the point group leave the density Fourier coefficients invariant except for a phase factor. These phases are central to our definition of the space group.

In Sec. II.A we review the concept of a standard lattice (Rokhsar, Mermin, and Wright, 1987; Mermin, Rokhsar, and Wright, 1987) and the classification of three-dimensional standard axial quasicrystallographic lattices (Mermin, 1989; Mermin, Rabson, Rokhsar, and Wright, 1990). We describe the two categories of standard axial lattices: vertical stackings ($V$ lattices) and staggered stackings ($S$ lattices) of standard two-dimensional quasicrystallographic lattices. The staggered stackings (of which the crystallographic examples are centered tetragonal and rhombohedral) exist only for rotational symmetries $n$ that are powers of prime numbers. In Sec. II.B we organize the well-known catalog of three-dimensional axial point groups along lines particularly well suited to the computation of the space groups. In Sec. II.C we review the RWM definition of the phase functions $\Phi_g(\mathbf{k})$, which relate the density Fourier coefficients at wave vectors connected by point-group operations. The values of these functions for those pairs $g$ and $\mathbf{k}$ with $g\mathbf{k}=\mathbf{k}$ determine the extinctions and the space groups. This reformulation agrees with the conventional one when applied to ordinary crystals.[4] In Sec. II.D we give a brief overview of the procedure we shall be carrying out in Secs. III–V, and in Sec. II.E we specify which point groups are compatible with a given lattice.

Section III reviews and simplifies RWM's classification of two-dimensional crystallographic space groups on standard lattices as a preliminary to extending it to the three-dimensional axial space groups in Secs. IV and V.

In Sec. IV we compute the space groups for vertically stacked standard lattices, and in Sec. V for staggered stackings. Each section concludes with a compact tabular specification of all the quasicrystallographic space groups.

In Sec. VI we discuss the general nature of extinctions in quasicrystallographic diffraction patterns, compute the extinctions for all the axial space groups, and characterize those extinctions by a simple set of three-dimensional, geometric rules.

In Sec. VII, we give a much lengthier (but no more informative) specification along the lines of the International Tables (International Union of Crystallography, 1987)

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[1]Janssen (1986) had previously applied the method to icosahedral space groups but arrived at the wrong number. A correct derivation (Rokhsar, Wright, and Mermin, 1988b) uses the purely three-dimensional approach that we follow here.

[2]The only non-axial non-crystallographic space groups are the icosahedral, which have been treated elsewhere (Rokhsar, Wright, Mermin, 1988b). In a companion paper to be published in *Reviews of Modern Physics,* one of us (N.D.M.) will apply the reciprocal-space approach to a unified treatment of the icosahedral and (three-dimensional) cubic space groups, as well as to the other nonaxial crystallographic space groups (orthorhombic, monoclinic, and triclinic).

[3]Nonstandard lattices do not exist for rotational symmetries less than 23-fold. See Sec. II.A.

[4]Rabson, Ho, and Mermin (1988) (Appendix) have also described how a space group so defined has a formal group structure, but this structure has no importance in our treatment.

to emphasize the close resemblance to the three-dimensional axial crystallographic space groups. In each case, we also give the results of applying the extinction rules of Sec. VI.

In the Appendix, we collect together a series of "gauge transformations" (corresponding to choices of origin in the crystallographic case) used in the course of our analysis, which are likely to prove useful in further extensions of our method.

Readers more interested in the conceptual basis of our approach than in its detailed application may want to skip Secs. III–V and read only the introductory part of Sec. VI. Readers more interested in results than their derivation may limit their perusal of Secs. III–V to an examination of Tables V and VI, from which the extinction rules of Sec. VI follow.

## II. PRELIMINARY FACTS

### A. Lattices

Traditional crystallography begins with periodicity in real space; this periodicity and the requirement of a minimum distance between atoms (discreteness) permit axes of 2-, 3-, 4-, and 6-fold symmetry only. The set of translations that bring an infinite crystal into coincidence with itself constitutes the real-space lattice.

The reciprocal lattice is traditionally defined in terms of the real-space lattice, as its mathematical dual.[5] A diffraction experiment directly specifies the reciprocal lattice. Each Bragg peak determines a wave vector according to the familiar Laue rules, and the set of integral linear combinations of all these wave vectors is the reciprocal lattice.

Because quasicrystals lack global translational symmetry, they have no real-space lattice. Most approaches to classifying their symmetries have viewed quasicrystals as two- or three-dimensional projections of ordinary crystals in an unphysically large number of dimensions,[6] thereby reintroducing a "real-space" lattice in the higher-dimensional space. Quasicrystals, however, have well-defined Bragg peaks, so without the intermediary of a higher-dimensional real-space lattice we can directly *define* the reciprocal lattice to be the set of all integral linear combinations of wave vectors determined by the diffraction pattern.

The feature that distinguishes quasicrystallographic from crystallographic reciprocal lattices is that the former are dense in $k$-space: for quasicrystals there are bounded regions of $k$-space in which more and more Bragg peaks can be found as the resolution becomes better and better. Since there is no shortest distance between reciprocal-lattice vectors, there are no grounds for prohibiting 5-fold or higher than 6-fold symmetry axes, and indeed quasicrystal diffraction patterns of Bragg peaks have been reported with 5-, 8-, 10-, and 12-fold symmetry axes.[7]

Since the only lattice we can associate with a quasicrystal in the physical number of dimensions is the reciprocal lattice of wave vectors determined by the Bragg peaks, throughout this paper the term "lattice" will always mean reciprocal lattice.

#### 1. Two-dimensional lattices

The simplest example of an $N$-fold-symmetric lattice in two dimensions consists of the $N$th roots of unity $\zeta_N^j=\exp(2\pi ij/N)$ and all their integral linear combinations, a set known as the cyclotomic integers of order $N$. Since the negative of a lattice vector is also in the lattice, the lattice is invariant under a rotation through $\pi$, and we can take $N$ to be even. Mermin, Rokhsar, and Wright (1987) call this the *standard N lattice* and show that for $N$ less than 46 (and greater than 2), all two-dimensional lattices are standard up to an overall scale and arbitrary rotation. The twofold lattices, although pathological from this point of view, are crystallographic and therefore well understood. For $N \geq 46$ more exotic "nonstandard" lattices exist. Here we shall consider only three-dimensional axial lattices with standard two-dimensional sublattices. Our classification of axial space groups is nevertheless complete for symmetry axes less than 23-fold.

We say that a lattice is generated by any set of vectors all integral linear combinations of which define the lattice, and we call any $N$-fold-symmetric set of vectors (such as the $N$th roots of unity) that generate the lattice a generating star (or, when there is no possibility of ambiguity, simply a star).

The $N$th roots of unity are integrally dependent; i.e., there are vanishing linear combinations with integral coefficients. Often it will be convenient to generate the lattice with the integrally independent subset of star vectors $\zeta_N^0, \zeta_N^1, \ldots, \zeta_N^{\nu-1}$, where $\nu$ is the smallest number of vectors that together can generate the lattice. This num-

[5]Less formally, as the set of wave vectors of plane waves with the periodicity of the real-space lattice.

[6]See, for example, Janssen (1986; this article, however, overlooks a consequence of scale invariance of the icosahedral lattices, for which see Rokhsar, Wright, and Mermin, 1988b), Levitov and Rhyner (1988), and Gähler (1988, 1990).

[7]See, for example, Wang, Chen, and Kuo, 1987 (8-fold); Kortan *et al.*, 1989 (10-fold); and Chen, Li, and Kuo, 1988 (12-fold). Most relevant to the present work, Idziak, Heiney, and Bancel (1987), Yamamoto and Ishihara (1988), Idziak and Heiney (1990), and Yamamoto *et al.* (1990) report nonsymmorphic space groups in the decagonal system.

ber is called the *rank* of the lattice and is given by the Euler totient function,[8]

$$\nu=\phi(N)=N\frac{p_1-1}{p_1}\frac{p_2-1}{p_2}\cdots , \tag{2.1}$$

where $p_i$ are the distinct prime factors of $N$. An integrally independent generating set is called primitive.

When $N=4$ or 6, there is a minimum distance between cyclotomic integers, and they therefore cannot be invariant under a rescaling. When $N>6$, however, the cyclotomic integers are invariant under multiplication by certain complex numbers whose modulus is not unity.[9] As a result, the common magnitude of the vectors in a generating star is not unique in a quasicrystallographic lattice, nor need the star have a unique orientation. What is important for our analysis below is the possible ambiguity in orientation. When $N$ is twice a power of a single prime number, the vectors of any generating star point uniquely along the directions of the roots of unity $\zeta_N^j$: no star of vectors pointing between $N$th roots of unity can generate the whole lattice. However, when $N$ is not twice a prime power, there is a second possibility: the vectors in a generating star can lie either along or between the $N$th roots of unity.[10]

A cautionary point: When $N=2n$ and $n$ is odd, one can also generate the $N$ lattice with an $n$-fold star of the vectors $\zeta_n^j=\zeta_N^{2j}$ (from which the vectors with $j=0,\ldots,\nu-1$ again generate the lattice primitively.) We shall generally make this choice when describing the two-dimensional sublattice of the "staggered lattices" introduced below. However, the second, inequivalent set of directions for $n$-fold generating stars is no longer between the directions of the first $n$-fold star.[11] It continues, of course, to be between the directions of the original $2n$-fold star, and is therefore rotated from the directions of the $n$-fold star by a quarter of the angle between adjacent $n$-fold-star vectors.[12] This is illustrated in Fig. 1.

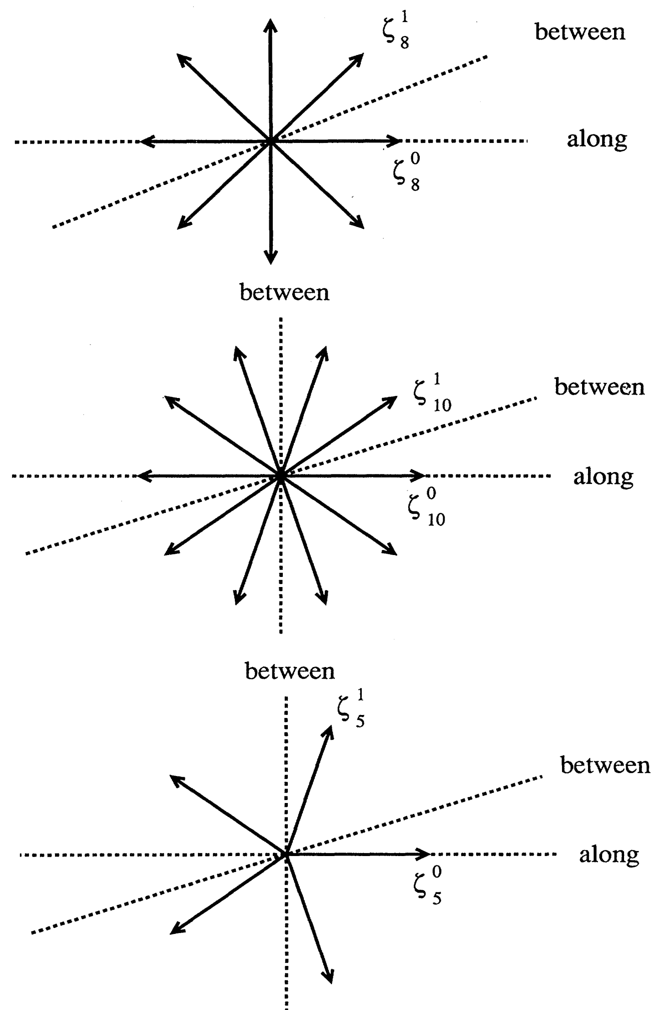


FIG. 1. Lattice directions along and between roots of unity (star vectors) for (a) $n=N$ twice even, (b) $n=N$ twice odd, and (c) $n$ odd, $N=2n$. Note that in case (c), the directions we designate "between" lie between $2n$th roots of unity, reflecting the fact that the $n$th and $2n$th roots of unity generate the same two-dimensional lattice. Note also in cases (b) and (c) that the directions between roots are perpendicular to directions along.

### 2. Three-dimensional axial lattices

An axial lattice has a unique axis of highest rotational symmetry (greater than twofold); while most crystallo-

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[8]See Lang (1984) p. 313 or Marcus (1977) p. 17 for the proof that the rank equals the Euler $\phi$ function. See the Appendix to Mermin, Rabson, Rokhsar, and Wright (1990) for a simple proof that $\nu$ angularly consecutive roots of unity do in fact generate the lattice.

[9]One of the attractions to viewing standard lattices in the complex plane is that rotations and rescaling are both represented as multiplication by a complex number.

[10]See RWM and references therein. For example, one can show that the vectors

$$\zeta_N'^j=\zeta_N^j+\zeta_N^{j+1}$$

constitute just such a star when $N$ is not twice a prime power. See Rabson (1991).

[11]The star between the directions of the first $n$-fold star is just its negative—i.e., the original star rescaled by the real factor $-1$.

[12]One easily sees that these directions are perpendicular to the directions of the original $n$-fold star.

TABLE I. Lattices and point groups. The possible stackings into three-dimensional axial lattices of the two-dimensional standard $N$ lattice depend on $N$ (which is necessarily an even number). If $N$ is twice a prime power, the stacking may be vertical or staggered (extreme top and bottom rows). Otherwise, only the vertical stacking is possible (middle rows). The column on the right shows the rotational orders $n$ of the points groups compatible with each lattice as discussed in Sec. II.E.

<table>
<tr><th>$N$-fold standard two-dimensional sublattice</th><th>stacking</th><th>Crystallographic Examples</th><th>Lattice Point Group (holohedry)</th><th>Rotational orders $n$ of compatible point groups</th></tr>
<tr><td rowspan="2">$N$ twice an odd prime power</td><td>Staggered $\frac{1}{2}N$-fold</td><td>rhombohedral</td><td>$\overline{\frac{1}{2}N}m$</td><td>$n=\frac{1}{2}N$</td></tr>
<tr><td rowspan="4">Vertical $N$-fold</td><td>hexagonal</td><td rowspan="5">$N/mmm$</td><td rowspan="2">$n=\frac{1}{2}N,\ N$</td></tr>
<tr><td>$N$ twice an odd number not an odd prime power</td><td>*none*</td></tr>
<tr><td>$N$ twice an even number not a power of two</td><td>*none*</td><td rowspan="3">$n=N$</td></tr>
<tr><td rowspan="2">$N$ a power of two</td><td>simple tetragonal</td></tr>
<tr><td>Staggered $N$-fold</td><td>centered tetragonal</td></tr>
</table>

graphic lattices are not axial, among quasicrystals only the icosahedral lattices[13] have more than a single axis of highest symmetry. We have calculated elsewhere the ways of stacking two-dimensional standard lattices to give three-dimensional axial lattices (which we shall refer to as "standard axial lattices," reminding the reader that all axial lattices with less than 23-fold symmetry are standard). We state below the pertinent elementary facts about standard axial lattices, referring the reader to Mermin, Rabson, Rokhsar, and Wright (1990) for proofs.

The obvious stacking places standard two-dimensional lattices directly atop each other: to generate it, one adds to the horizontal generating star of the two-dimensional sublattice an additional vertical lattice vector $\mathbf{z}$ of arbitrary length.[14] The rotational symmetry of the vertically stacked lattice is just the rotational symmetry $N$ of its two-dimensional, horizontal sublattice, which is always even. Except when $N$ is twice a power of a single prime number, this vertical stacking of standard lattices is the only standard axial lattice.

When $N$ is twice a prime power there exists one additional standard axial lattice, which is a staggered stacking of $N$-fold standard lattices, with a horizontal shift from layer to layer, analogous to the rhombohedral ($N=6$) and centered tetragonal ($N=4$) crystallographic lattices.[15] When $N$ is a power of 2, the staggered stacking continues to have the full $N$-fold symmetry; when $N$ is twice an odd prime power, however, the rotational symmetry $n$ of the staggered lattice is half that of its two-dimensional horizontal sublattice. This is the only way to get a three-dimensional axial lattice with odd rotational symmetry; the threefold rhombohedral lattice, for example, is such a stacking of sixfold hexagonal plane lattices.

The staggered lattice with $n$-fold symmetry ($n=p^s, p$ prime) repeats every $p$ layers and so includes the vector $p\mathbf{z}$ but not $\mathbf{z}$ itself. A vector connecting neighboring layers in the stacking is $\mathbf{z}+\alpha$, where the horizontal shift $\alpha$ between layers is given (up to an arbitrary horizontal lattice vector) by[16]

[13]The three icosahedral lattices are derived from the present point of view by Rokhsar, Mermin, and Wright (1987); the icosahedral space groups are derived in Rokhsar, Wright, and Mermin (1988b).

[14]In the crystallographic case $N=4$, there is a restriction on the magnitude of $\mathbf{z}$ to avoid accidental cubic symmetry.

[15]Mermin, Rabson, Rokhsar, and Wright (1990) show that, for given $N$, all possible staggered stackings differ only by scale factors and rotations.

[16]The reader may easily confirm that this gives the right shift for the rhombohedral ($N=6$) and centered tetragonal ($N=4$) lattices. The magnitude of $\mathbf{z}$ is again arbitrary except that in the crystallographic cases, there are restrictions to prevent accidental cubic symmetry.

$$\alpha = \frac{1}{\zeta_n - 1} . \tag{2.2}$$

We shall always treat the three-dimensional axial lattices as generated primitively by horizontal vectors (cyclotomic integers) and a single out-of-plane vector, $\mathbf{z}$ (vertical lattice) or $\mathbf{z}+\alpha$ (staggered lattice).

Table I summarizes the basic facts about standard axial lattices.

### B. The axial point groups and their generators

In constructing the space groups we shall make essential use of the fact that every point-group operation can be expressed as a product of powers of a small number (three, in the most complicated case) of group generators, a judicious choice of which can simplify the task considerably. In this subsection we therefore organize the axial point groups—three-dimensional point groups with a unique axis of highest symmetry at least threefold—according to their generating elements, giving the particular choices of generators we shall use throughout the paper, together with the relations among the generators that determine the group multiplication tables. Nothing foreign to conventional crystallography appears in this subsection, so knowledgeable readers might wish to skip it except to glance at Table III to note our particular choice of point-group generators.

We shall take each point group $G$ to be generated by at most three of the following operations: an $n$-fold rotation $r$, an $n$-fold rotoinversion $\bar{r}=ir$ (where $i$ is the three-dimensional inversion), a vertical mirror $m$ whose invariant plane includes the $n$-fold axis, a horizontal mirror $h$ whose plane is perpendicular to the $n$-fold axis, and a twofold (dihedral) axis $d$ perpendicular to the $n$-fold axis. We list these elements in Table II. We follow the convention of the International tables (International Union of Crystallography, 1987) by using the rotoinversion (rather than the rotomirror) as a generator.[17]

We now enumerate the axial point groups according to the elements from Table II that generate them, listing the generating relations and remarking on other features that will later prove useful. Although the particular choices of generators that follow are not unique, we shall adhere to them throughout the remainder of the paper: whenever we refer to the generators of a point group we shall always mean one of the seven sets that follow.

TABLE II. Symbols for point-group elements. We shall take every axial point group to be generated by at most three of these operations.

| | |
|---|---|
| $e$ | identity |
| $r$ | $n$-fold rotation |
| $\bar{r}$ | $n$-fold rotoinversion ($\bar{r} = ir$) |
| $m$ | vertical mirror including $n$-fold axis |
| $h$ | horizontal mirror perpendicular to $n$-fold axis |
| $d$ | dihedral axis perpendicular to $n$-fold axis |

($r$): The $n$-fold rotation $r$ generates the point group called $n$ in International notation; the generating relation is $r^n=e$.

($\bar{r}$): The $n$-fold rotoinversion $\bar{r}$ generates the point group $\bar{n}$. If $n$ is odd, $\bar{r}^n$ is the inversion, and the generating relation is $\bar{r}^{2n}=e$. When $n$ is even, the inversion is not present, and the generating relation is $\bar{r}^n=e$. When $n$ is twice odd, the group includes the horizontal mirror $h=\bar{r}^{n/2}$.

($r,h$): We may add the horizontal mirror $h$ to the group generated by the rotation $r$ to get the group called $\frac{n}{m}$ or $n/m$ when $n$ is even. When $n$ is odd, the International convention is to regard the group generated by $r$ and $h$ as the group $\overline{2n}$ generated by the $2n$-fold rotoinversion alone, as noted in the preceding case.[18] (Thus one regards $3/m$ as $\bar{6}$.) The generating relations are $r^n=h^2=e$ and $rh=hr$.

