these null results with silicon powder. It is clear from other measurements (*e.g.* electron microscopy) that powder grains are not prefect crystals, even if they happen to be spheres.

References

BORN, M. & WOLF, E. (1980). *Principles of Optics.* New York: Pergamon.

HART, M. (1981). *J. Cryst. Growth*, **55**, 409-427.

HASTINGS, J. B., THOMLINSON, W. & COX, D. E. (1984). *J. Appl. Cryst.* **17**, 85-95.

HUBBARD, C. R. (1983). *Adv. X-ray Anal.* **26**, 35-44.

HUBBARD, C. R., SWANSON, H. E. & MAUER, F. A. (1975). *J. Appl. Cryst.* **8**, 45-48.

JAMES, R. W. (1948). *The Optical Principles of the Diffraction of X-rays.* London: Bell.

JAMES, R. W. (1963). *Solid State Phys.* **15**, 53-220.

LIM, G., PARRISH, W., ORTIZ, C., BELLOTTO, M. & HART, M. (1987). *J. Mater. Res.* **2**, 471-477.

LIPSON, H. & WILSON, A. J. C. (1941). *J. Sci. Instrum.* **18**, 144-148.

PARRISH, W. (1960). *Acta Cryst.* **13**, 838-850.

PARRISH, W. & HART, M. (1985). *Trans. Am. Crystallogr. Assoc.* **21**, 51-55.

PARRISH, W., HART, M. & HUANG, T. C. (1986). *J. Appl. Cryst.* **19**, 92-100.

PARRISH, W., HART, M., HUANG, T. C. & BELLOTTO, M. (1987). *Adv. X-ray Anal.* **30**, 373-382.

THOMSON, J. S. & BURR, A. E. (1968). *Am. J. Phys.* **36**, 803-810.

WILSON, A. J. C. (1940). *Proc. Cambridge Philos. Soc.* **36**, 485-489.

ZACHARIASEN, W. H. (1945). *Theory of X-ray Diffraction in Crystals.* New York: Wiley.

Acta Cryst. (1988). A**44**, 197-211

The Two-Dimensional Quasicrystallographic Space Groups with Rotational Symmetries less than 23-Fold

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Abstract

The crystallographic concepts of lattice and space group are extended to describe materials with crystallographically forbidden point groups, and a complete classification of all two-dimensional space groups with rotational order less than 23 is given.

1. Introduction

The complete classification of the symmetries of periodic crystals, carried out in the nineteenth century by Bravais, Fedorov, Schoenflies and others, is an essential tool for determining and describing the structures of materials with diffraction patterns consisting of Bragg peaks. The classification is organized by the 32 crystallographic point groups (ten in two dimensions), which specify the symmetry of the macroscopic translationally invariant features of crystals - crystal habit, responses to external perturbations *etc.* Within this classification the description of the 14 Bravais lattices and 230 space groups in three dimensions (five and 17 in two dimensions) relies heavily on periodicity, as specified by the real-space lattices which describe the microscopic translational symmetries of crystalline materials.

Quasicrystalline materials have point groups which are incompatible with periodicity; their diffraction patterns consist of sharp well defined Bragg-like peaks, arranged with crystallographically forbidden point-group symmetries. The absence of periodicity precludes their description in terms of the standard classification system. We present here a reformulation of the concepts of space groups and lattices which, while reducing to the conventional scheme in the crystallographic case, is general enough to provide a classification of quasicrystalline materials by their lattices and space groups. This generalization is entirely based in reciprocal (wave-vector) space, where quasicrystals and crystals have the common

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feature of a point diffraction pattern; rather than starting from real-space translational symmetry we work directly with relations between Fourier coefficients, which can be meaningfully formulated in both the crystalline and the quasicrystalline cases.

The basis for this reformulation is that the set of wave vectors of a point diffraction pattern can be extended to a set which is closed under addition and subtraction; this set is simply the *reciprocal lattice* **L**. In the crystallographic case, **L** is dual to a lattice of real-space translations; as defined here, however, the reciprocal lattice has nothing to do with real-space periodicity. Nor is it necessary to view either the reciprocal lattice or the real-space structure itself as a lower-dimensional projection of a structure that is periodic in a higher dimension. The reciprocal lattice emerges as a natural construct for dealing with the fact that, except for systematic extinctions, a diffraction pattern generally contains sums and differences of vectors in the pattern. (Most, of course, will have intensities too low to be observed.)