To each of these three groups, we may add vertical mirrors or dihedral axes.

($\bar{r},m$): The group generated by $\bar{r}$ and a vertical mirror $m$ is called $\bar{n}\frac{2}{m}$ or $\bar{n}m$, if $n$ is odd, and $\bar{n}2m$ if $n$ is even. This group also contains the dihedral axis $d=\bar{r}m$, so ($\bar{r},d$) generates the same group, and so does ($m,d$). As noted above, when $n$ is twice odd, $\bar{r}^{n/2}$ is the horizontal mirror $h$, so the dihedral axes lie in the planes of the vertical mirrors. When $n$ is not twice odd, the planes of the vertical mirrors interleave the dihedral axes. To the generating relation for $\bar{n}$, we add $m^2=(\bar{r}m)^2=e$.

We can add to the group generated by $r$ either $d$ or $m$, but not both, without introducing $h$.

[17] A major advantage of the International scheme persists in the quasicrystallographic case: when $n$ is an odd prime power (the only case where the problem arises) the International nomenclature provides a simple way to determine on which of two possible types of lattice a given point group can exist. Every $n$-fold point group is compatible with both the $n$-fold staggered lattice and the vertical $2n$-fold lattice, while every $2n$-fold point group is compatible only with the vertical $2n$-fold lattice. (In the Schönflies scheme some $n$-fold groups are compatible only with the $2n$-fold lattice, and one $2n$-fold group is compatible with the $n$-fold lattice.)

[18] Warning: when $n$ is odd the $n$-fold rotoinversion—the product of an $n$-fold rotation with the inversion—is of group-theoretic order $2n$, as noted above; it should not thereby be confused with the $2n$-fold rotoinversion, which is also of group-theoretic order $2n$.

TABLE III. The three-dimensional axial point groups. We list here the point-group generators we shall use throughout the paper and a complete set of independent generating relations for each point group. Whenever we subsequently refer to the generators of a point group, we shall mean the particular choice of generators specified here. The group operations are defined in Table II. Our choice of $\bar{r}$ as a generator agrees with the International scheme, in which there are seven axial point groups for even rotational order $n$ and five for odd. (The Schönflies scheme uses the rotomirror $\tilde{r}=hr$ rather than the rotoinversion $\bar{r}$ as a generator. The International scheme is preferable because it incorporates naturally the compatibility of point groups with certain lattices, as noted in footnote 17).

| generators | generating relations | International (Hermann-Mauguin) | Schönflies |
|---|---|---|---|
| $\bar{r}$ | $\bar{r}^n = e$ $n$ even<br>$\bar{r}^{2n} = e$ $n$ odd | $\bar{n}$ | $S_n$ $n$ twice even<br>$C_{\frac{n}{2}h}$ $n$ twice odd<br>$S_{2n}$ or $C_{ni}$ $n$ odd |
| $\bar{r}, m$ | $m^2 = \bar{r}^n = (\bar{r}m)^2 = e$ $n$ even<br>$m^2 = \bar{r}^{2n} = (\bar{r}m)^2 = e$ $n$ odd | $\bar{n}2m$ $n$ even<br>$\bar{n}\frac{2}{m} = \bar{n}m$ $n$ odd | $D_{\frac{n}{2}d}$ $n$ twice even<br>$D_{\frac{n}{2}h}$ $n$ twice odd<br>$D_{nd}$ $n$ odd |
| $r$ | $r^n = e$ | $n$ | $C_n$ |
| $r, m$ | $r^n = m^2 = (rm)^2 = e$ | $nmm$ $n$ even<br>$nm$ $n$ odd | $C_{nv}$ |
| $r, d$ | $r^n = d^2 = (rd)^2 = e$ | $n22$ $n$ even<br>$n2$ $n$ odd | $D_n$ |
| $r, h$<br>($n$ even only) | $r^n = h^2 = e$;<br>$rh = hr$ | $\frac{n}{m} = n/m$ | $C_{nh}$ |
| $r, h, m$<br>($n$ even only) | $r^n = h^2 = m^2 = (rm)^2 = e$;<br>$rh = hr$;<br>$mh = hm$ | $\frac{n}{m}\frac{2}{m}\frac{2}{m} = n/mmm$ | $D_{nh}$ |

$(r,d)$: When $n$ is odd, the dihedral axes $d$ and $d'=rd$ are conjugate,[19] and the group generated by $r$ and $d$ is called $n2$. When $n$ is even, $d$ and $d'$ are not conjugate, and the group is called $n22$. The generating relations are $r^n=d^2=(rd)^2=e$.

$(r,m)$: When $n$ is odd, the vertical mirrors $m$ and $m'=rm$ are conjugate and the group is called $nm$. When $n$ is even, $m$ and $m'$ are not conjugate, and the group is called $nmm$. The generating relations are $r^n=m^2=(rm)^2=e$.

$(r,m,h)$: Either $d$ or $m$ added to the group generated by $(r,h)$ implies the other; the resulting group is called $\frac{n}{m}\frac{2}{m}\frac{2}{m}$ or $n/mmm$. As noted for the generators $(r,h)$, this case arises only when $n$ is even. When $n$ is odd, the International convention adds $d$ or $m$ to the group generated by the $2n$-fold rotoinversion, yielding the group $\overline{2n}2m$. The generating relations are just those for $(r,m)$ and $(r,h)$ with the additional fact that $h$ commutes with $m$.

Tables III summarizes the axial point groups, the generators we shall be using, the generating relations, and the International (and Schönflies) nomenclature.

### C. Space groups and point groups in reciprocal space

We review here the theory and terminology of Rokhsar, Wright, and Mermin (1988a, "RWM"), who generalize the reciprocal-space derivation of crystallographic space groups by Bienenstock and Ewald (1962) to include quasicrystals as well.

Two materials with density Fourier coefficients $\rho(\mathbf{k})$ and $\rho'(\mathbf{k})$ have identical translationally invariant macroscopic properties if

$$\rho'(\mathbf{k}_1)\rho'(\mathbf{k}_2)\rho'(\mathbf{k}_3)\cdots=\rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\rho(\mathbf{k}_3)\cdots \quad (2.3)$$

[19]When we come to consider extinctions (Sec. VI) we shall need to examine one element from each conjugacy class of the point group, so we pause to remark that if $n$ is odd then all dihedral axes $d$ are conjugate in every point group, as are all vertical mirrors $m$. If $n$ is even, however, then $d'=rd$ is a member of a second family of conjugate axes that are not conjugate to $d$ (and similarly for $m'=rm$ and $m$). The conjugacy for odd $n$ is easily established analytically. The generating relations $d^2=(rd)^2=e$ imply $r^kd=dr^{-k}$, so when $n=2k+1$, multiplying by $r^{k+1}$ on the left gives the relation $d=r^k(rd)r^{-k}$, which expresses the conjugacy of $d$ and $rd$.

for all sets of reciprocal-lattice vectors with vanishing sums $\sum \mathbf{k}_i = 0$. We may equivalently write this condition as

$$\rho'(\mathbf{k}) = e^{2\pi i \chi(\mathbf{k})} \rho(\mathbf{k}) , \tag{2.4}$$

where $\chi$, called a gauge function, is linear modulo an integer on the reciprocal lattice.[20] Two densities so related by a gauge function are called gauge equivalent and correspond to macroscopically indistinguishable systems.

The point group $G$ of a material with density $\rho$ is the set of operations $g$ that do not change any of the macroscopic properties of a sample. These are just the operations for which there is a gauge function linking $\rho(g\mathbf{k})$ to $\rho(\mathbf{k})$ for every lattice vector:

$$\rho(g\mathbf{k}) = e^{2\pi i \Phi_g(\mathbf{k})} \rho(\mathbf{k}) . \tag{2.5}$$

The gauge functions $\Phi_g$ are called phase functions. Equation (2.5) defines phase functions only up to integers; we use the symbol $\equiv$ to indicate equality modulo an integer.

Two sets of phase functions $\Phi$ and $\Phi'$ describing gauge-equivalent densities $\rho$ and $\rho'$ (2.4) must be related by

$$\Phi'_g(\mathbf{k}) \equiv \Phi_g(\mathbf{k}) + \chi((g-1)\mathbf{k}) \tag{2.6}$$

for every $g$ in the point group and every $\mathbf{k}$ in the lattice;[21] we call such sets of phase functions gauge equivalent and Eq. (2.6) a gauge transformation. Note that since $\chi(0) \equiv 0$, if $g\mathbf{k} = \mathbf{k}$ then the value of $\Phi_g(\mathbf{k})$ is gauge invariant. This simple fact will be of critical importance in enabling us to establish the inequivalence of distinct space groups. It also plays a crucial role in the treatment of extinctions, since Eq. (2.5) requires $\rho(\mathbf{k})$ to vanish if $g\mathbf{k} = \mathbf{k}$ and $\Phi_g(\mathbf{k}) \neq 0$.

All the symmetry-determined properties of a material reside in the phase functions defined by Eq. (2.5), but a gauge transformation changes none of these properties. We are therefore interested in classifying families of gauge-equivalent phase functions. We say that the members of each family of gauge-equivalent phase functions belong to the same space group. In the crystallographic case there is a one-to-one correspondence between the families of gauge-equivalent phase functions and the axial space groups as traditionally defined.[22]

In a small number of the axial quasicrystallographic cases, there can be two gauge-inequivalent families of phase functions that describe the same structure, viewed with respect to the two alternative families of lattice-generating stars described in Sec. II.A.1; those two families should clearly be viewed as constituting only a single space group. A closely related identification of gauge-inequivalent families occurs in the icosahedral case (Rokhsar, Wright, and Mermin, 1988b), where the ambiguity that results in the identification of gauge-inequivalent families of phase functions stems not from a nontrivial reorientation of the lattice-generating vectors but from a change in their scale at fixed orientation. (In the axial case the change in orientation is accompanied by a change in scale as well.) Gauge-inequivalent families of phase functions that have been further identified in this way are called *scale equivalent.*

The quasicrystallographic space groups are the scale-equivalent families of gauge-equivalent phase functions. The question of scale equivalence, which never arises in the crystallographic case, is easily settled[23] (although also easily overlooked). The main part of determining the space groups lies in establishing the distinct classes of gauge-equivalent phase functions.

A space group is called *symmorphic* if there is a gauge in which all its phase functions vanish.

### D. Determination of the phase functions (overview)

The phase functions for the point-group generators entirely determine the phase functions for the whole point group, $G$. This follows from the trivial fact that $\rho((fg)\mathbf{k}) = \rho(f(g\mathbf{k}))$ for any $f$ and $g$ in $G$. It then follows from the definition (2.5) of the phase function that

$$\begin{aligned} \exp[2\pi i \Phi_{fg}(\mathbf{k})]\rho(\mathbf{k}) &= \exp[2\pi i \Phi_f(g\mathbf{k})]\rho(g\mathbf{k}) \\ &= \exp[2\pi i \Phi_f(g\mathbf{k})] \\ &\quad \times \exp[2\pi i \Phi_g(\mathbf{k})]\rho(\mathbf{k}) . \end{aligned} \tag{2.7}$$

[20]By linearity we mean only that $\chi(\mathbf{k}_1 - \mathbf{k}_2) = \chi(\mathbf{k}_1) - \chi(\mathbf{k}_2)$ (modulo 1) for all reciprocal lattice vectors $\mathbf{k}_1$ and $\mathbf{k}_2$. In ordinary crystals, the most general gauge function, $\chi(\mathbf{k}) = \mathbf{a}\cdot\mathbf{k}$, corresponds to a uniform translation by $\mathbf{a}$. A general quasicrystallographic change of gauge corresponds to a real-space translation and a phason shift.

[21]By $(g-1)\mathbf{k}$ we mean, of course, the lattice vector $g\mathbf{k} - \mathbf{k}$.

[22]See Bienenstock and Ewald (1962) and the Appendix to Rabson, Ho, and Mermin (1988), as well as RWM. This will also emerge explicitly from our computations below. In the more general crystallographic cases (e.g., cubic, orthorhombic) there can be a further identification of gauge-inequivalent classes analogous to that described below for axial quasicrystals. This will be illustrated in the companion paper.

[23]For the axial space groups we discuss here it arises only for the two entries of "3" in Table V (which would have been 4 if scale equivalence had not been taken into account), as discussed below in Sec. IV.B.1 and as noted in the caption of Table XII. This was first pointed out for dodecagonal quasicrystals by Gähler (1988, 1990).

Therefore the phase functions $\Phi_f$ and $\Phi_g$ determine $\Phi_{fg}$ up to an integer:

$$\Phi_{fg}(\mathbf{k}) \equiv \Phi_f(g\mathbf{k}) + \Phi_g(\mathbf{k}) \ . \tag{2.8}$$

We shall refer to Eq. (2.8) as the group compatibility condition. As a special case of (2.8) [or directly from the definition (2.5)], note that

$$\Phi_e(\mathbf{k}) \equiv 0 \ , \tag{2.9}$$

where $e$ is the identity operation in $G$.

Since any element of $G$ can be expressed as a product of generators, by repeatedly applying the group compatibility condition we can express all phase functions in terms of the phase functions at the generators of $G$, of which there are at most three. There are, however, many different ways of expressing an element of $G$ as a product of generators. The group generating relations can be viewed as a set of identities satisfied by the generators that insures the identity of all such expressions. If they are to yield unambiguous phase functions for every element of $G$, the phase functions at the generators must therefore be constrained by the application of the group compatibility condition (2.8) to all of the group generating relations.

The generating relations in Table III can be cast into just two general forms: either they relate some power of a single group generator to the identity, $f^a = e$, or they relate two group generators $f$ and $g$ by $fgf = g$. Corresponding to these two forms, the group compatibility condition (2.8) requires either

$$0 \equiv \Phi_f((1 + f + \cdots + f^{a-1})\mathbf{k}) \quad (f^a = e) \tag{2.10}$$

or

$$0 \equiv \Phi_f(gf\mathbf{k}) + \Phi_g(f\mathbf{k}) + \Phi_f(\mathbf{k}) - \Phi_g(\mathbf{k}) \quad (fgf = g) \ . \tag{2.11}$$

Because the phase functions are linear on the lattice, phase functions at arbitrary lattice vectors can be expressed as integral linear combinations of phase functions at a set of vectors that generates the lattice.[24] It therefore suffices to determine the phase functions only for the group generators and only at the lattice-generating vectors. This set of phases is restricted only by the application of constraints of the form (2.10) or (2.11) evaluated at each lattice-generating vector. Application of the constraints leads to an infinite family of solutions for each gauge equivalence class, reflecting the freedom to alter any set of phase functions by an arbitrary gauge transformation. The analysis is greatly simplified by not carrying along this considerable degeneracy, seeking instead a unique representative of each gauge equivalence class, by introducing a series of particular gauges (summarized in the Appendix) that pin down the values of the phase functions. We do this in stages, first (Sec. III) introducing gauges that fix the values of the phase functions in the $z=0$ plane and then [Secs. IV (vertical lattices) and V (staggered lattices)] introducing gauges that further determine the values of the phase functions at the single out-of-plane lattice-generating vector.

In this way we arrive at a finite number of choices for the phase functions. We note that any two of these choices disagree in some of their gauge-invariant values, which insures that each choice provides a single representative for a distinct class of gauge-equivalent phase functions.

This procedure thus establishes for the axial space groups by explicit computation that two phases functions that agree in all their gauge-invariant values are gauge equivalent.[25] (The converse is trivial.)

### E. Compatibility of a quasicrystal's point group with its lattice

The point group (about any lattice point) of the vertical lattice with $n$-fold symmetry,[26] and of the staggered lattices with $n = 2^s$, is $n/mmm$. The point group of the staggered lattices with $n$ an odd prime power is $\bar{n}2/m$ (Mermin, Rabson, Rokhsar, and Wright, 1990).

Since the point group of a quasicrystal is the point group of all its macroscopic translationally invariant properties, the point group of a quasicrystal must be a subgroup of the point group of the lattice determined by its diffraction pattern. We also adopt the crystallographic rule that the point group of a vertical or staggered lattice should be no larger than required to accommodate the point group of the quasicrystal with that stacking.[27]

[24]More precisely, linearity is modulo an integer because phase functions are defined only to within an integer. We shall not continually remind the reader of this, understanding phase function arithmetic always to be conduced modulo an integer. [We shall, however, distinguish in equations between strict equality ("=") and equality modulo an integer ("≡").]

[25]For an alternative proof of this result for axial space groups that does not rely on explicit computation, see Rabson, Cornell Ph.D. thesis (1991). For a few nonaxial crystallographic cases, the result need not hold, as will be noted in the companion paper.

[26]Recall that the rotational symmetry $n$ of the vertical stacking is the same as the rotational symmetry $N$ of its horizontal sublattice, which is always even.

[27]In the crystallographic case there is nothing to prevent a lattice from distorting to the minimum symmetry compatible with that of the unit cell. For example, a square lattice decorated at its vertices with scalene triangles would distort to a skew lattice. In a quasicrystal there is no real-space unit cell, and the grounds for imposing a similar restriction are not well established. We do not pursue the point further here, but warn the reader that it has not been resolved.

The two rules together require that: (1) If a quasicrystal with a point group of even order $n$ has a vertical lattice, the rotational symmetry of the lattice is also $n$-fold; (2) If a quasicrystal with a point group of odd order $n$ has a vertical lattice, the rotational symmetry of the lattice is $2n$-fold; (3) A quasicrystal with a point group of order $n$ can have a staggered lattice only if $n$ is a prime power equal to the rotational order of the staggered lattice. The last column of Table I lists the point groups of quasicrystals compatible with each type of lattice.

When discussing point groups of rotational order $n$, we shall always use the star of $n$th roots of unity $\zeta_n^j$ to generate the lattice. Henceforth, we drop the subscript and write $\zeta$ for $\zeta_n$. By $\nu$ we shall mean the rank of the horizontal sublattice, so the rank of the full three-dimensional lattice is always $\nu+1$.

## III. THE PHASES IN THE $z=0$ PLANE

We show below[28] for both primitive and staggered lattices that if the rotational order $n$ of the lattice is not a power of 2, then we can choose a gauge in which all phase functions vanish in the $z=0$ plane. When $n$ is a power of 2 we can choose a gauge in which all phase functions vanish in the $z=0$ plane, with two possible exceptions: (a) If the horizontal mirror $h$ is a generator of $G$, then it is also possible for the associated phase function to be nonzero, with $\Phi_h(\zeta^j)\equiv\frac{1}{2}$ (for all $j$); (b) If a vertical mirror $m$ or a dihedral axis $d$ is a generator of $G$, then it is also possible for the associated phase functions to be nonzero with $\Phi_d(\zeta^j)\equiv\frac{1}{2}$ or $\Phi_m(\zeta^j)\equiv\frac{1}{2}$. If the generators of $G$ include both $h$ and $m$ (as happens only when $G$ is $n/mmm$), then both possibilities can be independently realized, leading to four gauge-inequivalent choices of phase functions in the $z=0$ plane.[29]

The steps leading to these conclusions are simple but require breaking the problem up into many different cases. As an aid to the reader, we give in Fig. 2 a diagram of the logical structure of Sec. III.

### A. Making $\Phi_r$ and $\Phi_{\bar r}$ vanish in the $z=0$ plane

If $r$ is a generator of $G$, we can make $\Phi_r(\zeta^j)$ vanish in the $z=0$ plane with a gauge transformation given by the gauge function[30]

$$\chi(\zeta^j)=\frac{1}{n}\Phi_r\left[\frac{n\zeta^j}{1-\zeta}\right],\quad j=0,\ldots,\nu-1\,. \tag{3.1}$$

(By linearity, this form extends to $j=0,\ldots,n-1$.) Since $\Phi_r$ is defined only at lattice vectors, it is important to note that $n\zeta^j/(1-\zeta)$ is indeed a lattice vector, as a consequence of the identity[31]

$$n=(1-\zeta)(1-\zeta^2)\cdots(1-\zeta^{n-1})\,. \tag{3.2}$$

Since $r\beta=\zeta\beta$ for any vector $\beta$ in the $z=0$ plane, the gauge transformation (2.6) determined by Eq. (3.1) changes $\Phi_r(\zeta^j)$ by

$$\Delta\Phi_r(\zeta^j)\equiv\chi((r-1)\zeta^j)=\chi((\zeta-1)\zeta^j)\equiv\frac{1}{n}\Phi_r(-n\zeta^j)\equiv-\Phi_r(\zeta^j)\,. \tag{3.3}$$

Thus $\Phi_r$ vanishes in this gauge for all lattice-generating vectors in the $z=0$ plane and hence for the entire plane.

Similarly, if $\bar r$ is a generator of $G$, we can make $\Phi_{\bar r}(\zeta^j)$ vanish with a gauge transformation given by the gauge function

$$\chi(\zeta^j)=\frac{1}{n}\Phi_{\bar r}\left[\frac{n\zeta^j}{1+\zeta}\right],\quad j=0,\ldots,\nu-1 \tag{3.4}$$

(which form also extends to $j=0,\ldots,n-1$). The fact that $n\zeta^j/(1+\zeta)$ is a lattice vector follows directly from $n/(1+\zeta)=n(1-\zeta)/(1-\zeta^2)$ in view of the identity (3.2). Since the rotoinversion gives $\bar r\beta=-\zeta\beta$ for any $\beta$ in the $z=0$ plane, the gauge transformation given by Eq. (3.4) changes $\Phi_{\bar r}(\zeta^j)$ by

$$\Delta\Phi_{\bar r}(\zeta^j)\equiv\chi((\bar r-1)\zeta^j)=\chi((-\zeta-1)\zeta^j)\equiv\frac{1}{n}\Phi_{\bar r}(-n\zeta^j)\equiv-\Phi_{\bar r}(\zeta^j)\,. \tag{3.5}$$

Thus $\Phi_{\bar r}$ vanishes in this gauge throughout the $z=0$ plane.

We next investigate the phase functions for the remaining generators of $G$ in the gauges in which $\Phi_r(\zeta^j)$ or

[28]Many of the results that follow were established by Rokhsar, Wright, and Mermin (RWM, 1988a) in the course of classifying the two-dimensional space groups on standard lattices. We rederive them here in a somewhat simpler way from the slightly different three-dimensional perspective.

[29]For vertical lattices, the in-plane phases are completely independent of the out-of-plane phases, and all of these possibilities are available. For staggered lattices, the in-plane and out-of-plane phases are not always independent, and we shall find further restrictions on the in-plane phases.

[30]Because they are linear, gauge functions are defined by their values on a set of vectors that generate the lattice. Throughout this section we require the value of the gauge function only in the $z=0$ plane, so there is no need to specify $\chi(\mathbf{z})$ for the vertically stacked lattices or $\chi(\mathbf{z}+\alpha)$ for the staggered lattices. We shall examine the consequences of this additional gauge degree of freedom in the sections that follow.

[31]This follows from factoring $z-1$ from both sides of the polynomial identity $z^n-1=(z-1)(z-\zeta)\cdots(z-\zeta^{n-1})$, and then setting $z$ to 1.

$\Phi_{\bar{r}}(\xi^j)$ vanishes. Note that if a generator is either a vertical mirror $m$ or a dihedral axis $d$, then it does not matter which particular such mirror or dihedral axis we examine. Consider, for example, the case in which $r$ and $m$ are generators. Any other vertical mirror $m'$ is related to $m$ by $m'=r^k m$, so an application of the group compatibility condition (2.8) gives $\Phi_{m'}(\xi^j)\equiv\Phi_{r^k}(m\xi^j)+\Phi_m(\xi^j)$. But if $\Phi_r$ vanishes in the $z=0$ plane, then Eq. (2.10) gives $\Phi_{r^k}(m\xi^j)\equiv\Phi_r((1+r+\cdots+r^{k-1})m\xi^j)\equiv 0$, and therefore $\Phi_m\equiv\Phi_{m'}$ in the $z=0$ plane. The same argument can be given when the rotoinversion $\bar{r}$ is a generator instead of the rotation $r$ or when a dihedral axis $d$ is the group generator instead of a vertical mirror $m$.

We now consider separately the cases in which the rotation $r$ or the rotoinversion $\bar{r}$ is a generator of $G$.

## B. The point groups with $r$ among the generators

### 1. The horizontal mirror

When $r$ is a generator, $G$ may also have the horizontal mirror $h$ as a generator. Since $h$ leaves every vector in the $z=0$ plane invariant, the generating relation $h^2=e$ leads via Eq. (2.10) to

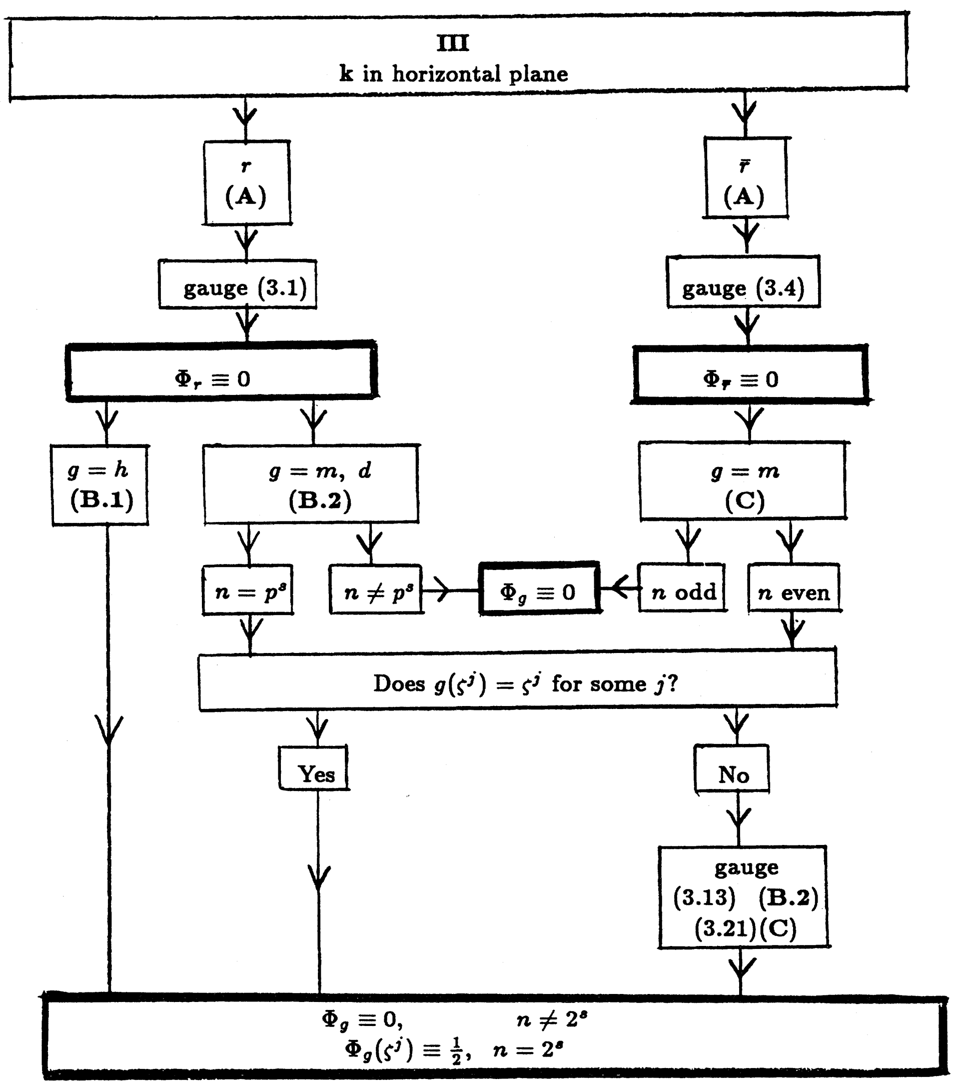


FIG. 2. The logical structure of Sec. III. Conclusions are in boxes with heavy borders. If an arrow passes through a box marked "gauge," a gauge (specified by the accompanying equation number) is required to reach the conclusion to which the arrow points.

$$2\Phi_h(\zeta^j)\equiv 0 \ . \tag{3.6}$$

Because we are in a gauge with $\Phi_r(\zeta^j)\equiv 0$, the generating relation $hrh=r$ gives via Eq. (2.11) the further condition $\Phi_h(\zeta^j)\equiv\Phi_h(\zeta^{j+1})$, or, equivalently,

$$\Phi_h(\zeta^j)\equiv\Phi_h(\zeta^0) \ . \tag{3.7}$$

Note, finally, that if $n$ is divisible by $a$, then

$$\zeta^0+\zeta^{n/a}+\zeta^{2n/a}+\cdots+\zeta^{(a-1)n/a}=0 \ , \tag{3.8}$$

which, with Eq. (3.7) and the linearity of phase functions, gives

$$a\Phi_h(\zeta^j)\equiv 0 \ . \tag{3.9}$$

With Eq. (3.6) this requires $\Phi_h(\zeta^j)\equiv 0$ if $n$ has any prime factors $a$ other than 2.

We have thus established that the $\Phi_h(\zeta^j)$ vanish unless $n$ is a power of 2, in which case they can also all have the value $\frac{1}{2}$.

### 2. Vertical mirrors or dihedral axes

In addition to (or instead of) $h$ there can be a generator $g$ of $G$ that acts as a mirror line in the $z=0$ plane (either a vertical mirror $m$ or a dihedral axis $d$). Since we are in a gauge with $\Phi_r(\zeta^j)\equiv 0$, the generating relation $rgr=g$ gives via Eq. (2.11) the further condition $\Phi_g(\zeta^{j+1})\equiv\Phi_g(\zeta^j)$, or

$$\Phi_g(\zeta^j)\equiv\Phi_g(\zeta^0) \ . \tag{3.10}$$

As in the case of $\Phi_h$ this condition with the identity (3.8) requires that if $a$ divides $n$ then

$$a\Phi_g(\zeta^j)\equiv 0 \ . \tag{3.11}$$

If $n$ has two distinct prime factors, it follows immediately that $\Phi_g(\zeta^j)\equiv 0$.

Furthermore, if $g$ is a mirror or dihedral axis that leaves one of the $\zeta^j$ invariant, then the generating relation $g^2=e$ requires $2\Phi_g(\zeta^j)\equiv 0$, which, with Eq. (3.11), requires $\Phi_g(\zeta^j)$ to vanish unless $n$ is a power of 2, when it can also have the value $\frac{1}{2}$.

There remains the case in which $g$ is a mirror or dihedral axis that leaves no $\zeta^j$ invariant. We show that if $n$ is a power of an odd prime $p$, then there is a gauge in which $\Phi_g(\zeta^j)\equiv 0$, just as in the other case. It suffices to consider the mirror or dihedral axis that contains the imaginary axis, satisfying

$$g\zeta^j=-\zeta^{-j} \ . \tag{3.12}$$

Equation (3.11) with $a=p$ requires that $\Phi_g(\zeta^j)\equiv c/p$ for some integer $c$. Consider now the gauge function $\chi(\zeta^j)=1/p$ for the lattice generators $\zeta^j, j=0,\ldots,\nu-1$. Since $n=p^s$, each of the remaining $\zeta^j$ can be expressed [using Eq. (3.8) with $a=p$] as minus the sum of $(p-1)$ of the generating vectors. For $j=\nu,\ldots,n-1$, we then have $\chi(\zeta^j)\equiv(1-p)\chi(\zeta^0)\equiv 1/p$, and therefore

$$\chi(\zeta^j)\equiv 1/p \tag{3.13}$$

for the entire star. We then have

$$\Delta\Phi_g(\zeta^0)\equiv\chi((g-1)\zeta^0)\equiv\chi(-2\zeta^0)\equiv -2/p \ . \tag{3.14}$$

If 2 does not divide $p$, repeated application of this gauge transformation can change the phase $\Phi_g(\zeta^j)$ by an arbitrary multiple of $1/p$. Note, finally, that the gauge transformation does not change the value of $\Phi_r(\zeta^j)\equiv 0$, since[32]

$$\Delta\Phi_r(\zeta^j)\equiv\chi(\zeta^{j+1}-\zeta^j)\equiv 0 \ . \tag{3.15}$$

Thus, for either type of mirror or dihedral axis, we can take $\Phi_g(\zeta^j)\equiv 0$ unless $n=2^s$, when it can also have the value $\frac{1}{2}$.

## C. The point groups with $\bar{r}$ among the generators

When $\bar{r}$ is a generator of $G$, the only other generator we have to consider is a vertical mirror $m$ (see Table III). The generating relation $m=\bar{r}m\bar{r}$ and the vanishing of $\Phi_{\bar{r}}(\zeta^j)$ lead via Eq. (2.11) to

$$\Phi_m(\zeta^j)\equiv\Phi_m(\bar{r}\zeta^j)\equiv-\Phi_m(\zeta^{j+1}) \ . \tag{3.16}$$

When $n$ is odd, repeated application of this condition gives

$$\Phi_m(\zeta^0)\equiv-\Phi_m(\zeta^1)\equiv+\Phi_m(\zeta^2)\equiv\cdots\equiv-\Phi_m(\zeta^0) \ , \tag{3.17}$$

leading to the requirement

$$\Phi_m(\zeta^j)\equiv\Phi_m(\zeta^0)\equiv \ 0 \text{ or } \tfrac{1}{2} \ . \tag{3.18}$$

Since, however, $\zeta^0+\zeta+\cdots+\zeta^{n-1}=0$, we also have $n\Phi_m(\zeta^0)\equiv 0$, which with $n$ odd is consistent only with the alternative $\Phi_m(\zeta^0)\equiv 0$.

It remains to consider the case of even $n$, where repeated application of Eq. (3.16) gives

$$\Phi_m(\zeta^{2j})\equiv-\Phi_m(\zeta^{2j+1})\equiv\Phi_m(\zeta^0) \ . \tag{3.19}$$

If $n$ has two distinct odd prime factors $a$ and $b$, we can apply $\Phi_m$ to the identity (3.8), noting that only even powers of $\zeta$ appear there, to conclude from Eq. (3.19) that both $a\Phi_m(\zeta^j)\equiv 0$ and $b\Phi_m(\zeta^j)\equiv 0$, which again requires $\Phi_m(\zeta^j)\equiv 0$. This leaves only the case $n=2p^s$ and the condition

$$p\Phi_m(\zeta^j)\equiv 0 \ . \tag{3.20}$$

As in the corresponding case with $r$ a generator, if $m$ is a mirror that leaves one of the $\zeta^j$ invariant, then we must also have $2\Phi_m(\zeta^j)\equiv 0$, which with Eq. (3.20) requires

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[32]Since $h\zeta^j=\zeta^j$, the $\Phi_h(\zeta^j)$ are gauge invariant and therefore will also be unshifted.

$\Phi_m(\zeta^j)\equiv 0$ unless $p=2$. If $m$ leaves no $\zeta^j$ invariant, then it again suffices to consider $m$ to be the mirror that takes $\zeta^j$ into $-\zeta^{-j}$, and we can again eliminate the phases $\Phi_m(\zeta^j)\equiv(-1)^j c/p$ compatible with Eq. (3.20) by a gauge transformation, unless $p=2$. We choose

$$\chi(\zeta^j)=(-1)^j/p \ . \tag{3.21}$$

As in the preceding case this can be taken to hold for the entire symmetric star.[33]

We now have

$$\Delta\Phi_m(\zeta^j)\equiv\chi((m-1)\zeta^j)\equiv\chi(-\zeta^{-j}-\zeta^j)$$
$$\equiv-(-1)^j 2/p \ . \tag{3.22}$$

Thus, as before, unless $p=2$, by repeated application of this gauge transformation we can change the phase $\Phi_m(\zeta^j)$ by an arbitrary multiple of $(-1)^j/p$. The gauge transformation given by Eq. (3.21) does not, however, alter the values $\Phi_{\bar{r}}(\zeta^j)\equiv 0$, since

$$\Delta\Phi_{\bar{r}}(\zeta^j)\equiv\chi((\bar{r}-1)\zeta^j)=\chi(-\zeta^{j+1}-\zeta^j)\equiv 0 \ . \tag{3.23}$$

## IV. THE SPACE GROUPS FOR VERTICAL LATTICES

The vertically stacked lattices are given by adding to the generators of the $z=0$ sublattice the vector $\mathbf{z}$ perpendicular to the plane. The group compatibility conditions (2.8)–(2.11) applied to the generating relations of the point group determine the distinct classes of phase functions. Since every element $g$ of the point group either leaves $\mathbf{z}$ invariant or takes it into $-\mathbf{z}$, these constraints on the additional phases $\Phi_g(\mathbf{z})$ do not couple them back to the in-plane phases $\Phi_g(\zeta^j)$ determined earlier. We may therefore independently determine the phases $\Phi_g(\mathbf{z})$ associated with the out-of-plane lattice-generating vector $\mathbf{z}$.[34]

### A. Determination of the phase functions

#### 1. The gauge-invariant phases $\Phi_m(\mathbf{z})$ and $\Phi_r(\mathbf{z})$

The operations $m$ and $r$ leave $\mathbf{z}$ invariant, so the phases $\Phi_m(\mathbf{z})$ and $\Phi_r(\mathbf{z})$ are gauge invariant. The generating relations $m^2=e$ and $r^n=e$ constrain these phases:

$$0\equiv\Phi_{m^2}(\mathbf{z})\equiv\Phi_m(m\mathbf{z})+\Phi_m(\mathbf{z})=2\Phi_m(\mathbf{z}) \ , \tag{4.1}$$

or

$$\Phi_m(\mathbf{z})\equiv 0,\tfrac{1}{2} \ ; \tag{4.2}$$

and

$$0\equiv\Phi_{r^n}(\mathbf{z})\equiv\Phi_r((1+r+\cdots+r^{n-1})\mathbf{z})\equiv n\Phi_r(\mathbf{z}) \ , \tag{4.3}$$

or

$$\Phi_r(\mathbf{z})\equiv 0,\frac{1}{n},\ldots,\frac{n-1}{n} \ . \tag{4.4}$$

We shall see below that the presence in the point group of a horizontal or vertical mirror further restricts $\Phi_r(\mathbf{z})$.

#### 2. Gauge-transforming away the phase $\Phi_g(\mathbf{z})$ when $g\mathbf{z}=-\mathbf{z}$

In addition to $m$ and $r$, each of the seven point groups in Table III may also have among its generators at most one of the operations $g=\bar{r}$, $d$, or $h$ that take $\mathbf{z}$ into $-\mathbf{z}$. Since we have earlier specified the gauge function $\chi$ only in the $z=0$ plane, we may still choose a value for $\chi(\mathbf{z})$ without altering the phase functions in that plane. We exploit this additional gauge freedom to make $\Phi_g(\mathbf{z})$ vanish for $g=\bar{r}$, $d$, or $h$ by taking

$$\chi(\mathbf{z})=\tfrac{1}{2}\Phi_g(\mathbf{z}) \ , \tag{4.5}$$

since we then have

$$\Delta\Phi_g(\mathbf{z})\equiv\chi((g-1)\mathbf{z})=\chi(-2\mathbf{z})\equiv-2\chi(\mathbf{z})=-\Phi_g(\mathbf{z}) \ . \tag{4.6}$$

#### 3. General form for the remaining generating relations

Since the generating relations $\bar{r}^n=e$ (or $\bar{r}^{2n}=e$), $d^2=e$, or $h^2=e$ impose no further constraint on a phase function that already vanishes, the only additional generating relations we need consider are those involving two distinct generators $f$ and $g$. As noted above, these can always be cast in the form $fgf=g$, so that the corresponding group compatibility conditions take the previously derived form

$$0\equiv\Phi_f(gf\mathbf{z})+\Phi_g(f\mathbf{z})+\Phi_f(\mathbf{z})-\Phi_g(\mathbf{z}) \ . \tag{2.11}$$

Since every element of the point group either leaves $\mathbf{z}$ invariant or takes it into $-\mathbf{z}$, the particular realizations of Eq. (2.11) are quite simple.

#### 4. Restriction of $\Phi_r(\mathbf{z})$ in the presence of mirrors

The relation (2.11) further constrains the form (4.4) for $\Phi_r(\mathbf{z})$ if $G$ also contains either the vertical mirror $m$ or

[33] In this case take as the independent vectors at which $\chi$ is defined $\zeta^{2j}, j=0\cdots\nu-1$. The extension to the remaining even powers of $\zeta$ is exactly as in the previous case, and since the odd powers of $\zeta$ are just the negatives of even powers, the rest of Eq. (3.21) follows from linearity.