Since the density has a non-zero Fourier component for each vector in the diffraction pattern, we will therefore be considering densities of the form

$$\rho(\mathbf{r}) = \sum_{\mathbf{k}\in\mathbf{L}} \rho(\mathbf{k}) \exp i\mathbf{k}\cdot\mathbf{r}. \qquad (1.1)$$

For a generic material we expect the Fourier coefficients $\rho(\mathbf{k})$ to be non-zero for general reciprocal-lattice vectors $\mathbf{k}$, though some may be required to vanish by symmetry.

Within the conventional framework of point groups and real-space periodicity, a symmetry element contained in a crystallographic space group is a compound operation consisting of a point-group operation g followed by an associated translation $\mathbf{t}_g$ which leaves the density unchanged:

$$\rho(g\mathbf{r}+\mathbf{t}_g) = \rho(\mathbf{r}). \qquad (1.2)$$

This implies that the Fourier coefficients of ρ are related by

$$\rho(g\mathbf{k}) = \rho(\mathbf{k}) \exp(-ig\mathbf{k}\cdot\mathbf{t}_g). \qquad (1.3)$$

Starting with this relation, the problem of classifying ordinary crystal structures can be equally well posed in reciprocal space (Bienenstock & Ewald, 1962).

In the case of a structure with a general noncrystallographic point group, there are no real-space translational symmetries, and we cannot assume *a priori* a phase relationship of the form (1.3). We begin instead with the entirely general relation

$$\rho(g\mathbf{k}) = \rho(\mathbf{k}) \exp[2\pi i\Phi_g(\mathbf{k})], \qquad (1.4)$$

and determine the *phase function* $\Phi_g(\mathbf{k})$ by imposing the condition that any translationally invariant macroscopic property of the quasicrystal should be invariant under the operations of the point group. When the point group and reciprocal lattice are crystallographic, it is easy to show that the more general phase functions appearing in (1.4) necessarily reduce to the forms appearing in (1.3), so that solving for the allowed classes of phases functions $\Phi_g(\mathbf{k})$ gives back the familiar crystallographic space groups.

In this paper we apply this general formulation to the particular case of two dimensions, considering arbitrary two-dimensional point groups. It is convenient to represent a two-dimensional lattice as a set of complex numbers. For example, the set of all integral linear combination of the Nth roots of unity, the *cyclotomic integers* Z_N, represents a lattice with N-fold symmetry. The sets Z_4 and Z_6 are just the familiar two-dimensional square and triangular nets. These two lattices are the *only* two-dimensional crystallographic lattices (to within a scale factor and rotation) with fourfold and sixfold symmetry. This happy coincidence between the cyclotomic integers of order N and the reciprocal lattices with N-fold symmetry is maintained for all $N<46$; for higher N, however, lattices which are not equivalent to Z_N may occur in addition to the 'standard' lattice Z_N (Mermin, Rokhsar & Wright, 1987). We limit ourselves here to classifying space groups for the standard lattice with arbitrary N, thereby arriving at a complete classification when the rotational order of the point group is less than 23.

There is a body of earlier work on the question of generalizing space groups. Our approach is inspired by the work of Bienenstock & Ewald (1962), who were the first to formulate the problem of determining crystallographic space groups entirely in reciprocal space. Their solution, like ours, is based on constructing linear phase functions that satisfy compatibility conditions imposed by the point-group symmetry. Bienenstock & Ewald use the real-space translational symmetry of crystals only in establishing their initial formulation of the problem. From this perspective the point of our analysis in § 2 is to reach that stage without the assumption of translational symmetry.

More recently the space-group problem has been formulated for quasicrystals using techniques initially developed to treat the classification of incommensurately modulated structures (Janner & Janssen, 1977). Alexander (1986), Janssen (1986*a*, *b*) and Bak (1985*b*, 1986) have given descriptions of such approaches. These authors discuss quasicrystallographic space groups by viewing a general quasiperiodic density in physical space as a slice through a density in a higher-dimensional space; only certain crystallographic space groups in this hyperspace are consistent with the noncrystallographic symmetry in physical space.

We caution the reader that although some aspects of quasicrystals are perhaps more transparent when considered in terms of these higher-dimensional spaces, such a treatment of space groups can be misleading. In particular, it is important to note that quasicrystallographic reciprocal lattices can have

scale invariances, which must be taken into account in the determination of their space groups. As a consequence of scale invariance, space groups which are distinct in higher dimensions can be physically indistinguishable. Our approach also differs from others in dealing systematically with the difficult problem of enumerating the lattices with noncrystallographic point-group symmetry. [This problem is addressed in detail in the first two papers in this series (Rokhsar, Mermin & Wright, 1987; Mermin, Rokhsar & Wright, 1987), the relevant results of which are summarized in § 3.]