[34] In contrast, when the lattice is staggered, the compatibility conditions couple the in-plane phases $\Phi_g(\zeta^j)$ to those at the out-of-plane generating vector, $\Phi_g(\mathbf{z}+\alpha)$.

TABLE IV. The out-of-plane gauge-invariant phases (vertical stacking). When $n \neq 2^s$, these are the only nontrivial gauge-invariant phases. [When $n=2^s$, one can also have $\Phi_h(\zeta^j)\equiv 0,\frac{1}{2}$, $\Phi_d(\zeta^j)\equiv 0,\frac{1}{2}$, and $\Phi_m(\zeta^j)\equiv 0,\frac{1}{2}$.]

| | | |
|---|---|---|
| 1. $m$ present: | $\boxed{\Phi_m(\mathbf{z}) \equiv j/2\,, \quad j=0,1}$ | $(\bar{n}2m,\ \bar{n}2/m,\ nmm,\ nm,\ n/mmm)$ |
| 2. $r$ present: | | |
| a) $m$ and $h$ absent: | $\boxed{\Phi_r(\mathbf{z}) \equiv j/n\,, \quad j=0,\ldots,n-1}$ | $(n,\ n22,\ n2)$ |
| b) $m$ or $h$ present and $n$ even: | $\boxed{\Phi_r(\mathbf{z}) \equiv j/2\,, \quad j=0,1}$ | $(nmm,\ n/m,\ n/mmm)$ |
| c) $m$ present and $n$ odd: | $\boxed{\Phi_r(\mathbf{z}) \equiv 0}$ | $(nm)$ |

the horizontal mirror $h$. Since $\mathbf{z}$ is invariant under both $r$ and $m$, Eq. (2.11) applied to the generating relation $rmr=m$ immediately gives

$$2\Phi_r(\mathbf{z})\equiv 0\ . \tag{4.7}$$

Applying Eq. (2.11) to the generating relation $hrh=r$, and noting that $h$ reverses the sign of $\mathbf{z}$, leads to the same condition.

If $n$ is even, Eq. (4.7) reduces the range of possibilities allowed by (4.4) to two:

$$\Phi_r(\mathbf{z})\equiv\ 0 \text{ or } \tfrac{1}{2},\quad n \text{ even, } m \text{ or } h \text{ generators}\ . \tag{4.8}$$

If $n$ is odd (which is never the case when $h$ is taken as a generator), then all possibilities are excluded except for

$$\Phi_r(\mathbf{z})\equiv 0,\quad n \text{ odd, } m \text{ a generator}\ . \tag{4.9}$$

### 5. Absence of additional constraints on the phase functions

The above analysis exhausts the generating relations for four of the seven point groups [$\bar{n},n,nmm$ (or $nm$), and $n/m$]; we next show that the remaining generating relations impose no further constraints on the other three point groups (see Table III):

(1) For the group $\bar{n}2m$ (or $\bar{n}2/m$) generated by the pair $(\bar{r},m)$, there is an additional generating relation $\bar{r}m\bar{r}=m$. Since $\Phi_{\bar{r}}(\mathbf{z})\equiv 0$, the additional group compatibility condition (2.11) becomes $0\equiv -2\Phi_m(\mathbf{z})$, which Eq. (4.2) already guarantees.

(2) For $n22$ (or $n2$) generated by the pair $(r,d)$, there is an additional relation $rdr=d$. Since we work in a gauge with $\Phi_d(\mathbf{z})\equiv 0$, the additional compatibility condition becomes $\Phi_r(-\mathbf{z})+\Phi_r(\mathbf{z})\equiv 0$, which linearity insures.

(3) We can view $n/mmm$ generated by $(r,m,h)$ as given by adding $h$ to the pair $(r,m)$. There is then an additional relation $hmh=m$. Since $\Phi_h(\mathbf{z})\equiv 0$, the additional compatibility condition becomes $\Phi_m(-\mathbf{z})-\Phi_m(\mathbf{z})\equiv 0$, which Eq. (4.2) already guarantees.

The nonzero out-of-plane phases for each of the seven point groups are summarized for vertical lattices in Table IV.

## B. Determination of the space groups with vertical lattices

The number of space groups for each point group is not the same as the number of distinct phase functions $\Phi_g(\mathbf{z})$ listed in Table IV for two reasons. The first stems from the question of whether or not there is a unique orientation of the point group with respect to the lattice. The second (and simpler) reason is that when (and only when) $n$ is a power of 2, in addition to the phases at $\mathbf{z}$ we have just determined, there can be gauge-invariant nonzero phases in the $z=0$ plane, as noted in Sec. III.

### 1. The orientation of $m$ or $d$ with respect to the lattice

#### *a. N twice a prime power*

If the rotational symmetry $N$ of the lattice is twice a prime power (i.e., when the rotational symmetry of the point group $n$ is either a prime power or twice a prime power), then as noted in Sec. II.A.1, the vectors of any generating star must lie along the cyclotomic integers $\zeta_N^j$. A group element $m$ or $d$ may be oriented either along one of these directions or between two adjacent ones.[35] When $n$ is an odd prime power, this choice doubles the number of space groups for the point groups with $n$ vertical mirrors ($nm$), $n$ dihedral axes ($n2$), and $n$ mirrors interleaved with $n$ dihedral axes ($\bar{n}2/m$). When $n$ is either twice an odd prime power or a power of 2, the doubling

[35] As noted earlier, when we say the vertical mirror $m$ lies along a horizontal direction we mean the direction is in the invariant plane of the mirror.

TABLE V. The space groups for vertically stacked lattices. We summarize here the complete classification of axial space groups on vertically stacked lattices. The lattice is $n$-fold symmetric if the rotational order $n$ of the point group is even and $2n$-fold symmetric if $n$ is odd. By $p$ we mean any prime (including 2), while $p_o$ stands for any odd prime. The appropriate column on the right gives the number of space groups. The ticks mark the possible nonzero gauge-invariant out-of-plane phases at **z**. (The parameter $j$ can assume any integral value between 0 and $n-1$.) The number of space groups is simply the number of choices of out-of-plane phases, with the following exceptions (described in detail in Secs. IV.B.1 and 2): (1) When neither $n$ nor $n/2$ is a prime power, the two entries of 3 are down from 4 because the orientation of two families of vertical mirrors with respect to the lattice cannot be distinguished, resulting in the scale equivalence of two gauge-inequivalent choices of phases for the two families; (2) when $n$ or $n/2$ is a prime power (odd or even), the two orientations can be distinguished, and some entries are doubled; (3) when $n$ is a power of 2, there is an additional doubling if the generators include either $m$ or $h$, and a quadrupling if they include both, because $\Phi_m(\zeta^j)$ and independently $\Phi_h(\zeta^j)$ can be either 0 or $\frac{1}{2}$.

| generators | point groups | parity of $n$ | nonzero out-of-plane phases | | | numbers of space groups | | |
|---|---|---|---|---|---|---|---|---|
| | | | $\Phi_m(\mathbf{z}) \equiv 0, 1/2$ | $\Phi_r(\mathbf{z}) \equiv j/n$ | $\Phi_r(\mathbf{z}) \equiv 0, 1/2$ | $n \neq p^s$, $n \neq 2p^s$ | $n = p_o^s$, $n = 2p_o^s$ | $n = 2^s$ |
| $\bar{r}$ | $\bar{n}$ | either | | | | 1 | 1 | 1 |
| $\bar{r}, m$ | $\bar{n}2m$ | even | ✓ | | | 2 | 4 | 8 |
| | $\bar{n}\frac{2}{m}$ | odd | ✓ | | | 2 | 4 | — |
| $r$ | $n$ | either | | ✓ | | $n$ | $n$ | $n$ |
| $r, m$ | $nmm$ | even | ✓ | | ✓ | 3 | 4 | 8 |
| | $nm$ | odd | ✓ | | | 2 | 4 | — |
| $r, d$ | $n22$ | even | | ✓ | | $n$ | $n$ | $2n$ |
| | $n2$ | odd | | ✓ | | $n$ | $2n$ | — |
| $r, h$ | $n/m$ | even | | | ✓ | 2 | 2 | 4 |
| $r, h, m$ | $\frac{n}{m}\frac{2}{m}\frac{2}{m}$ | even | ✓ | | ✓ | 3 | 4 | 16 |

cannot occur for $nmm$, $n22$, or $n/mmm$, because mirrors or dihedral axes necessarily lie along both families of directions; the doubling occurs only for $\bar{n}2m$, which can still discriminate between the two families of directions, either because it interleaves mirrors and dihedral axes (when $n$ is twice even) or because its $n$ mirrors and $n$ dihedral axes lie along the same family of directions (when $n$ is twice odd).[36]

### b. N not twice a prime power

When $N$ is not twice a prime power (i.e., when neither $n$ nor $n/2$ is a prime power), the lattice admits a second set of generating stars whose vectors lie in the directions between those of the original star, as described in Sec. II.A.1. There is then no way to distinguish between the two possible orientations of mirrors or dihedral axes, and no doubling can occur. There can, however, be a *reduction* in the apparent number of space groups for even $n$ and the point groups $nmm$ and $n/mmm$. This is because these groups possess two distinct families of nonconjugate vertical mirrors, $m$ and $m'=rm$, oriented along the two possible sets of directions for a star of primitive generating vectors for the horizontal sublattice. We are free to take a mirror from either family as the group generator. The phase functions for the two are related by the group compatibility condition (2.8):

$$\Phi_{m'}(\mathbf{z})\equiv\Phi_{rm}(\mathbf{z})\equiv\Phi_r(m\mathbf{z})+\Phi_m(\mathbf{z})\equiv\Phi_r(\mathbf{z})+\Phi_m(\mathbf{z}) \ . \tag{4.10}$$

Therefore, when $\Phi_r(\mathbf{z})\equiv\frac{1}{2}$, the two choices of phase $\Phi_m(\mathbf{z})\equiv 0,\frac{1}{2}$ can equally well be viewed as $\Phi_{m'}(\mathbf{z})\equiv\frac{1}{2},0$. Since the lattice-generating stars provide no basis for distinguishing the two types of mirrors (as they do when $n=2^s$), these two choices of phase correspond to a single

[36]A perusal of Table III confirms that this exhausts all cases.

space group, and the number of space groups when $n$ is even and not a prime power drops from four to three for the point groups $nmm$ and $n/mmm$. (This reduction first occurs at $n=12$.)

### 2. The nonzero phases in the $z=0$ plane when $n=2^s$

As we found in Sec. III, when (and only when) $n=2^s$, if the horizontal mirror $h$ is present, the phases $\Phi_h(\zeta^j)$ can either all be zero or all be $\frac{1}{2}$; independently of this, if the point group has a generator $m$ or $d$ (either of which reduces to a mirror line in the $z=0$ plane), then the phases associated with that generator, $\Phi_m(\zeta^j)$ or $\Phi_d(\zeta^j)$, can also either all be zero or all be $\frac{1}{2}$.

Consequently when $n=2^s$ there is a doubling of the number of space groups for those point groups ($n/m$, $n22$, $\bar{n}2m$, and $nmm$) that have just one of $h$, $m$, or $d$ as a generator, and a quadrupling for the point group ($n/mmm$) that has both $h$ and $m$.

Table V collects all these results together and specifies the space groups for the vertically stacked lattices.

## V. THE SPACE GROUPS FOR STAGGERED LATTICES

The rotational symmetry $n$ of a staggered lattice is necessarily a power of a prime number, $n=p^s$. These are precisely the values of $n$ for which the vectors of a star generating the horizontal sublattice lie along a unique set of directions. Except when $n=2^s$ and the point group is $\bar{n}2m$, however, there is no freedom in the orientation of mirrors or dihedral axes with respect to this unique set of directions, for when $n$ is an odd prime power the shift vector $\alpha$ [Eq. (2.2)], which lies between adjacent vectors in a generating star, breaks the full symmetry of the vertical stacking.[37] As a result, vertical mirror planes are required to lie in directions between star vectors, and dihedral axes can lie only along the directions of star vectors (Mermin, Rabson, Rokhsar, and Wright, 1990). Only when $n$ is a power of 2 is it also possible to have things the other way around, with dihedral axes in directions between star vectors and mirrors along such directions. When $n=2^s$, however, every point group that has a family of mirrors (or dihedral axes) in one of the possible orientations also has a second family of mirrors (or dihedral axes) in the other, with the sole exception of the point group $\bar{n}2m$, which has a single family of mirrors interleaved with a single family of dihedral axes.

[37] Recall that when $n$ is odd, as it is in staggered lattices except when $n=2^s$, the phrases "between" and "between star vectors" refer to directions lying between the vectors of the $2n$-fold star consisting of the $n$-fold star vectors and their negatives, as illustrated in Figs. 1(b) and 1(c). (This possibility for confusion does not exist for "along.")

Therefore only in the case of the point group $\bar{n}2m$ with $n=2^s$ is there an issue of how the point group is to be oriented in the staggered lattice. In all other cases we may take a generating dihedral axis $d$ to lie along $\zeta^0$ and a generating vertical mirror $m$ to lie in the plane of $\mathbf{z}+\alpha$.

### A. Constraints on the out-of-plane phases

#### 1. The gauge-invariant phase $\Phi_m(\mathbf{z}+\alpha)$ for $m$ along $\alpha$

Except for the one case noted above, the generator $m$ can be chosen to leave $\mathbf{z}+\alpha$ invariant, so the phase function $\Phi_m(\mathbf{z}+\alpha)$ is gauge invariant. The generating relation $m^2=e$ then gives

$$\Phi_m(\mathbf{z}+\alpha)\equiv c/2,\quad c=0,1 \quad \text{whenever } m(\mathbf{z}+\alpha)=\mathbf{z}+\alpha\ . \tag{5.1}$$

Other group compatibility conditions may further restrict Eq. (5.1).

#### 2. The gauge-invariant phase $\Phi_r(p\mathbf{z})$ and the phase $\Phi_r(\mathbf{z}+\alpha)$

We show here that $\Phi_r(\mathbf{z}+\alpha)$ can have only the values $c/n$, $c=0,1,\ldots,(n/p)-1$.

The generating relation $r^n=e$ gives from the group compatibility condition (2.10)

$$\begin{aligned}0\equiv\Phi_{r^n}(\mathbf{z}+\alpha)&\equiv\Phi_r((1+r+\cdots+r^{n-1})(\mathbf{z}+\alpha))\\&=\Phi_r(n\mathbf{z})\ .\end{aligned} \tag{5.2}$$

Since $p\mathbf{z}$ is a lattice vector and is left invariant by $r$, Eq. (5.2) gives the gauge-invariant phases

$$\Phi_r(p\mathbf{z})\equiv\frac{c}{n/p},\quad c=0,1,\ldots,\frac{n}{p}-1\ . \tag{5.3}$$

If we wish to determine $\Phi_r$ at arbitrary lattice vectors, we need, in addition, to specify the gauge-dependent phase $\Phi_r(\mathbf{z}+\alpha)$. The stacking repeats after $p$ layers, so $p\alpha$ is a vector in the two-dimensional sublattice. Since $\Phi_r$ vanishes in that sublattice, we have $\Phi_r(p\mathbf{z})\equiv\Phi_r(p\mathbf{z}+p\alpha)\equiv p\Phi_r(\mathbf{z}+\alpha)$, and therefore

$$\Phi_r(\mathbf{z}+\alpha)\equiv\frac{c}{n}+\frac{c'}{p}\ ,\qquad c=0,\ldots,\frac{n}{p}-1,\quad c'=0,\ldots,p-1\ . \tag{5.4}$$

We now make a further gauge transformation that shifts $\Phi_r(\mathbf{z}+\alpha)$ by $-c'/p$, thereby allowing us to set $c'$ to zero. Define

$$\chi(\mathbf{z}+\alpha)=0,\quad \chi(\zeta^j)=\frac{-c'}{p},\quad j=0,1,\ldots,\nu-1\ . \tag{5.5}$$

When $n=p^s$, each of the remaining $\zeta^j$ in the full star can be written as minus the sum of $p-1$ of the powers of $\zeta$

appearing in Eq. (5.5). We then have $\chi(\zeta^j) \equiv (1-p)\chi(\zeta^0) \equiv -c'/p$ for $j=\nu,\ldots,n-1$. We can therefore drop the restriction in (5.5):

$$\chi(\mathbf{z}+\alpha)=0, \quad \chi(\zeta^j)\equiv\frac{-c'}{p}, \quad j \text{ arbitrary} . \tag{5.6}$$

We now have

$$\begin{aligned}\Delta\Phi_r(\mathbf{z}+\alpha)&\equiv\chi((r-1)(\mathbf{z}+\alpha))\\ &=\chi\left[(\zeta-1)\frac{1}{\zeta-1}\right]=\chi(\zeta^0)=-c'/p ,\end{aligned} \tag{5.7}$$

so that Eq. (5.4) can indeed be simplified to the set of values

$$\Phi_r(\mathbf{z}+\alpha)\equiv\frac{c}{n}, \quad c=0,\ldots,\frac{n}{p}-1 . \tag{5.8}$$

The gauge transformation given by Eq. (5.6) does not alter any of the phases $\Phi_g$ specified in Sec. III in the $z=0$ plane, for every point-group element $g$ takes $\zeta^j$ into some other power $\zeta^k$, so that

$$\Delta\Phi_g(\zeta^j)\equiv\chi((g-1)\zeta^j)\equiv\chi(\zeta^k)-\chi(\zeta^j)\equiv 0 . \tag{5.9}$$

Although the values of $\Phi_r(\mathbf{z}+\alpha)$ given by Eq. (5.8) are not themselves gauge invariant, they imply the distinct values (5.3) for the gauge-invariant phases $\Phi_r(p\mathbf{z})$ and are therefore associated with distinct space groups.

### 3. Gauge-transforming away the phase $\Phi_g(\mathbf{z}+\alpha)$ for $g\mathbf{z}=-\mathbf{z}$

As noted in the vertical case, we can pick generators of each point group so that at most one of the operations $\bar{r}$, $d$, or $h$ that reverse the sign of $\mathbf{z}$ is among them. We can then find a gauge in which the phase $\Phi_g(\mathbf{z}+\alpha)$ vanishes for $g=\bar{r}$, $d$, or $h$:

$$\begin{aligned}&\chi(\mathbf{z}+\alpha)=\tfrac{1}{2}\Phi_g(\mathbf{z}+\alpha) ,\\ &\chi=0 \quad \text{in the } z=0 \text{ plane} .\end{aligned} \tag{5.10}$$

This changes $\Phi_g(\mathbf{z}+\alpha)$ by

$$\begin{aligned}\Delta\Phi_g(\mathbf{z}+\alpha)&\equiv\chi((g-1)(\mathbf{z}+\alpha))\\ &\equiv\chi(-2\mathbf{z}-2\alpha)+\chi(g\alpha+\alpha) .\end{aligned} \tag{5.11}$$

Since $g\alpha+\alpha$ is in the $z=0$ plane, where $\chi$ vanishes,

$$\Delta\Phi_g(\mathbf{z}+\alpha)\equiv-\Phi_g(\mathbf{z}+\alpha) , \tag{5.12}$$

as required.

The gauge transformation given by Eq. (5.10) clearly changes no phases in the $\mathbf{z}=0$ plane, nor can it alter $\Phi_r(\mathbf{z}+\alpha)$ from the form (5.8), since

$$\begin{aligned}\Delta\Phi_r(\mathbf{z}+\alpha)&\equiv\chi((r-1)(\mathbf{z}+\alpha))\\ &=\chi((\zeta-1)\alpha)=\chi(\zeta^0)=0 .\end{aligned} \tag{5.13}$$

[We have used the specific form (2.2) of $\alpha$.]

### 4. General form for the remaining generating relations

As noted in the vertical case, all generating relations between two distinct generators can be put in the form $fgf=g$. This gives the group compatibility condition (2.11), which can also be cast in the form

$$0\equiv\Phi_f((gf+1)(\mathbf{z}+\alpha))+\Phi_g((f-1)(\mathbf{z}+\alpha)), \quad (fgf=g) . \tag{5.14}$$

## B. Determination of the space groups with staggered lattices

We now examine each of the seven point groups. We always work in the gauges constructed above. If $r$ is a generator, we take $\Phi_r(\mathbf{z}+\alpha)$ to be one of the gauge-inequivalent choices (5.8), and if $\bar{r}$, $d$, or $h$ is a generator, we work in a gauge that makes $\Phi_{\bar{r}}(\mathbf{z}+\alpha)$, $\Phi_d(\mathbf{z}+\alpha)$, or $\Phi_h(\mathbf{z}+\alpha)$ vanish. If $m$ is a generator and leaves $\mathbf{z}+\alpha$ invariant, $\Phi_m(\mathbf{z}+\alpha)$ is determined by the gauge-invariant relation (5.1). Our task is to determine the additional constraints on the out-of-plane phases $\Phi_g(\mathbf{z}+\alpha)$ imposed by the group compatibility conditions (5.14) and (when relevant) the conditions coming from generating relations $d^2=e, h^2=e$, and (in the single case where $m$ does not leave $\mathbf{z}+\alpha$ invariant) $m^2=e$.

#### Generator: $\bar{r}$; point group: $\bar{n}$

Since $\Phi_{\bar{r}}(\mathbf{z}+\alpha)=0$, there is only one (symmorphic) space group.

#### Generators: $\bar{r},m$; point group: $\bar{n}2m$ ($n$ even), $\bar{n}2/m$ ($n$ odd)

Since $\Phi_{\bar{r}}\equiv 0$ and $\bar{r}(\mathbf{z}+\alpha)=-\mathbf{z}-\zeta\alpha$, the group compatibility relation (5.14) for the generating relation $\bar{r}m\bar{r}=m$ gives

$$\begin{aligned}0&\equiv\Phi_m((\bar{r}-1)(\mathbf{z}+\alpha))\\ &\equiv\Phi_m(-2(\mathbf{z}+\alpha)-(\zeta-1)\alpha) .\end{aligned} \tag{5.15}$$

Since $(\zeta-1)\alpha=1=\zeta^0$, we have

$$2\Phi_m(\mathbf{z}+\alpha)\equiv-\Phi_m(\zeta^0) . \tag{5.16}$$

If $m$ leaves $\mathbf{z}+\alpha$ invariant, Eq. (5.1) holds, requiring $2\Phi_m(\mathbf{z}+\alpha)\equiv 0$. Since $\Phi_m(\zeta^0)\equiv 0$ where $n$ is an odd prime power, Eq. (5.16) has no additional content except in the case $n=2^s$, where it prohibits the additional possibility $\Phi_m(\zeta^0)\equiv\frac{1}{2}$. For this orientation of the mirrors, there are thus just two space groups, and the only nonzero phase is the one allowed by Eq. (5.1): $\Phi_m(\mathbf{z}+\alpha)\equiv\frac{1}{2}$.

When $n$ is a power of two, however, and only for the point group $\bar{n}2m$, the mirror $m$ may instead lie along the lattice generator $\zeta^0$, so that $m\alpha=\alpha^*$. In this case the generating relation $m^2=e$ yields

$$0\equiv\Phi_m(m(\mathbf{z}+\alpha))+\Phi_m(\mathbf{z}+\alpha)\equiv\Phi_m(2\mathbf{z})-\Phi_m(\zeta^0)\ , \tag{5.17}$$

since $\alpha+\alpha^*=-\zeta^0$ as a consequence of $\alpha=1/(\zeta-1)$. We may rewrite Eq. (5.17) as

$$2\Phi_m(\mathbf{z}+\alpha)\equiv\Phi_m(\zeta^0)\ , \tag{5.18}$$

because[38] when $n=2^s$,

$$\Phi_m(2\alpha)\equiv 0\ . \tag{5.19}$$

Since $\Phi_m(\zeta^0)\equiv c/2$, $c=0$ or 1, Eq. (5.18) gives

$$\Phi_m(\mathbf{z}+\alpha)\equiv\frac{c}{4}+\frac{c'}{2},\quad c,c'=0,1\ . \tag{5.20}$$

The gauge function

$$\chi(\mathbf{z}+\alpha)=1/4\ ,\qquad \chi(\zeta^j)\equiv 1/2\ , \tag{5.21}$$

gives

$$\begin{aligned}\Delta\Phi_m(\mathbf{z}+\alpha)\equiv\chi((m-1)(\mathbf{z}+\alpha))&=\chi(\alpha^*-\alpha)\\&=\chi(\alpha^*+\alpha-2\alpha)\\&\equiv-\chi(\zeta^0)\equiv\tfrac{1}{2}\ ,\end{aligned} \tag{5.22}$$

permitting us to set $c'$ to zero in Eq. (5.20).

We must verify that the gauge transformation given by Eq. (5.21) does not change the phase $\Phi_{\bar r}\equiv 0$:

$$\begin{aligned}\Delta\Phi_{\bar r}(\mathbf{z}+\alpha)&\equiv\chi((\bar r-1)(\mathbf{z}+\alpha))\\&=\chi(-2\mathbf{z}-\zeta\alpha-\alpha)\\&=\chi(-2\mathbf{z}-(\zeta-1)\alpha-2\alpha)\\&\equiv-2\chi(\mathbf{z}+\alpha)-\chi(\zeta^0)\equiv 0\ .\end{aligned} \tag{5.23}$$

Nor does this gauge transformation (5.21) alter any of the phases in the $\mathbf{z}=0$ plane—see the paragraph containing Eq. (5.9).

We conclude that when $n=2^s$ and $\zeta^0$ lies in a vertical mirror plane, there can be a nonsymmorphic space group with the nonvanishing out-of-plane phase

$$\Phi_m(\mathbf{z}+\alpha)\equiv 1/4 \tag{5.24}$$

accompanied by the in-plane phases $\Phi_m(\zeta^j)\equiv\frac{1}{2}$. When combined with the case in which a vertical mirror plane contains $\mathbf{z}+\alpha$, this results in one symmorphic and one nonsymmorphic space group for each of the two orientations of the vertical mirrors, for a total of four space groups with point group $\bar n 2m$, $n=2^s$.

### Generator: *r*; point group: *n*

The only generator is $r$, so the phases at $\mathbf{z}+\alpha$ are given by Eq. (5.8), and there are $n/p=p^{s-1}$ space groups.

### Generators: *r*, *d*; point group: *n*22 (*n* even), *n*2 (*n* odd)

This group adds to $r$ the generator $d$, which we may take to lie along the vector $\zeta^0$. Since $d(\mathbf{z}+\alpha)=-\mathbf{z}+\alpha^*$, the generating relation $d^2=e$ gives

$$\begin{aligned}0\equiv\Phi_{d^2}(\mathbf{z}+\alpha)&\equiv\Phi_d((d+1)(\mathbf{z}+\alpha))\\&=\Phi_d(\alpha+\alpha^*)\equiv-\Phi_d(\zeta^0)\ ,\end{aligned} \tag{5.25}$$

so $\Phi_d(\zeta_0)$ must vanish (modulo 1) even in the one case ($n=2^s$) where for the vertical stacking it could have had the value $\frac{1}{2}$. The remaining generating relation, $rdr=d$, leads via Eq. (5.14) to the same conclusion:

$$\begin{aligned}0&\equiv\Phi_r((dr+1)(\mathbf{z}+\alpha))+\Phi_d((r-1)(\mathbf{z}+\alpha))\\&=\Phi_r(\zeta^*\alpha^*+\alpha)+\Phi_d((\zeta-1)\alpha)\\&\equiv\Phi_d(\zeta^0)\ ,\end{aligned} \tag{5.26}$$

since $\Phi_r$ vanishes in the $z=0$ plane.

Thus adding $d$ as a generator to the point group $n$ changes nothing. There continue to be $n/p$ space groups, associated with the $n/p=p^{s-1}$ choices for the phase $\Phi_r(\mathbf{z}+\alpha)$, corresponding to $n/p$ distinct choices for the gauge-invariant phase $\Phi_r(p\mathbf{z})$.

### Generators: *r*, *m*; point group: *nmm* (*n* even), *nm* (*n* odd)

This group adds to $r$ the generator $m$. The gauge-invariant phase $\Phi_m(\mathbf{z}+\alpha)$ is given by Eq. (5.1). The additional group generating relation $rmr=m$ gives for the compatibility condition (5.14)

$$\begin{aligned}0&\equiv\Phi_r((mr+1)(\mathbf{z}+\alpha))+\Phi_m((r-1)(\mathbf{z}+\alpha))\\&\equiv\Phi_r(2\mathbf{z}+\alpha+\zeta^*\alpha)+\Phi_m(\zeta^0)\\&\equiv 2\Phi_r(\mathbf{z}+\alpha)+\Phi_m(\zeta^0)\ ,\end{aligned} \tag{5.27}$$

the last equivalence following, again, because $\zeta^*\alpha-\alpha$ is a lattice vector in the $\mathbf{z}=0$ plane, where $\Phi_r\equiv 0$.

When $n$ is an odd prime power, $\Phi_m(\zeta^0)\equiv 0$, so this requires $\Phi_r(\mathbf{z}+\alpha)\equiv 0$ or $\frac{1}{2}$, which is compatible with $\Phi_r(\mathbf{z}+\alpha)\equiv c/n$ [Eq. (5.8)] only if $\Phi_r(\mathbf{z}+\alpha)\equiv 0$. There are thus only two space groups for odd $n$, the nonsymmorphic one coming from the choice $\Phi_m(\mathbf{z}+\alpha)\equiv\frac{1}{2}$.

When $n=2^s$, however, Eq. (5.27) again restricts the range of choices (5.8) gives for $\Phi_r(\mathbf{z}+\alpha)$ to 0 when $\Phi_m(\zeta^0)\equiv 0$, and to 1/4 when $\Phi_m(\zeta^0)\equiv\frac{1}{2}$. There are therefore four space groups, associated with the two ine-

[38]Note that $(\zeta-1)(\zeta^0+\zeta^1+\cdots+\zeta^{\nu-1})=\zeta^\nu-\zeta^0=-2$ when $n=2^s$, so that $\Phi_m(2\alpha)=\Phi_m[2/(\zeta-1)]\equiv-\nu\Phi_m(\zeta^0)=-2^{s-1}\Phi_m(\zeta^0)$. But $\Phi_m(\zeta^0)$ is 0 or 1/2.

quivalent choices 0 or $\frac{1}{2}$ for $\Phi_m(\mathbf{z}+\alpha)$ and the two additional choices 0 or $\frac{1}{4}$ for $\Phi_r(\mathbf{z}+\alpha)$ [going with the choices 0 or $\frac{1}{2}$ for $\Phi_m(\zeta^j)$].

Generators: *r*,*h*; point group: *n*/*m*

(This occurs only for even $n$—i.e., for $n=2^s$ in the staggered lattices; the case of odd $n$ is described as $\overline{2n}$.)

The generating relation $h^2=e$ gives $0\equiv\Phi_h((h+1)(\mathbf{z}+\alpha))\equiv\Phi_h(2\alpha)$, which is consistent with either of the values 0 or $\frac{1}{2}$ available to $\Phi_h(\zeta^j)$ when $n=2^s$, for exactly the same reasons as in the case of $\Phi_m$ (see footnote 38). Applied to the remaining generating relation, $hrh=r$, Eq. (5.14) gives

$$0\equiv\Phi_h((rh+1)(\mathbf{z}+\alpha))+\Phi_r((h-1)(\mathbf{z}+\alpha))$$
$$\equiv\Phi_h((\zeta+1)\alpha)-\Phi_r(2\mathbf{z}) \ . \qquad (5.28)$$

Because $\Phi_h(2\alpha)\equiv0$, because $\Phi_r$ vanishes for any lattice vector in the $\mathbf{z}=0$ plane, and because $(\zeta-1)\alpha=\zeta^0$, Eq. (5.28) can be rewritten as

$$2\Phi_r(\mathbf{z}+\alpha)\equiv\Phi_h(\zeta^0) \ . \qquad (5.29)$$

This restricts the range of choices allowed by Eq. (5.8) for $\Phi_r(\mathbf{z}+\alpha)$ to 0 when $\Phi_h(\zeta^0)\equiv0$, and to $\frac{1}{4}$ when $\Phi_h(\zeta^0)\equiv\frac{1}{2}$. There are therefore just two space groups, the nonsymmorphic one being associated with the phase $\Phi_r(\mathbf{z}+\alpha)\equiv\frac{1}{4}$, $\Phi_h(\zeta^j)\equiv\frac{1}{2}$.

Generators: *r*, *m*, *h*; point group: *n*/*mmm*

(This occurs only for even $n$; the case of odd $n$ is described as $\overline{2n}2m$.)

The phases $\Phi_r$ and $\Phi_m$ for this group are subject to all the conditions we found above for $nmm$. Additional conditions are imposed by the presence of the third generator $h$. As noted in the case of $n/m$, the generating relation $h^2=e$ imposes no restrictions, and the generating relation $hrh=r$ imposes the condition (5.29). Since our analysis of $nmm$ led to the condition (5.27) that $2\Phi_r(\mathbf{z}+\alpha)\equiv-\Phi_m(\zeta^0)$, we conclude that

$$\Phi_h(\zeta^0)\equiv-\Phi_m(\zeta^0)\equiv\Phi_m(\zeta^0) \ . \qquad (5.30)$$

The final generating relation, $mhm=h$, gives

$$0\equiv\Phi_m((hm+1)(\mathbf{z}+\alpha))+\Phi_h((m-1)(\mathbf{z}+\alpha)) \ , \qquad (5.31)$$

which reduces to $0\equiv\Phi_m(2\alpha)$, the validity of which we have already noted [Eq. (5.19)]. The same four solutions for the phases we found in the case $nmm$ are therefore still available, and the additional phase $\Phi_h(\zeta^j)$ produces

TABLE VI. The space-groups for staggered lattices. We summarize here the complete classification of axial space groups on staggered lattices. The rotational symmetry of the staggered lattice is $n=p^s$ for a prime number $p$. The horizontal shift from layer to layer is $\alpha=1/(\zeta_n-1)$. Except for the single case noted, $m\alpha=\alpha^*$ ($m$ along star vectors), we always take the vertical mirror $m$ to leave $\alpha$ invariant ($m$ between star vectors). In each row, the number of space groups in the right-most column is simply the number of choices of phases in the previous two.

| generators | point groups | parity of $n$ | nonzero out-of-plane phases | nonzero in-plane phases | number of space groups |
|---|---|---|---|---|---|
| $\bar{r}$ | $\bar{n}$ | even or odd | — | — | 1 |
| $\bar{r},m$ | $\bar{n}2m$ | even, $m\alpha=\alpha^*$ | $\Phi_m(\mathbf{z}+\alpha)\equiv\frac{1}{2}\Phi_m(\zeta^0)$ | $\Phi_m(\zeta^0)\equiv 0,\ ^1/_2$ | 2 } 4 |
| | | even, $m\alpha=\alpha$ | $\Phi_m(\mathbf{z}+\alpha)\equiv 0,\ ^1/_2$ | — | 2 |
| | $\bar{n}\frac{2}{m}$ | odd | $\Phi_m(\mathbf{z}+\alpha)\equiv 0,\ ^1/_2$ | — | 2 |
| $r$ | $n$ | even or odd | $\Phi_r(\mathbf{z}+\alpha)\equiv {}^j/_n$, $j=0,\ldots,{}^n/_p-1$ | — | $n/p$ |
| $r,m$ | $nmm$ | even | $\Phi_r(\mathbf{z}+\alpha)\equiv\frac{1}{2}\Phi_m(\zeta^0)$; $\Phi_m(\mathbf{z}+\alpha)\equiv 0,\ ^1/_2$ | $\Phi_m(\zeta^0)\equiv 0,\ ^1/_2$ | 4 |
| | $nm$ | odd | $\Phi_m(\mathbf{z}+\alpha)\equiv 0,\ ^1/_2$ | — | 2 |
| $r,d$ | $n22$; $n2$ | even; odd | $\Phi_r(\mathbf{z}+\alpha)\equiv {}^j/_n$, $j=0,\ldots,{}^n/_p-1$ | — | $n/p$ |
| $r,h$ | $n/m$ | even | $\Phi_r(\mathbf{z}+\alpha)\equiv\frac{1}{2}\Phi_h(\zeta^0)$ | $\Phi_h(\zeta^0)\equiv 0,\ ^1/_2$ | 2 |
| $r,h,m$ | $\frac{n}{m}\frac{2}{m}\frac{2}{m}$ | even | $\Phi_r(\mathbf{z}+\alpha)\equiv\frac{1}{2}\Phi_h(\zeta^0)$; $\Phi_m(\mathbf{z}+\alpha)\equiv 0,\ ^1/_2$ | $\Phi_h(\zeta^0)\equiv\Phi_m(\zeta^0)\equiv 0,\ ^1/_2$ | 4 |

no further possibilities because it is constrained by Eq. (5.30) to be the same as $\Phi_m(\zeta^j)$.

Table VI collects these results together and specifies the space groups for the staggered lattices.

## VI. EXTINCTIONS

Extinctions—lattice vectors that do not correspond to points in the diffraction pattern—are the most direct experimental manifestation of the space group. As noted in Sec. II.A, the Bragg peaks in a diffraction pattern determine a set of wave vectors, and the lattice is the set of all integral linear combinations of those wave vectors. When the space group is symmorphic, nothing prohibits a Bragg peak from being associated with any lattice vector, although its intensity may well be below the threshold of observability. When the space group is nonsymmorphic, however, density Fourier coefficients must vanish at certain wave vectors, whose corresponding Bragg peaks are forbidden from appearing in the diffraction pattern.

The condition for a lattice vector $\mathbf{k}$ to be extinct is that there should be some point-group operation $g$ which leaves $\mathbf{k}$ invariant, such that $\Phi_g(\mathbf{k})$ does not vanish (modulo an integer). This follows directly from the definition (2.5) of the phase functions which, when $g\mathbf{k}=\mathbf{k}$, reduces to

$$\rho(\mathbf{k})=e^{2\pi i\Phi_g(\mathbf{k})}\rho(\mathbf{k}) , \tag{6.1}$$

thereby requiring $\rho(\mathbf{k})$ to vanish for nonintegral $\Phi_g(\mathbf{k})$. It follows from the definition (2.6) of a gauge transformation that $\Phi_g(\mathbf{k})$ is gauge invariant when $g\mathbf{k}=\mathbf{k}$, so this condition for an extinction is (as it clearly must be) independent of the choice of gauge.

To determine the extinctions for a given space group we simply note the invariant space of every point-group operation (not just those we have chosen to be generators); we calculate the phase functions on these invariant spaces by expressing each element in terms of the group generators and applying the group compatibility condition (2.8) to the values we have already determined for those generators.

It suffices to determine the extinctions for one element from each conjugacy class of the point group. This is geometrically obvious since the invariant spaces of conjugate vertical mirrors—the same remarks hold for dihedral axes—differ by point-group operations, under which the diffraction pattern is invariant. It also follows analytically from the group compatibility conditions. If $m'$ and $m$ are conjugate mirrors so that $m'=gmg^{-1}$ for some $g$, then $g\mathbf{k}$ and $\mathbf{k}$ are corresponding points in their respective invariant subspaces, and we have $\Phi_{m'}(g\mathbf{k})\equiv\Phi_g(\mathbf{k})+\Phi_m(\mathbf{k})+\Phi_{g^{-1}}(g\mathbf{k})\equiv\Phi_m(\mathbf{k})$ [the last equivalence following from the expansion of $0\equiv\Phi_{g^{-1}g}(\mathbf{k})$].

We shall specify the orientations of vertical mirrors and dihedral axes by the horizontal directions of their invariant spaces.[39] In all cases those directions lie either *along* or *between* the directions of the vectors in the star of $N$th roots of unity.[40] We also describe a lattice vector as *along* or *between* star vectors according to the direction of its horizontal component. When the point group contains mirrors (or dihedral axes) both along and between star directions (which can happen only when $n$ is even), we must consider the extinctions produced by one of each type of mirror (or dihedral axis), since the two types are in different conjugacy classes.

When we mention values of the phase functions that are not gauge invariant, we shall always have in mind the particular gauges used above to construct them—i.e., we shall always be referring to the values given in Tables V and VI. (The condition for extinctions, as noted above, is gauge invariant.) Similarly, when we refer to the generators of point groups, we shall always be referring to the particular set of generators specified in Table III.

In the following two subsections we derive the extinctions for all the axial space groups. Readers interested only in the conclusions can skip to Sec. VI.C, where the results of this analysis are concisely summarized.