The paper is organized as follows: In § 2 we formulate the relationship between the diffraction pattern and the reciprocal lattice, we briefly review the relationship between the point symmetry of a material and the point symmetry of its diffraction pattern, and we specify the restrictions placed upon the phases of $\rho(\mathbf{k})$ by point-group symmetry. We then define generalized space groups, and give the conditions under which point-group symmetry prohibits a vector in the lattice from appearing in the diffraction pattern. A distinction between quasicrystalline and incommensurate crystals is drawn, without which the classification problem is unmanageable. § 3 summarizes the properties of two-dimensional lattices and introduces their representation as sets of complex numbers. We describe some important features of the scale invariance of two-dimensional lattices with noncrystallographic symmetry. § 4 begins with an outline of the major steps in the computation of the two-dimensional space groups for the standard lattice, then explicitly gives the details of this calculation. The results are summarized in the initial outline and in Table 3. In § 5 we describe, as an example, the simplest 'non-symmorphic' non-crystallographic two-dimensional space group.

The reader who wants to use these space groups (without deriving them) is encouraged to skip all of § 4 except for the opening summary.

2. Diffraction patterns and space-group symmetry

A. Diffraction patterns and reciprocal lattices

A diffraction pattern gives information about the magnitudes of Fourier coefficients of the density ρ of a material. We restrict ourselves to diffraction patterns with well defined Bragg-like peaks, and assume the specimen is macroscopically homogeneous - *i.e.* the diffraction pattern is independent of the region of the specimen illuminated by the incident beam. Such complications as multiple scattering, anomalous dispersion, peak widths *etc.* will be ignored. In view of these simplifications we can identify the symmetries of the diffraction pattern with the symmetries of the magnitudes of the Fourier coefficients of the density.

Thus the diffraction pattern provides us with a set $\mathbf{D}$ of wave vectors at which the density has non-vanishing Fourier coefficients, together with a set of intensities which are measures of the magnitudes of those Fourier coefficients. It will be convenient to refer to the set of wave vectors $\mathbf{D}$ as 'the diffraction pattern', even though a full specification of the diffraction pattern includes both the wave vectors and the associated intensities.

One expects in general that if $\mathbf{k}_1$ and $\mathbf{k}_2$ are wave vectors appearing in the density, then ρ will also have Fourier components at $\mathbf{k}_1 \pm \mathbf{k}_2$, unless such wave vectors are forbidden by extinction rules determined by symmetry. The presence of such sums reflects the underlying nonlinearity of the mechanisms that determine the equilibrium density of a material. We define the *reciprocal lattice* $\mathbf{L}$ [or, more fully, $\mathbf{L}(\mathbf{D})$] determined by the set of wave vectors $\mathbf{D}$ in the diffraction pattern to be the set of all integral linear combinations of wave vectors in the diffraction pattern. It is thus the smallest set of vectors which (1) is closed under addition and subtraction and (2) contains all wave vectors in the diffraction pattern. As so defined, the term retains its usual meaning in the crystallographic case. Whenever we use the term 'lattice' we shall always mean 'reciprocal lattice'; 'lattice' alone is unambiguous, since quasicrystals have no real-space lattices.

Given a diffraction pattern, we infer that the density has a Fourier expansion

$$\rho(\mathbf{r}) = \sum_{\mathbf{k}\in L} \rho(\mathbf{k}) \exp i\mathbf{k}\cdot\mathbf{r}. \qquad (2.1)$$

For a generic material we expect the Fourier coefficients in (2.1) to be non-zero, unless they are required to vanish by symmetry, as discussed in § 2.*E*.

B. Point groups, Laue groups and holohedries

The macroscopic symmetry of a material - crystal or quasicrystal - is characterized by its *point group* G, the symmetry group of all macroscopic translationally invariant properties such as elasticity, conductivity *etc.* The point group G of the material is not in general directly determined by the diffraction pattern; there are, however, two larger groups which do characterize a diffraction pattern:

(1) The point group G_D of the diffraction pattern. Known as the *Laue group*, G_D is the symmetry group of the magnitudes of the density Fourier coefficients: g is a symmetry operation in the Laue group G_D if $|\rho(g\mathbf{k})| = |\rho(\mathbf{k})|$. Since the reality of $\rho(\mathbf{r})$ gives $\rho(-\mathbf{k}) = \rho(\mathbf{k})^*$, the vectors $\mathbf{k}$ and $-\mathbf{k}$ are related by a Laue-group operation even though the point group G need not contain the inversion. With each point group G is associated a unique smallest Laue group G_D obtained by adjoining the inversion. Barring accidental symmetry (as we shall), the observation of a Laue group G_D implies that G is one of the point groups giving G_D when the inversion is adjoined.