### A. The extinctions when $n\neq 2^s$

When the rotational order $n$ of the point group is not a power of 2, all phase functions vanish modulo unity in the horizontal plane, so there are no extinctions in that plane. The only point-group operations that leave out-of-plane vectors invariant are rotations about $\mathbf{z}$ and vertical mirrors containing $\mathbf{z}$. Among the rotations, it suffices to examine just the generator $r$, since $\Phi_{r^j}\equiv j\Phi_r$ everywhere on the $z$ axis, so that $\Phi_{r^j}$ can be nonintegral only if $\Phi_r$ is.

The rules for the extinctions when $n\neq 2^s$ are conveniently extracted by considering two cases:

#### 1. No vertical mirrors in the point group

This case includes the point groups generated by $r$, the pair $(r,d)$, or the pair $(r,h)$.[41] (The only other point group without $m$, generated by $\bar{r}$ alone, has no nonsymmorphic space group.)

[39]The International system specifies a dihedral axis in this way but specifies a vertical mirror by the direction of its normal.

[40]When the rotational order $n$ of the point group is odd, $N=2n$. Putting it another way, for purposes of defining "between," the star should be thought of as containing both the $n$th roots of unity and their negatives, as noted in Sec. II.A.1 and as illustrated in Figs. 1(b) and 1(c).

[41]In discussing extinctions it is most convenient to identify the point groups by their generators; to connect these point-group specifications with the International nomenclature, see Table III.

*Vertical stackings*: When the generators are $r$ or the pair $(r,d)$, the only nontrivial phase function is

$$\Phi_r(\mathbf{z})\equiv c/n, \quad c=1,2,\ldots,n-1 , \tag{6.2}$$

which assigns the phases

$$\Phi_r(j\mathbf{z})\equiv cj/n \tag{6.3}$$

on the $z$ axis. The vector $j\mathbf{z}$ is therefore extinct unless $cj$ is a multiple of $n$. When the generators are $(r,h)$, the only nonintegral phase is

$$\Phi_r(\mathbf{z})\equiv \tfrac{1}{2} , \tag{6.4}$$

which gives extinctions along $\mathbf{z}$ at all odd layers.

*Staggered stackings*: These occur only when $n=p^s$ for a prime number $p$. The lattice vectors along the $z$ axis are multiples of $p\mathbf{z}$. The pair of generators $(r,h)$ does not occur when $p\neq 2$. When the generators are $r$ or the pair $(r,d)$, there are nonsymmorphic space groups if $s$ is at least 2, with

$$\Phi_r(jp\mathbf{z})\equiv cj/p^{s-1}, \quad c=1,\ldots,p^{s-1} . \tag{6.5}$$

The vector $jp\mathbf{z}$ is therefore extinguished unless $cj$ is a multiple of $p^{s-1}$.

### 2. Vertical mirrors in the point group

This case includes the point groups generated by the pair $(\bar{r},m)$, the pair $(r,m)$, or the trio $(r,m,h)$. Extinctions now turn out to be entirely determined by the phases associated with the vertical mirror $m$ and, if $n$ is even, the nonconjugate vertical mirror $m'=rm$.

*Vertical stackings*: In all cases (see Table V) there are nonsymmorphic space groups with $\Phi_m(\mathbf{z})\equiv\frac{1}{2}$, which extinguishes all lattice vectors in the plane of the mirror in odd layers. When $n$ is even there is a second nonconjugate family of mirrors containing $m'=rm$ that interleaves the first. It follows from the group compatibility condition (2.8) that

$$\Phi_{m'}(\mathbf{z})\equiv\Phi_r(\mathbf{z})+\Phi_m(\mathbf{z}) , \tag{6.6}$$

so that when $\Phi_r(\mathbf{z})\equiv 0$ both (or in the symmorphic case neither) families of mirror planes have these extinctions, but when $\Phi_r(\mathbf{z})\equiv\frac{1}{2}$ (the only other possibility in this case) just one of the families has the extinctions. (As noted in Sec. IV.B.1, only when $N$ is twice a prime power is it possible to specify whether the family with extinctions is along or between a lattice-generating star.) Note that the extinctions associated with $\Phi_r$ being nonintegral on its invariant space (a twofold screw axis) add nothing new, since when $\Phi_r(\mathbf{z})\equiv\frac{1}{2}$, one or the other families of mirrors will have extinctions in the odd layers in its planes.

*Staggered stackings*: The trio of generators $(r,m,h)$ does not occur when $n$ is an odd prime power; for either of the other two pairs $(\bar{r},m)$ or $(r,m)$, the mirror $m$ can be taken in the plane of $\mathbf{z}+\alpha$ (so that the family of mirrors is necessarily *between* the directions in a generating star) and the only nonsymmorphic space group has $\Phi_m(\mathbf{z}+\alpha)\equiv\frac{1}{2}$. Thus, as in the case of vertical lattices, all lattice vectors in the planes of vertical mirrors with nonintegral phase functions are extinct when they lie in odd layers of the stacking.

The extinctions when $n\neq 2^s$ can thus be summarized in two simple rules:

*Rule I.* If the point group lacks vertical mirrors, then only points on the $z$ axis can be extinct *(screw axis)*. Forbidden lattice points occur wherever $\Phi_r\not\equiv 0$ [as specified in Eq. (6.2) for vertical lattices or (6.5) for staggered lattices].

*Rule II.* If the point group contains vertical mirrors, then the only extinct points are those in odd layers lying in the planes of the mirrors with nonintegral phase functions (vertical *glide planes*).

## B. The extinctions when $n=2^s$

When (and only when) the rotational order is a power of 2, there can be nonvanishing gauge-invariant phases in the $z=0$ plane. This modifies the conclusions of the preceding section in two ways: (1) There can be additional extinctions at horizontal invariant vectors of the point-group elements (dihedral axes or the horizontal mirror)[42] that reverse the sign of $\mathbf{z}$; (2) When the phases $\Phi_m(\xi^j)$ do not vanish, there is a nontrivial contribution to $\Phi_m(\mathbf{k})$ from the components of $\mathbf{k}$ along the $\xi^j$, which alters the character of extinct points in the planes of vertical mirrors. Note that the mirror $m'=rm$ (which is not conjugate to $m$ for even $n$) has $\Phi_{m'}(\xi^j)\equiv\Phi_m(\xi^j)$ as a consequence of the group compatibility condition (2.8) and the fact that $\Phi_r\equiv 0$ in the $z=0$ plane.

### 1. Extinctions from dihedral axes or horizontal mirrors

If the horizontal mirror $h$ is present with $\Phi_h(\xi^j)\equiv\frac{1}{2}$, then a point in the $z=0$ plane of the form $\sum n_j\xi^j$ is extinguished if and only if $\sum_j n_j$ is odd. We call points "odd" or "even" depending on the parity of this sum, and note that for $n=2^s$ whether a point is odd or even does not depend on the particular primitive (or nonprimitive) collection of star vectors in which we expand it.[43] We also call "odd" points in other layers of the stacking directly above the odd points in the $z=0$ plane. Odd

[42]The rotoinversion also reverses the sign of $\mathbf{z}$ but has no horizontal invariant vectors (and, in fact, we always chose a gauge with $\Phi_{\bar{r}}\equiv 0$).

[43]This follows simply from the fact that when $n=2^s$ all primitive subsets of the stars are the same except for the signs of their vectors.

points can thus be distinguished in all layers of the vertical stacking and in even layers of the staggered stacking with $n=2^s$.

If a dihedral axis $d$ is present with $\Phi_d(\xi^j)\equiv\frac{1}{2}$, then odd points in the $z=0$ plane along its invariant line are extinct. Since all points in directions between star vectors have even parity,[44] a dihedral axis can produce extinctions only if oriented along a star direction. [If that direction is $\xi^j$, then only the coefficients of $\xi^j$ (and $-\xi^j$) have to be examined to determine the parity.]

These conclusions give two additional rules for extinctions that come into play only when $n=2^s$:

*Rule III.* If the point group contains a horizontal mirror with a nonintegral phase $\Phi_h(\xi^j)$ (a horizontal *glide plane*), then all odd points in the $z=0$ plane are extinct.

*Rule IV.* If the point group contains dihedral axes along star directions with nonzero phases $\Phi_d(\xi^j)$ (horizontal *twofold screw axes*), then all odd points along star directions in the $z=0$ plane are extinct.

2. Vertical mirrors

*Vertical stackings.* If a mirror lies between star vectors, then $\Phi_m(\xi^j)\equiv\frac{1}{2}$ has no consequences, since, as noted in footnote 44, lattice vectors between star vectors always have even parity. For a mirror along a star vector, the effect of changing $\Phi_m(\xi^j)$ from 0 to $\frac{1}{2}$ is to reverse the status of odd-parity points in the plane of the mirror. Thus they are extinct if $\Phi_m(\mathbf{z})\equiv 0$; if $\Phi_m(\mathbf{z})\equiv\frac{1}{2}$ odd-parity points along star vectors are extinct in even layers, but only even-parity points along star vectors are extinct in odd layers.[45]

*Staggered stackings.* An additional complication when $n=2^s$ is that in this one case a staggered stacking can have vertical mirrors along as well as between star directions; this complication is mitigated by the fact that $2^s$-fold staggered lattices have points along star directions only in even layers.[46]

When the point group is generated by the pair $(\bar{r},m)$, vertical mirrors can lie either along or between star directions (alternating with dihedral axes between or along the star directions.) When the vertical mirrors lie between star directions, $\Phi_m(\xi^j)$ always vanishes, and, as earlier, all points in odd layers in the plane of the mirror are extinct when $\Phi_m(\mathbf{z}+\alpha)\equiv\frac{1}{2}$. When the vertical mirrors lie along star directions, then we need consider only even layers of the stacking (since the only points along star directions occur in even layers). We have

$$\Phi_m(2\mathbf{z}+2\alpha)\equiv\Phi_m(\xi^0)\equiv 0 \text{ or } \tfrac{1}{2}\ . \tag{6.7}$$

When $\Phi_m(\xi^0)\equiv\frac{1}{2}$ this gives extinctions in the plane of the mirror at points of odd parity in layers a multiple of 4 away from the $z=0$ layer and at points of even parity in the other even layers.

If the generators are $(r,m)$ or $(r,m,h)$, then the possibility $\Phi_m(\xi^j)\equiv\frac{1}{2}$ is always accompanied by $\Phi_r(\mathbf{z}+\alpha)\equiv\frac{1}{4}$. There are now mirrors both along $(m_a)$ and between $(m_b)$ star vectors. Since $m_b=rm_a$, the phases associated with the two types of mirrors are related by the group compatibility condition (2.8):

$$\Phi_{m_b}(\mathbf{k})\equiv\Phi_r(m_a\mathbf{k})+\Phi_{m_a}(\mathbf{k})\ . \tag{6.8}$$

Because all vectors *between* star vectors in the $z=0$ plane have even parity, for the mirror $m_b$ whose plane contains $\mathbf{z}+\alpha$, any vector in that plane in the $j$th layer differs from $j(\mathbf{z}+\alpha)$ by an even-parity vector and therefore has phase $j\Phi_{m_b}(\mathbf{z}+\alpha)$ whether or not $\Phi_{m_b}(\xi^j)\equiv 0$. Thus when $\Phi_{m_b}(\mathbf{z}+\alpha)\equiv\frac{1}{2}$ all points in the plane of the mirror $m_b$ in odd layers continue to be extinct. For the additional mirrors *along* generating vectors, we need consider only even layers (there being no points along generators in odd layers). An application of the group compatibility condition (2.8)[47] gives $\Phi_{m_a}(2\mathbf{z}+2\alpha)\equiv\Phi_{m_a}(\xi^0)$ indepen-

[44]Suppose there were such a point $\beta$ with odd parity. Expand $\beta$ in the integrally independent set consisting of the $\nu/2=2^{s-2}$ pairs of vectors angularly closest to it, next closest, etc. Since $\beta$ is invariant under mirroring in itself, interchanging the coefficients in each pair must also give an expansion of $\beta$. Since the set is integrally independent, however, there can be only one expansion. Therefore both members of each pair must have the same coefficient, and the parity of $\beta$ is even.

[45]We say an out-of-plane lattice vector is along or between star vectors if its horizontal component is along or between star vectors.

[46]Proof: It follows from the general form (2.2) of $\alpha$ that if $n=2^s$ then $\alpha=-\frac{1}{2}\sum_{j=0}^{\nu-1}\xi^j$. Thus the horizontal part $\beta$ of any lattice vector in an odd layer has an expansion in any primitive set of star vectors in which every coefficient is half integral (i.e., an integer plus $\frac{1}{2}$). Given any horizontal part $\beta$ and any star vector, we expand $\beta$ in the integrally independent set built up by taking the given star vector, the pair of star vectors angularly closest to it, the pair next closest, etc., until we finally add a single unbalanced star vector (since $\nu$ is even) perpendicular to the given one. If $\beta$ were invariant under mirroring in the given star vector, then, since an integrally independent set is also "half-integrally independent," not only would both members of each pair have to have the same coefficient, but the coefficient of the unbalanced star vector would also have to be zero. This last requirement is impossible, since every coefficient must be half integral.

[47]Applied to $m_a=r^{-1}m_b$ and using the fact that $\Phi_r(\mathbf{z}+\alpha)\equiv\frac{1}{2}\Phi_m(\xi^0)$.

dently of whether $\Phi_{m_b}(\mathbf{z}+\alpha)$ is 0 or $\frac{1}{2}$. Thus when $\Phi_{m_a}(\zeta^0)\equiv\frac{1}{2}$ this produces extinctions at points of odd parity that are multiples of four layers from the $z=0$ layer and at points of even parity in the other even layers.

### C. General rules for extinctions

We summarize the rules derived above, stating them in a form that unless otherwise noted applies to both lattice types (vertical or staggered) and all values of $n$:

#### 1. Extinctions out of the $z=0$ plane

*Rule I.* If the point group lacks vertical mirrors, then extinct points are on the $z$ axis. Extinctions occur at points with nonintegral values of $\Phi_r$, given by Eq. (6.2) in vertical stackings or (6.5) in staggered stackings (*screw axes*).[48]

*Rule II.* If the point group contains vertical mirrors between star vectors, then the extinct points are all those in odd layers lying in the planes of the mirrors that have nonintegral phase functions $\Phi_m(\mathbf{z})$ or $\Phi_m(\mathbf{z}+\alpha)$ (vertical *glide planes*).

*Rule IIA.* Rule II also holds for vertical mirrors along star vectors with two exceptions that can arise only when $n=2^s$: (i) In a vertical stacking, if $\Phi_m(\zeta^j)\equiv\frac{1}{2}$, then the extinct points in the plane of the mirror have odd parity[49] if $\Phi_m(\mathbf{z})\equiv 0$; if $\Phi_m(\mathbf{z})\equiv\frac{1}{2}$, they have odd parity in even layers and even parity in odd layers; (ii) In a staggered stacking, if $\Phi_m(\zeta^j)\equiv\frac{1}{2}$, then the extinct points in the plane of the mirror have odd parity when they are multiples of four layers from the $z=0$ plane and even parity in the other even layers. (There are no points along star vectors in odd layers of the staggered lattice.)

#### 2. Extinctions in the $z=0$ plane ($n=2^s$ only)

*Rule III.* If the point group contains a horizontal mirror with a nonintegral phase function (a horizontal *gilde plane*), then all odd-parity points in the $z=0$ plane are extinct.

*Rule IV.* If the point group contains dihedral axes along star directions with nonzero phase functions (horizontal *twofold screw axes*), then all odd-parity points along star directions in the $z=0$ plane are extinct.

## VII. QUASICRYSTALLOGRAPHIC NOMENCLATURE

Tables V and VI contain in compact form the complete classification of all the axial space groups, crystallographic and quasicrystallographic, on standard lattices, and the Rules I–IV at the end of Sec. VI, used in conjunction with these tables, specify the extinctions that characterize each space group. We present this information below in a more expanded form, along the lines of the International Tables of X-ray crystallography. We do this to emphasize that the conventional crystallographic axial space groups are quite naturally contained within the general quasicrystallographic scheme (or, if you prefer, the quasicrystallographic categories are very simple generalizations of the crystallographic ones) and also to suggest some obvious generalizations of conventional crystallographic nomenclature that apply to all the standard axial quasicrystallographic space groups. We stress, however, that all five of Tables IX–XIII contain no information not in the very brief Tables V and VI and the extinction rules I–IV given in Sec. VI.C.

### A. The five axial quasicrystal types

Five tables are required to list the space groups for arbitrary point-group rotational symmetry $n$: (1) $n$ any power of an odd prime (which contains as its two lowest-order members the trigonal crystal system and the pentagonal quasicrystal system); (2) $n$ any power of 2 greater than the first (which contains the tetragonal crystal system and the octagonal quasicrystal system); (3) $n$ twice a power of an odd prime (which contains the hexagonal crystal system and the decagonal quasicrystal system); (4) $n$ even, but not twice a prime power (which contains no crystal system and first occurs for the dodecagonal quasicrystal system); and (5) $n$ odd, but not a prime power (which first occurs at $n=15$ and contains no crystal system or previously investigated quasicrystal system).

Because the organization is by point group, the first category contains space groups with $p_o^s$-fold point groups on $2p_o^s$-fold vertical lattices as well as $p_o^s$-fold staggered lattices ($p_o$ any odd prime). The remaining space groups on the $2p_o^s$-fold vertical lattices (with $2p_o^s$-fold point groups) are in the third category.[50] Space groups in the third, fourth, and fifth categories must have vertical lattices; only the first and second categories contain both staggered and vertical lattices.

[48]Note that for given $n$ the extinctions produced by the phase functions (6.2) or (6.5) can be identical for many different values of $j$. (If $n$ is prime, for example, all values of $j$ between 1 and $p-1$ give the same extinctions.) This contrasts with the crystallographic case, in which only $j$ and $n-j$ (enantiamorphic pairs) give the same extinctions.

[49]See the first paragraph of Sec. VI.B.1 for the definition of parity, which applies only when $n=2^s$.

[50]This follows the crystallographic convention of grouping all space groups on rhombohedral lattices and space groups with 3-fold point groups on hexagonal lattices into the single trigonal crystal system.

We refer to these five categories as quasicrystal types and name each type for the lowest-order structure (crystal or quasicrystal) it can describe. Thus we have the (1) trigonal, (2) tetragonal, (3) hexagonal, (4) dodecagonal, and (5) pentadecagonal quasicrystal types. We call members of a quasicrystal type with a given $n$ quasicrystal systems. (Thus the trigonal quasicrystal type contains the trigonal (quasi)crystal system, the pentagonal quasicrystal system, the septagonal, the nonagonal, etc.)

### B. Specifying a space group

The first column in the tables that follow (Tables IX–XIII) identifies each type of space group in a way that directly reflects the way in which we constructed it:

(1) We denote the vertical lattice by $V$ and the staggered by $S$. $V$ corresponds to $P$ (for primitive) in the International nomenclature for simple tetragonal and hexagonal lattices, and $S$ becomes $R$ (for rhombohedral) and most commonly $I$ (for centered tetragonal with body-centered real-space indexing) in the two crystallographic examples of staggered lattices.[51]

(2) We specify the point group by the set of generators (see Table III) used in our construction of the space groups, e.g., $(r,h,m)$ for $n/mmm$. If one needs to be explicit about the order of rotation (or rotoinversion) (i.e., the quasicrystal system), one can affix a subscript, e.g., $(r,h,m)_8$ for $8/mmm$. Since each of the tables that follows holds for an infinite family of rotational orders $n$ (an entire quasicrystal type), we specify the allowed values of $n$ at the head of the table and omit the generic subscript $n$ from individual entries.[52]

(3) For mirrors and dihedral axes we use a prime ($m'$ or $d'$) to indicate alignment between horizontal reciprocal-lattice star vectors. (When $n$ is odd, "between" means between the vectors of a $2n$-fold star.) Otherwise the mirror ($m$) or dihedral axis ($d$) is aligned along star vectors.

(4) To indicate the nonzero values of the phase functions associated with the generators at the reciprocal-lattice-generating vectors, we add a superscript or a subscript to the generators. A superscript specifies the phase above the $z=0$ plane at $\mathbf{z}$ or $\mathbf{z}+\alpha$, depending on whether the lattice is vertical or staggered. Subscripts (which occur only in the tetragonal quasicrystal type) specify the phases associated with vertical mirrors or dihedral axes at $\zeta^j$. We always give these in a gauge in which all vertical mirrors (or all dihedral axes) have the same phase for all $j$.