Table 1. *Two-dimensional Laue groups G_D and associated point groups G*

The relation between G_D and G depends on whether the rotational order n of the point group is even or odd. The two (isomorphic) point groups $nm1$ and $n1m$ reflect the fact that there are two distinct such subgroups of $[2n]mm$, depending which half of the $2n$ mirrorings the subgroup contains. (Here and in what follows, we use International notation to name point groups.)

	Laue group	Point group
n even	n	n
	nmm	nmm
n odd	$2n$	n
	$[2n]mm$	$nm1, n1m$

(2) The point group G_L of the associated lattice. In classical crystallography the point group of the real-space lattice is called the *holohedral group* of the lattice. This is, of course, identical to the point group of the corresponding (crystallographic) reciprocal lattice, so it is natural in the non-crystallographic case to refer to the point group G_L of the lattice of wave vectors $\mathbf{L}(\mathbf{D})$ as the holohedral group. Since lattices are by definition closed under subtraction, if $\mathbf{k}$ is in the lattice so is $-\mathbf{k}$, so holohedral groups necessarily contain the inversion. A *holohedry* is the set of lattices with a particular point group.

Since any symmetry of the diffraction pattern is a symmetry of the (reciprocal) lattice it gives rise to, the Laue group G_D of the diffraction pattern will be a subgroup of the holohedral group G_L. Indeed, barring accidental vanishings of Fourier coefficients, G_L will be just the symmetry group of the wave vectors in $\mathbf{D}$ without regard for their intensities. Note that because they contain the inversion, in two dimensions both G_L and G_D must contain a rotation by π, and therefore their rotational order N is necessarily even. If the rotational order n of the point group G is odd, the rotational order N of the associated Laue group G_D (and holohedral group G_L) is $2n$.

In two dimensions the catalogue of point groups and their associated Laue groups is quite simple; a complete list is given in Table 1. Note that when n is odd there is a pair of isomorphic point groups, $nm1$ and $n1m$, both consisting of n-fold rotations and n mirrorings perpendicular to the rotation axis. These must be viewed as separate cases because they correspond to the two distinct ways in which the point group nm can be a subgroup of the lattice group $[2n]mm$. In the familiar crystallographic cases, $3m1$ and $31m$ correspond to the two possible orientations of the point group $3m$ relative to a sixfold symmetric reciprocal lattice — the mirror lines can either be along the shortest vectors or between them (Fig. 1). Crystallographically these cases can be distinguished, but we will see below that quasicrystallographically the two cases remain distinguishable only when n is a power of an odd prime, owing to the scale invariances of the corresponding reciprocal lattice.

C. Point groups and phase relations

Since the Laue group G_D of the diffraction pattern is the symmetry group of the *magnitudes* of the Fourier coefficients $\rho(\mathbf{k})$, knowledge of the Laue group gives no phase information. Knowledge of the point group G of the material, however, provides restrictions on the *phases* of the $\rho(\mathbf{k})$. The determination of these symmetry-imposed phase relations (which in the crystallographic case is tantamount to determination of the space group) is the primary aim of this paper.

Consider, as an example of a macroscopic translationally invariant quantity,

$$\rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\ldots\rho(\mathbf{k}_m)\delta(\mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_m). \quad (2.2)$$

Since by definition of the point group such products must be equal when related by point-group symmetries, we must have

$$\rho(\mathbf{k}_1)\rho(\mathbf{k}_2)\ldots\rho(\mathbf{k}_m)=\rho(g\mathbf{k}_1)\rho(g\mathbf{k}_2)\ldots\rho(g\mathbf{k}_m)$$
$$\text{whenever}\quad \mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_m=0, \quad (2.3)$$

for each element g of the point group G, and all wave vectors $\mathbf{k}_1,\ldots,\mathbf{k}_m$ in the diffraction pattern $\mathbf{D}$.

The equations (2.3) place constraints on the relative phases of the Fourier amplitudes of symmetry-related wave vectors. We can specify these phase relationships by defining for each g in the point group G and all $\mathbf{k}$ in the diffraction pattern $\mathbf{D}$ the *phase function* $\Phi_g(\mathbf{k})$:

$$\rho(g\mathbf{k})=\exp[2\pi i\Phi_g(\mathbf{k})]\rho(\mathbf{k}). \quad (2.4)$$

The phase function Φ_g gives the *relative* phases of $\rho(g\mathbf{k})$ and $\rho(\mathbf{k})$. It is real and defined only to within an integer.