Thus the symbol $V(r,h_{1/2},m^{1/2}_{1/2})_8$ specifies the space group in the octagonal quasicrystal system with $\Phi_h(\zeta^j)\equiv\Phi_m(\zeta^j)\equiv\Phi_m(\mathbf{z})\equiv\frac{1}{2}$.

Of course the symbol is not unique, depending as it does on our original choice of point-group generators. The above example can also be written[53] as $V(m^{1/2}_{1/2},m'^{1/2}_{1/2},h_{1/2})_8$.

The generalized International space-group symbol is given in the second column. For purposes of comparing the orthodox notation to the generalization we propose, we also list, when one exists, the single crystallographic case. The individual table captions comment on when these differ from the general form by more than simply replacing the general $n$ by 3, 4, or 6 for the first three quasicrystal types.[54]

The final column locates the extinct lattice vectors following the four rules of Sec. VI.

Readers unfamiliar with or uninterested in the International (Hermann-Mauguin) space-group notation should go directly to a perusal of the tables, ignoring the second column and the further discussion below.

### C. Generalized International axial space-group symbols

The remarks that follow and the accompanying Tables VII and VIII are intended to explain in a little more detail our treatment of the axial quasicrystallographic space

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[51]Note, however, that our $V$ and $S$ denote only the lattice type, making no reference to any indexing scheme. (Our analysis above used only primitive indexing, and our description of extinctions is based on that primitive indexing.)

[52]In a few instances this generic rotational $n$ clashes with the $n$ used to denote glide plane type in the International nomencalture. Such glide planes arise for axial quasicrystals only of the tetragonal type. The two $n$'s can always be distinguished because the rotational $n$ occurs only in primary position and never in the denominator, while the glide plane $n$, if in primary position, appears always in the denominator. In any specific case, the rotational $n$ would be a particular number.

[53]The phases for any other choice of generators or any other point-group operations can easily be found from the information given in any version of the symbol by expressing the operation in terms of the given generators and applying the group compatibility condition (2.8). Indeed, as a consequence of working in a gauge with $\Phi_{\bar{r}}\equiv 0$ or $\Phi_r(\zeta^j)\equiv 0$, one easily establishes that, in going from the pair $(r,m)$ to the pair $(m,m')$ or from $(\bar{r},m)$ to $(m,d)$ or $(m,d')$, the superscripts and subscripts for the new generator ($m'$ or $d'$) are simply the sums of the superscripts and subscripts of the original pair. In some cases, a different gauge choice may further simplify this kind of derived space-group symbol. The simple summation rule breaks down when applied on a staggered lattice to a dihedral axis $d=hm$ expressed in terms of the horizontal mirror $h$ and a vertical mirror $m$ lying along a star vector, for then one finds $\Phi_d(\mathbf{z}+\alpha)\equiv\Phi_h(\mathbf{z}+\alpha)+\Phi_h(\zeta^0)+\Phi_m(\mathbf{z}+\alpha)$. In this case, however, one can use the gauge function (5.10) to set either $\Phi_d(\mathbf{z}+\alpha)$ or $\Phi_h(\mathbf{z}+\alpha)$ (but not both) to zero.

[54]The last two types contain no crystal systems.

TABLE VII. Between and along directions in international notation. When the rotational symmetry $N$ of the horizontal sublattice of the reciprocal lattice is twice a prime power ($p_o$ stands for any odd prime), there is a unique orientation for an $N$-fold star that generates the lattice. The dihedral axes or the planes of vertical mirrors can lie either along ($m$ and $d$) or between ($m'$ and $d'$) these directions. The table indicates whether such operations appear in the secondary or tertiary positions of our generalization of the International space-group symbols (for both the $P$ and the $S$ lattices). When $N$ is not twice a prime power, i.e., when the rotational order $n$ of the point group is neither a prime power nor twice a prime power, there is no distinction between secondary and tertiary positions: exchanging the two entries does not change the space group. (The commonly used $I$ setting for the centered tetragonal crystallographic space groups ($N=4$) implies a nonprimitive, face-centered indexing of reciprocal space. This has the effect of rotating through $\pi/4$ the axes with respect to which "secondary" and "tertiary" are defined. As a result, our generalization of the International space-group symbols for lattices of the centered tetragonal type differs from the $I$ setting in interchanging secondary and tertiary positions.)

| GENERATORS | $N=2^s$ ($n=N$) | $N=2p_o^s$ ($n=N$ or $\frac{1}{2}N$) | other $N$ |
|---|---|---|---|
| $m$ along | secondary | secondary | |
| $m'$ between | tertiary | tertiary | *no* |
| $d$ along | secondary | tertiary | *distinction* |
| $d'$ between | tertiary | secondary | |

groups to readers familiar with the International nomenclature.[55]

We give each space group a generalized International (Hermann-Mauguin) symbol. Because the rhombohedral and centered tetragonal lattices are simply the first two members of the infinite quasicrystallographic family of staggered lattices that exists whenever the rotational order of the point group is a power of a prime number, we have replaced the symbols $I$ (or $F$) (centered tetragonal) and $R$ (rhombohedral) by the single symbol $S$ (staggered).[56] We have retained the conventional symbol $P$ (primitive) for the vertically stacked lattices.

The International nonmenclatural treatment of the alignment of mirrors and dihedral axes in axial point groups is not perfectly adapted to the quasicrystallographic generalization. International notation refers to primary, secondary, and tertiary directions (information about which is listed in the first, second, and third positions after the letter identifying the lattice). For axial point groups, the primary direction is perpendicular to the layers; the secondary and tertiary directions are sometimes what we refer to as "along" and "between" reciprocal-lattice generators and sometimes "between" and "along." Since the distinction between "along" and "between" is meaningful in the quasicrystallographic case only when $n$ is a prime power or twice a prime power, this problem arises only for the trigonal, tetragonal, and hexagonal quasicrystal types (which, of course, include all the crystallographic cases) but not the dodecagonal or pentadecagonal.

We specify the orientation of a vertical mirror by a horizontal direction in the plane of the mirror.[57] When $n$ is a prime power or twice a prime power, our "along" directions for vertical mirrors or (horizontal) dihedral axes lie along the unique set of directions in a star of vectors, all integral linear combinations of which generate the horizontal two-dimensional sublattice of the reciprocal lattice; our "between" directions lie between the directions of a $2n$-fold ($n$ odd) or $n$-fold ($n$ even) star.

In the International scheme, on the other hand, the direction of a vertical mirror is given by its normal, and the distinction between secondary and tertiary directions is tied to a conventional choice of real-space lattice generators. The rules for translating between these conventions are very simple but depend on quasicrystal type:

*Dodecagonal and pentadecagonal quasicrystal types.* Here the issue does not arise: there is no distinction between directions along or between generating stars, since generating stars can be found in both sets of directions. Reflecting this, generalized International space-group symbols that differ only by an interchange of secondary and tertiary positions describe the same space group.[58]

*Trigonal and hexagonal quasicrystal types.* Here the horizontal sublattice of the reciprocal lattice is generated by an $N$-fold star, where $N$ is twice an odd prime power. The normal to a vertical mirror containing (i.e., along) reciprocal-lattice generators lies between the generators and vice versa. In the crystallographic case, $N=6$, directions along generators in real space lie between them in

[55]They may also serve a secondary purpose of introducing that nomenclature to curious innocents, whose knowledge of space groups is limited to what we have taught them above.

[56]Although none of the primitive generators of the staggered lattice lie along the $z$ axis perpendicular to the layers, we continue to use a $c$ to label glide planes for which the translation (plus phason) required to undo the mirroring has a component perpendicular to the layers of the stacking. Because our $S$ lattice is primitive, there are no "included extinctions." Our specification of the space group in the left-hand column requires no further nomenclatural convention ($a,b,c,n$, or $d$) for identifying glide planes, since specifying the phase associated with a mirror entirely determines the translation (plus phason) that undoes it. [For an ordinary crystal with phase functions $\Phi_g(\mathbf{k})$, one readily establishes that $\rho(g\mathbf{r})=\rho(r+\sum \mathbf{a}^i\Phi_g(\mathbf{b}^i))$, where the vectors $\mathbf{a}^i$ generate the real-space lattice dual to the reciprocal lattice generated by $\mathbf{b}^i$, so that $\mathbf{a}^i\cdot\mathbf{b}^j=2\pi\delta^{ij}$.]

[57]We do this so that the actions of mirrors and dihedral axes on the horizontal two-dimensional sublattice can be treated on an equal footing.

[58]This was pointed out by RWM for the two-dimensional space groups with standard lattices.

TABLE VIII. Space-group element symbols. We indicate the correspondence between the phases associated with point-group generators and the generalized International symbols. A subscripted generator $x_f$ means that $\Phi_x(\xi^j)\equiv f$; a superscripted symbol $x^f$ means either $\Phi_x(\mathbf{z})\equiv f$ or $\Phi_x(\mathbf{z}+\alpha)\equiv f$, depending on the lattice. A prime on the symbol $m$ or $d$ indicates that the operation lies between roots of unity; otherwise it lies along a root. Note that directions along or between roots of unity (and therefore entries in secondary and tertiary positions) can be distinguished only for the trigonal, tetragonal, and hexagonal quasicrystal types. Symbols for the dodecagonal and pentadecagonal types that differ only by an interchange of secondary and tertiary entries describe the same space group. [For the centered tetragonal lattice ($n=4$), the International Tables use a nonprimitive $I$ setting, which differs from the $S$ setting shown here in reversing secondary and tertiary positions and in replacing the glide $n$ in the denominator of primary position with a glide $a$].

| Generating Symbol | International Symbol |
|---|---|
| $\bar{r}$ | primary $\bar{n}$ |
| $r$ | primary $n$ |
| $r^{j/n}$ | primary $n_j$ |
| $d$ without subscript (arbitrary superscript) | secondary 2 ($n$ a multiple of 4)<br>tertiary 2 ($n$ not a multiple of 4) |
| $d_{1/2}$ (found only on vertical stacking, $n=2^s$) | secondary $2_1$ ($n$ a multiple of 4) |
| $d'$ of any kind | tertiary 2 ($n$ a multiple of 4)<br>secondary 2 ($n$ not a multiple of 4) |
| no generator<br>(used when needed to clarify positional notation) | secondary or tertiary 1 |
| $h$ | primary $m$ |
| $h_{1/2}$ | primary $n$ (glide plane) |
| $m$ | secondary $m$ |
| $m^{1/2}$ (staggered stacking) | secondary $m$, $S$ setting |
| $m^{1/2}$ (vertical stacking) | secondary $c$, $P$ setting |
| $m_{1/2}$ (found only on vertical stacking) | secondary $b$ |
| $m_{1/2}^{1/2}$ (found only on vertical stacking) | secondary $n$ (glide plane) |
| $m_{1/2}^{1/4}$ or $m_{1/2}^{3/4}$ (found only on staggered stacking) | secondary $d$ |
| $m'$ or $m'_{1/2}$ | tertiary $m$ |
| $m'^{1/2}$ or $m'^{1/2}_{1/2}$ | tertiary $c$ |

reciprocal space and vice versa.[59] Consequently, in extending the International notation to the trigonal and hexagonal quasicrystal types, because of these two reversals, we list vertical mirrors along ($m$) or between ($m'$) reciprocal-lattice-generating stars in secondary or tertiary positions, respectively. On the other hand, dihedral axes along ($d$) or between ($d'$) reciprocal-lattice-generating vectors are listed in tertiary or secondary position.

*Tetragonal quasicrystal type.* Here the horizontal sublattice of the reciprocal lattice is generated by an $N$-fold

[59]When $N$ exceeds 6, there is no real-space lattice.

TABLE IX. The axial space groups—$n$ a power of an odd prime (trigonal type). Note that the space groups $S(r^{j/n})$ and $S(r^{j/n},d)$ have no crystallographic analogs and first arise in the $n=3^2$ nonagonal system. When a vertical mirror is among the point-group generators for a staggered lattice with odd $n$, it must lie between roots of unity, and we denote it here by $m'$. ("Included extinctions" in the $R$ lattice due to a nonprimitive basis are not shown; our primitively indexed $S$ lattice implies no such extinctions.)

| | | | |
|---|---|---|---|
| $V(\bar{r})$ | $P\bar{n}$ | $P\bar{3}$ | no extinctions |
| $S(\bar{r})$ | $S\bar{n}$ | $R\bar{3}$ | no extinctions |
| $V(\bar{r},\ m)$ | $P\bar{n}\frac{2}{m}1$ | $P\bar{3}\frac{2}{m}1$ | no extinctions |
| $V(\bar{r},\ m^{1/2})$ | $P\bar{n}\frac{2}{c}1$ | $P\bar{3}\frac{2}{c}1$ | odd layers along |
| $V(\bar{r},\ m')$ | $P\bar{n}1\frac{2}{m}$ | $P\bar{3}1\frac{2}{m}$ | no extinctions |
| $V(\bar{r},\ m'^{1/2})$ | $P\bar{n}1\frac{2}{c}$ | $P\bar{3}1\frac{2}{c}$ | odd layers between |
| $S(\bar{r},\ m')$ | $S\bar{n}\frac{2}{m}$ | $R\bar{3}\frac{2}{m}$ | no extinctions |
| $S(\bar{r},\ m'^{1/2})$ | $S\bar{n}\frac{2}{c}$ | $R\bar{3}\frac{2}{c}$ | odd layers between |
| $V(r)$ | $Pn$ | $P3$ | no extinctions |
| $V(r^{j/n})$ $j=1,\ldots,n-1$ | $Pn_j$ | $P3_j$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $S(r)$ | $Sn$ | $R3$ | no extinctions |
| $S(r^{j/n})$ $j=1,\ldots,{}^{n}/_{p}-1$ | $Sn_j$ | *(none)* | $kp\mathbf{z}$ when $jkp$ not a multiple of $n$ |
| $V(r,\ m)$ | $Pnm1$ | $P3m1$ | no extinctions |
| $V(r,\ m^{1/2})$ | $Pnc1$ | $P3c1$ | odd layers along |

star where $N$ is a power of 2. The normal to a vertical mirror containing ("along") reciprocal-lattice generators is also along them, and similarly for "between." In the crystallographic case $N=4$ a star that *primitively* generates the real-space square lattice also lies along the directions of the reciprocal-lattice-generating star. Therefore mirrors $(m)$ or dihedral axes $(d)$ along reciprocal-lattice-generating vectors are listed in secondary position, and mirrors $(m')$ or dihedral axes $(d')$ between reciprocal-lattice-generating vectors are listed in tertiary position. There is a further complication in the case of the $S$ lattice, because the International notation favors the $I$ (body-centered in real space) setting in its description of centered tetragonal lattices.[60] This setting views the centered tetragonal reciprocal lattice as face-centered, and the axes for the horizontal square lattice are taken at 45° to the axes that generate the square lattice primitively. Consequently the $S$ symbol for the tetragonal quasicrystal type differs from the symbol for the tetragonal crystallographic space groups in the $I$ setting by the interchange of entries in secondary and tertiary positions.[61]

These relations between our "along" and "between" and the "secondary" and "tertiary" of the International scheme are summarized in Table VII.

Table VIII gives the complete set of rules used to go from our specification of the space groups on the left to the generalized International symbols. In our opinion the **V** and **S** symbols in the first column of Tables IX–XIII are simpler and more informative than the conventional generalized International symbols in the second.

[60]The complication does not arise when the $F$ (face-centered in real space) setting is used instead.

[61]There are also three instances where the difference in setting requires a glide plane to change its name from $a$ to $n$.

TABLE IX. (*Continued*).

| | | | |
|---|---|---|---|
| $V(r,\ m')$ | $Pn1m$ | $P31m$ | no extinctions |
| $V(r,\ m'^{1/2})$ | $Pn1c$ | $P31c$ | odd layers between |
| $S(r,\ m')$ | $Snm$ | $R3m$ | no extinctions |
| $S(r,\ m'^{1/2})$ | $Snc$ | $R3c$ | odd layers between |
| $V(r,\ d)$ | $Pn12$ | $P312$ | no extinctions |
| $V(r^{j/n},\ d)$ $j=1,\ldots,n-1$ | $Pn_j12$ | $P3_j12$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r,\ d')$ | $Pn21$ | $P321$ | no extinctions |
| $V(r^{j/n},\ d')$ $j=1,\ldots,n-1$ | $Pn_j21$ | $P3_j21$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $S(r,\ d)$ | $Sn2$ | $R32$ | no extinctions |
| $S(r^{j/n},\ d)$ $j=1,\ldots,{}^n/_p-1$ | $Sn_j2$ | (*none*) | $kp\mathbf{z}$ when $jkp$ not a multiple of $n$ |

TABLE X. The axial space groups—$n$ a power of two (tetragonal type). The symbol $n$ in the numerator of primary position and in the subscripts $\frac{n}{2}$ and $\frac{n}{4}$ refers to the $n$-fold rotation axis. Anywhere else (denominator of primary position or anywhere in secondary or tertiary positions), $n$ refers to a glide plane. (This unfortunate clash between point-group rotational order and the conventional International glide plane nomenclature arises only for the tetragonal quasicrystal type.) When a point group on a staggered lattice includes mirrors both along $(m)$ and between $(m')$ roots of unity, we choose the latter as a generator, as we did in Sec. V. (Only the point group $\bar{n}2m$ has just one set of mirrors, and one of its two orientations puts them along roots of unity). In deducing the extinctions it may be necessary also to examine the phases for the "along" mirror $m$ (or the "along" dihedral axis $d$). Since $m'=rm$, one easily translates between the two choices of generator with the group compatibility relation (2.8). If $a$, $b$, and $c$ stand for arbitrary superscripts and subscripts, then $(r^a,m_b^c)=(r^a,m_b'^{a+c})$, on both $V$ and $S$ lattices. The same rule works for $d=\bar{r}m'$. (It fails for $d=hm$ on staggered lattices; see footnote 51.) Extinctions in the centered tetragonal $I$ lattice due to the nonprimitive basis ("included extinctions") are not shown; our primitive $S$ indexing has no included extinctions.

| | | | |
|---|---|---|---|
| $V(\bar{r})$ | $P\bar{n}$ | $P\bar{4}$ | no extinctions |
| $S(\bar{r})$ | $S\bar{n}$ | $I\bar{4}$ | no extinctions |
| $V(\bar{r},\ m)$ | $P\bar{n}m2$ | $P\bar{4}m2$ | no extinctions |
| $V(\bar{r},\ m_{1/2})$ | $P\bar{n}b2$ | $P\bar{4}b2$ | all layers, odd parity, along |
| $V(\bar{r},\ m^{1/2})$ | $P\bar{n}c2$ | $P\bar{4}c2$ | odd layers along |
| $V(\bar{r},\ m_{1/2}^{1/2})$ | $P\bar{n}n2$ | $P\bar{4}n2$ | even layers, odd parity, along<br>odd layers, even parity, along |

TABLE X. (*Continued*).

| | | | |
|---|---|---|---|
| $V(\bar{r},\ m')$ | $P\bar{n}2m$ | $P\bar{4}2m$ | no extinctions |
| $V(\bar{r},\ m'_{1/2})$ | $P\bar{n}2_1m$ | $P\bar{4}2_1m$ | zero layer, odd parity, along |
| $V(\bar{r},\ m'^{1/2})$ | $P\bar{n}2c$ | $P\bar{4}2c$ | odd layers between |
| $V(\bar{r},\ m'^{1/2}_{1/2})$ | $P\bar{n}2_1c$ | $P\bar{4}2_1c$ | odd layers between<br>zero layer, odd parity, along |
| $S(\bar{r},\ m)$ | $S\bar{n}m2$ | $I\bar{4}2m$ | no extinctions |
| $S(\bar{r},\ m^{1/4}_{1/2})$ | $S\bar{n}d2$ | $I\bar{4}2d$ | 2 mod 4 layers, even parity, along<br>0 mod 4 layers, odd parity, along |
| $S(\bar{r},\ m')$ | $S\bar{n}2m$ | $I\bar{4}m2$ | no extinctions |
| $S(\bar{r},\ m'^{1/2})$ | $S\bar{n}2c$ | $I\bar{4}c2$ | odd layers between |
| $V(r)$ | $Pn$ | $P4$ | no extinctions |
| $V(r^{j/n})$<br>$j=1,\ldots,n-1$ | $Pn_j$ | $P4_j$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $S(r)$ | $Sn$ | $I4$ | no extinctions |
| $S(r^{j/n})$<br>$j=1,\ldots,{}^{n}/_{2}-1$ | $Sn_j$ | $I4_1$ | $2k\mathbf{z}$ when $2jk$ not a multiple of $n$ |
| $V(r,\ m)$ | $Pnmm$ | $P4mm$ | no extinctions |
| $V(r,\ m_{1/2})$ | $Pnbm$ | $P4bm$ | all layers, odd parity, along |
| $V(r,\ m^{1/2})$ | $Pncc$ | $P4cc$ | odd layers,<br>along and between |
| $V(r,\ m^{1/2}_{1/2})$ | $Pnnc$ | $P4nc$ | odd layers, even parity, along<br>even layers, odd parity, along<br>odd layers, between |
| $V(r^{1/2},\ m)$ | $Pn_{\frac{n}{2}}mc$ | $P4_2mc$ | odd layers between |
| $V(r^{1/2},\ m_{1/2})$ | $Pn_{\frac{n}{2}}bc$ | $P4_2bc$ | odd layers between<br>all layers, odd parity, along |
| $V(r^{1/2},\ m^{1/2})$ | $Pn_{\frac{n}{2}}cm$ | $P4_2cm$ | odd layers along |
| $V(r^{1/2},\ m^{1/2}_{1/2})$ | $Pn_{\frac{n}{2}}nm$ | $P4_2nm$ | odd layers, even parity, along<br>even layers, odd parity, along |
| $S(r,\ m')$ | $Snmm$ | $I4mm$ | no extinctions |
| $S(r,\ m'^{1/2})$ | $Snmc$ | $I4cm$ | odd layers between |

TABLE X. (*Continued*).

| | | | |
|---|---|---|---|
| $S(r^{1/4},\ m'_{1/2})$ | $Sn_{\frac{n}{4}}dm$ | $I4_1md$ | 2 mod 4 layers, even parity, along<br>0 mod 4 layers, odd parity, along |
| $S(r^{1/4},\ m'^{1/2}_{1/2})$ | $Sn_{\frac{n}{4}}dc$ | $I4_1cd$ | 2 mod 4 layers, even parity, along<br>0 mod 4 layers, odd parity, along<br>odd layers between |
| $V(r,\ d)$ | $Pn22$ | $P422$ | no extinctions |
| $V(r,\ d_{1/2})$ | $Pn2_12$ | $P42_12$ | zero layer, odd parity, along |
| $V(r^{j/n},\ d)$<br>$j=1,\ldots,n-1$ | $Pn_j22$ | $P4_j22$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r^{j/n},\ d_{1/2})$<br>$j=1,\ldots,n-1$ | $Pn_j2_12$ | $P4_j2_12$ | zero layer, odd parity, along<br>$k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $S(r,\ d)$ | $Sn22$ | $I422$ | no extinctions |
| $S(r^{j/n},\ d)$<br>$j=1,\ldots,n/2-1$ | $Sn_j22$ | $I4_122$ | $2k\mathbf{z}$ when $2jk$ not a multiple of $n$ |
| $V(r,\ h)$ | $P\frac{n}{m}$ | $P\frac{4}{m}$ | no extinctions |
| $V(r,\ h_{1/2})$ | $P\frac{n}{n}$ | $P\frac{4}{n}$ | zero layer, odd parity |
| $V(r^{1/2},\ h)$ | $P\frac{n_{\frac{n}{2}}}{m}$ | $P\frac{4_2}{m}$ | $k\mathbf{z}$ when $k$ odd |
| $V(r^{1/2},\ h_{1/2})$ | $P\frac{n_{\frac{n}{2}}}{n}$ | $P\frac{4_2}{n}$ | zero layer, odd parity<br>$k\mathbf{z}$ when $k$ odd |
| $S(r,\ h)$ | $S\frac{n}{m}$ | $I\frac{4}{m}$ | no extinctions |
| $S(r^{1/4},\ h_{1/2})$ | $S\frac{n_{\frac{n}{4}}}{n}$ | $I\frac{4_1}{a}$ | zero layer, odd parity<br>$2k\mathbf{z}$ when $k$ odd |
| $V(r,\ h,\ m)$ | $P\frac{n}{m}\frac{2}{m}\frac{2}{m}$ | $P\frac{4}{m}\frac{2}{m}\frac{2}{m}$ | no extinctions |
| $V(r,\ h,\ m_{1/2})$ | $P\frac{n}{m}\frac{2_1}{b}\frac{2}{m}$ | $P\frac{4}{m}\frac{2_1}{b}\frac{2}{m}$ | all layers, odd parity, along |
| $V(r,\ h,\ m^{1/2})$ | $P\frac{n}{m}\frac{2}{c}\frac{2}{c}$ | $P\frac{4}{m}\frac{2}{c}\frac{2}{c}$ | odd layers, along and between |
| $V(r,\ h,\ m^{1/2}_{1/2})$ | $P\frac{n}{m}\frac{2_1}{n}\frac{2}{c}$ | $P\frac{4}{m}\frac{2_1}{n}\frac{2}{c}$ | odd layers, even parity, along<br>even layers, odd parity, along<br>odd layers, between |
| $V(r,\ h_{1/2},\ m)$ | $P\frac{n}{n}\frac{2_1}{m}\frac{2}{m}$ | $P\frac{4}{n}\frac{2_1}{m}\frac{2}{m}$ | zero layer, odd parity |

TABLE X. (*Continued*).

| | | | |
|---|---|---|---|
| $V(r,\ h_{1/2},\ m_{1/2})$ | $P\frac{n}{n}\frac{2}{b}\frac{2}{m}$ | $P\frac{4}{n}\frac{2}{b}\frac{2}{m}$ | all layers, odd parity, along<br>zero layer, odd parity |
| $V(r,\ h_{1/2},\ m^{1/2})$ | $P\frac{n}{n}\frac{2_1}{c}\frac{2}{c}$ | $P\frac{4}{n}\frac{2_1}{c}\frac{2}{c}$ | odd layers, along and between<br>zero layer, odd parity |
| $V(r,\ h_{1/2},\ m^{1/2}_{1/2})$ | $P\frac{n}{n}\frac{2}{n}\frac{2}{c}$ | $P\frac{4}{n}\frac{2}{n}\frac{2}{c}$ | odd layers, even parity, along<br>even layers, odd parity, along<br>odd layers, between<br>zero layer, odd parity |
| $V(r^{1/2},\ h,\ m)$ | $P\frac{n_{n/2}}{m}\frac{2}{m}\frac{2}{c}$ | $P\frac{4_2}{m}\frac{2}{m}\frac{2}{c}$ | odd layers between |
| $V(r^{1/2},\ h,\ m_{1/2})$ | $P\frac{n_{n/2}}{m}\frac{2_1}{b}\frac{2}{c}$ | $P\frac{4_2}{m}\frac{2_1}{b}\frac{2}{c}$ | odd layers, between<br>all layers, odd parity, along |
| $V(r^{1/2},\ h,\ m^{1/2})$ | $P\frac{n_{n/2}}{m}\frac{2}{c}\frac{2}{m}$ | $P\frac{4_2}{m}\frac{2}{c}\frac{2}{m}$ | odd layers along |
| $V(r^{1/2},\ h,\ m^{1/2}_{1/2})$ | $P\frac{n_{n/2}}{m}\frac{2_1}{n}\frac{2}{m}$ | $P\frac{4_2}{m}\frac{2_1}{n}\frac{2}{m}$ | odd layers, even parity, along<br>even layers, odd parity, along |
| $V(r^{1/2},\ h_{1/2},\ m)$ | $P\frac{n_{n/2}}{n}\frac{2_1}{m}\frac{2}{c}$ | $P\frac{4_2}{n}\frac{2_1}{m}\frac{2}{c}$ | odd layers, between<br>zero layer, odd parity |
| $V(r^{1/2},\ h_{1/2},\ m_{1/2})$ | $P\frac{n_{n/2}}{n}\frac{2}{b}\frac{2}{c}$ | $P\frac{4_2}{n}\frac{2}{b}\frac{2}{c}$ | odd layers, between<br>all layers, odd parity, along<br>zero layer, odd parity |
| $V(r^{1/2},\ h_{1/2},\ m^{1/2})$ | $P\frac{n_{n/2}}{n}\frac{2_1}{c}\frac{2}{m}$ | $P\frac{4_2}{n}\frac{2_1}{c}\frac{2}{m}$ | odd layers, along<br>zero layer, odd parity |
| $V(r^{1/2},\ h_{1/2},\ m^{1/2}_{1/2})$ | $P\frac{n_{n/2}}{n}\frac{2}{n}\frac{2}{m}$ | $P\frac{4_2}{n}\frac{2}{n}\frac{2}{m}$ | odd layers, even parity, along<br>even layers, odd parity, along<br>zero layer, odd parity |
| $S(r,\ h,\ m')$ | $S\frac{n}{m}\frac{2}{m}\frac{2}{m}$ | $I\frac{4}{m}\frac{2}{m}\frac{2}{m}$ | no extinctions |
| $S(r,\ h,\ m'^{1/2})$ | $S\frac{n}{m}\frac{2}{m}\frac{2}{c}$ | $I\frac{4}{m}\frac{2}{c}\frac{2}{m}$ | odd layers between |
| $S(r^{1/4},\ h_{1/2},\ m'_{1/2})$ | $S\frac{n_{n/4}}{n}\frac{2}{d}\frac{2}{m}$ | $I\frac{4_1}{a}\frac{2}{m}\frac{2}{d}$ | 2 mod 4 layers, even parity, along<br>0 mod 4 layers, odd parity, along<br>zero layer, odd parity |
| $S(r^{1/4},\ h_{1/2},\ m'^{1/2}_{1/2})$ | $S\frac{n_{n/4}}{n}\frac{2}{d}\frac{2}{c}$ | $I\frac{4_1}{a}\frac{2}{c}\frac{2}{d}$ | 2 mod 4 layers, even parity, along<br>0 mod 4 layers, odd parity, along<br>odd layers, between<br>zero layer, odd parity |

TABLE XI. The axial space groups—$n$ twice a power of an odd prime (hexagonal type). Here the notational correspondence between the general case and the one crystallographic example is perfect.

| | | | |
|---|---|---|---|
| $V(\bar{r})$ | $P\bar{n}$ | $P\bar{6}$ | no extinctions |
| $V(\bar{r},\ m)$ | $P\bar{n}m2$ | $P\bar{6}m2$ | no extinctions |
| $V(\bar{r},\ m^{1/2})$ | $P\bar{n}c2$ | $P\bar{6}c2$ | odd layers along |
| $V(\bar{r},\ m')$ | $P\bar{n}2m$ | $P\bar{6}2m$ | no extinctions |
| $V(\bar{r},\ m'^{1/2})$ | $P\bar{n}2c$ | $P\bar{6}2c$ | odd layers between |
| $V(r)$ | $Pn$ | $P6$ | no extinctions |
| $V(r^{j/n})$ $j=1,\ldots,n-1$ | $Pn_j$ | $P6_j$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r,\ m)$ | $Pnmm$ | $P6mm$ | no extinctions |
| $V(r,\ m^{1/2})$ | $Pncc$ | $P6cc$ | odd layers, along and between |
| $V(r^{1/2},\ m)$ | $Pn_{\frac{n}{2}}mc$ | $P6_3mc$ | odd layers between |
| $V(r^{1/2},\ m^{1/2})$ | $Pn_{\frac{n}{2}}cm$ | $P6_3cm$ | odd layers along |
| $V(r,\ d)$ | $Pn22$ | $P622$ | no extinctions |
| $V(r^{j/n},\ d)$ $j=1,\ldots,n-1$ | $Pn_j22$ | $P6_j22$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r,\ h)$ | $P\frac{n}{m}$ | $P\frac{6}{m}$ | no extinctions |
| $V(r^{1/2},\ h)$ | $P\frac{n_{\frac{n}{2}}}{m}$ | $P\frac{6_3}{m}$ | $k\mathbf{z}$ with $k$ odd |
| $V(r,\ h,\ m)$ | $P\frac{n}{m}\frac{2}{m}\frac{2}{m}$ | $P\frac{6}{m}\frac{2}{m}\frac{2}{m}$ | no extinctions |
| $V(r,\ h,\ m^{1/2})$ | $P\frac{n}{m}\frac{2}{c}\frac{2}{c}$ | $P\frac{6}{m}\frac{2}{c}\frac{2}{c}$ | odd layers, along and between |
| $V(r^{1/2},\ h,\ m)$ | $P\frac{n_{\frac{n}{2}}}{m}\frac{2}{m}\frac{2}{c}$ | $P\frac{6_3}{m}\frac{2}{m}\frac{2}{c}$ | odd layers between |
| $V(r^{1/2},\ h,\ m^{1/2})$ | $P\frac{n_{\frac{n}{2}}}{m}\frac{2}{c}\frac{2}{m}$ | $P\frac{6_3}{m}\frac{2}{c}\frac{2}{m}$ | odd layers along |

TABLE XII. The axial space groups—$n$ even, not twice a prime power (dodecagonal type). The lattice cannot distinguish mirror lines along generating vectors from those between them. Thus the space group designated $V(r^{1/2},m^{1/2})$ could equally well be called $V(r^{1/2},m'^{1/2})$, and the generalized International symbol $Pn_{n/2}mc$ specifies the same space group as $Pn_{n/2}cm$. Aside from this kind of identification, the space groups are the same as for the hexagonal type.

| | | |
|---|---|---|
| $V(\bar{r})$ | $P\bar{n}$ | no extinctions |
| $V(\bar{r},\ m)$ | $P\bar{n}2m$ | no extinctions |

TABLE XII. (*Continued*).

| | | |
|---|---|---|
| $V(\bar{r},\ m^{1/2})$ | $P\bar{n}2c$ | mirror lines in odd layers |
| $V(r)$ | $Pn$ | no extinctions |
| $V(r^{j/n})$ $j=1,\ldots,n-1$ | $Pn_j$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r,\ m)$ | $Pnmm$ | no extinctions |
| $V(r^{1/2},\ m^{1/2})$ | $Pn_{\frac{n}{2}}cm$ | one of the two families of mirror lines in odd layers |
| $V(r,\ m^{1/2})$ | $Pncc$ | both families of mirror lines in odd layers |
| $V(r,\ d)$ | $Pn22$ | no extinctions |
| $V(r^{j/n},\ d)$ $j=1,\ldots,n-1$ | $Pn_j22$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r,\ h)$ | $P\dfrac{n}{m}$ | no extinctions |
| $V(r^{1/2},\ h)$ | $P\dfrac{n_{\frac{n}{2}}}{m}$ | $k\mathbf{z}$ with $k$ odd |
| $V(r,\ h,\ m)$ | $P\dfrac{n}{m}\dfrac{2}{m}\dfrac{2}{m}$ | no extinctions |
| $V(r^{1/2},\ h,\ m^{1/2})$ | $P\dfrac{n_{\frac{n}{2}}}{m}\dfrac{2}{c}\dfrac{2}{m}$ | one of the two families of mirror lines in odd layers |
| $V(r,\ h,\ m^{1/2})$ | $P\dfrac{n}{m}\dfrac{2}{c}\dfrac{2}{c}$ | both families of mirror lines in odd layers |

TABLE XIII. The axial space groups—$n$ odd, not a prime power (pentadecagonal type). The $2n$-fold lattice cannot distinguish mirror lines along and between generating vectors. Thus the space group designated $V(r,m^{1/2})$ here could equally well be called $V(r,m'^{1/2})$. Aside from such identification of pairs, the space groups are the same as those for the trigonal type on vertical lattices. (For example, trigonal $Pn$c1 and $Pn$1c reduce to pentadecagonal $Pnc$.)

| | | |
|---|---|---|
| $V(\bar{r})$ | $P\bar{n}$ | no extinctions |
| $V(\bar{r},\ m)$ | $P\bar{n}\dfrac{2}{m}$ | no extinctions |
| $V(\bar{r},\ m^{1/2})$ | $P\bar{n}\dfrac{2}{c}$ | mirror lines in odd layers |
| $V(r)$ | $Pn$ | no extinctions |
| $V(r^{j/n})$ $j=1,\ldots,n-1$ | $Pn_j$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |
| $V(r,\ m)$ | $Pnm$ | no extinctions |
| $V(r,\ m^{1/2})$ | $Pnc$ | mirror lines in odd layers |
| $V(r,\ d)$ | $Pn2$ | no extinctions |
| $V(r^{j/n},\ d)$ $j=1,\ldots,n-1$ | $Pn_j2$ | $k\mathbf{z}$ when $jk$ not a multiple of $n$ |

TABLE XIV. Gauge functions used in Sections III–V. The first four rows summarize the gauge functions used in Sec. III to simplify the phases in the horizontal ($z=0$) plane. These gauge functions are all zero at $\mathbf{z}$ ($V$ lattice) or $\mathbf{z}+\alpha$ ($S$ lattice). They give gauge transformations that reduce all phase functions in the horizontal plane to zero except when $n$ is a power of two, in which case the phases $\Phi_g(\zeta^j)$, $g=m$, $d$, or $h$, can have nonzero gauge-invariant values. The gauge functions given by Eqs. (4.5) and (5.10) are zero in the horizontal plane and therefore do not alter the effects of the gauge functions of the first four rows in that plane. Gauge (5.21) is also useful in simplifying the phases at $m$ and $m'$ implied by a given set of phases at $r$ and $m'$.

| equation in text | purpose | when applied | definition $j=0,\ldots,\nu-1$ |
|---|---|---|---|
| (3.1) | make $\Phi_r \equiv 0$ in horizontal plane | when $r$ is a generator | $\chi(\zeta^j)=\frac{1}{n}\Phi_r\left(\frac{n\zeta^j}{1-\zeta}\right)$ |
| (3.4) | make $\Phi_{\bar{r}} \equiv 0$ in horizontal plane | when $\bar{r}$ is a generator | $\chi(\zeta^j)=\frac{1}{n}\Phi_{\bar{r}}\left(\frac{n\zeta^j}{1+\zeta}\right)$ |
| (3.13) | make $\Phi_x \equiv 0$ in horizontal plane; $x$ is $m$ or $d$ *between* roots | when $n$ is a power of an odd prime $p$ and either $m$ or $d$ is a generator between $2n^{\text{th}}$ roots of unity (perpendicular to an $n^{\text{th}}$ root of unity) | $\chi(\zeta^j)=\frac{1}{p}$ |
| (3.21) | make $\Phi_m \equiv 0$ in horizontal plane $m$ *between* roots of unity | when $n$ is twice a power of an odd prime $p$ and $m$ is a generator between $n^{\text{th}}$ roots of unity | $\chi(\zeta^j)=\frac{(-1)^j}{p}$ |
| (4.5) | make $\Phi_g(\mathbf{z}) \equiv 0$ | when $g$ is a group generator, $g\mathbf{z}=-\mathbf{z}$ — $V$ lattice | $\chi(\mathbf{z})=\frac{1}{2}\Phi_g(\mathbf{z})$ |
| (5.10) | make $\Phi_g(\mathbf{z}+\alpha) \equiv 0$ ($g$ is $h$, $d$, or $\bar{r}$) | $S$ lattice | $\chi(\mathbf{z}+\alpha)=\frac{1}{2}\Phi_g(\mathbf{z}+\alpha)$ |
| (5.5) | add $\frac{1}{p}$ to $\Phi_r(\mathbf{z}+\alpha)$ ($p$ a prime) | staggered lattices for groups with $r$ a generator that do not contain vertical mirrors $m$ | $\chi(\zeta^j)=\frac{1}{p}$ <br> $\chi(\mathbf{z}+\alpha)=0$ |
| (5.21) | add $\frac{1}{2}$ to $\Phi_m(\mathbf{z}+\alpha)$ | group $(\bar{r},m)$ when $m$ lies along a root of unity | $\chi(\zeta^j)=\frac{1}{2}$ <br> $\chi(\mathbf{z}+\alpha)=\frac{1}{4}$ |

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## APPENDIX: SUMMARY OF GAUGE FUNCTIONS

In Table XIV we list all the gauge transformations used to reduce the phase functions to the forms listed in Tables V and VI. We emphasize that although the gauge transformations given by these functions were of importance in arriving at those phase functions, it is not necessary to know them once the results are in hand, since the most general set of phase functions for a particular space group is given by applying an arbitrary gauge transformation to those listed in the tables. We gather them together here, because they are likely to prove useful in subsequent extensions of this analysis, for example, to double groups or magnetic groups.

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