In terms of the phase functions, the constraint equation (2.3) becomes

$$\Phi_g(\mathbf{k}_1)+\Phi_g(\mathbf{k}_2)+\ldots+\Phi_g(\mathbf{k}_m)\equiv 0$$
$$\text{whenever}\quad \mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_m=0,\quad \mathbf{k}_i\in\mathbf{D}, \quad (2.5)$$

where $\equiv$ denotes equality to within an integer, *i.e.* modulo one.

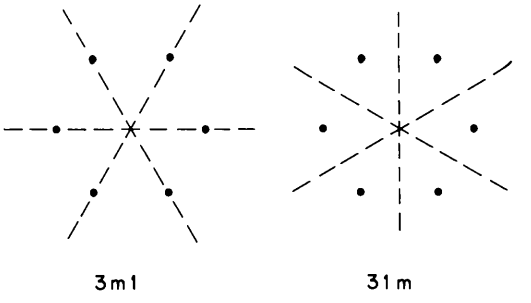

Fig. 1. The two possible orientations of the point group $3m$ relative to the shortest vectors of a sixfold symmetric reciprocal lattice. The solid circles indicate the shortest vectors; dashed lines denote mirror lines.

A further constraint on the phase functions follows from noting that for g and h in G, the phase functions for group elements g, h, and gh are interrelated by the group condition

$$\rho[(gh)\mathbf{k}] = \rho[g(h\mathbf{k})]. \tag{2.6}$$

Application of (2.4) to both sides of (2.6) gives

$$\begin{aligned}\exp[2\pi i\Phi_{gh}(\mathbf{k})]\rho(\mathbf{k}) &= \exp[2\pi i\Phi_g(h\mathbf{k})]\rho(h\mathbf{k}) \\ &= \exp\{2\pi i[\Phi_g(h\mathbf{k})+\Phi_h(\mathbf{k})]\}\rho(\mathbf{k}),\end{aligned} \tag{2.7}$$

which gives the group compatibility conditions

$$\Phi_{gh}(\mathbf{k}) \equiv \Phi_g(h\mathbf{k}) + \Phi_h(\mathbf{k}). \tag{2.8}$$

The equations (2.5) and (2.8) contain all information about the phase relations of the Fourier transform required by the point-group symmetry of the material. Although these conditions have been derived only for wave vectors appearing in the diffraction pattern, we shall see (§ 2.*E*) that they can be easily extended to the entire lattice. We shall describe procedures for finding the physically distinct solutions to (2.5) and (2.8) for a given lattice **L** and point group G.

D. Equivalent solutions: gauge functions

Two sets of phase functions are *equivalent* if they describe two densities that give identical values to all translationally invariant macroscopic quantities (2.2). It is our aim to determine the classes of *inequivalent* phase functions $\Phi_g(\mathbf{k})$ satisfying the linearity condition (2.5) and the group condition (2.8). In the crystallographic case these classes of solutions for a given point group G and lattice **L** are precisely the crystallographic space groups associated with **L** and G. We therefore regard the classes of solutions in the quasicrystallographic case as specifying the *quasicrystallographic space groups.* In agreement with conventional crystallographic nomenclature, we define a *symmorphic* space group to be a solution equivalent to the trivial phase functions $\Phi_g(\mathbf{k}) \equiv 0$ for all g in G and all **k** in **L**.

Two densities related by

$$\rho'(\mathbf{k}) = \exp[2\pi i\chi(\mathbf{k})]\rho(\mathbf{k}) \tag{2.9}$$

will give the same value for all quantities of the form (2.2) if and only if the difference in phase satisfies the condition

$$\begin{aligned}&\chi(\mathbf{k}_1)+\chi(\mathbf{k}_2)+\ldots+\chi(\mathbf{k}_m)\equiv 0 \\ &\text{whenever}\quad \mathbf{k}_1+\ldots+\mathbf{k}_m=0,\quad \mathbf{k}_i\in\mathbf{D}.\end{aligned} \tag{2.10}$$

We call such a function $\chi(\mathbf{k})$ a *gauge function* (in analogy with gauge transformations in electrodynamics) because no macroscopic physical properties depend on χ. The simplest (and in the crystallographic case the only) example of a gauge function is $2\pi\chi(\mathbf{k}) = \mathbf{k}\cdot\mathbf{r}$. In this case the two densities ρ and ρ' are related simply by a translation through **r**. In the quasicrystalline case gauge functions can contain 'phason' as well as translational shifts (Bak, 1985*a*; Levine, Lubensky, Ostlund, Ramaswamy, Steinhardt & Toner, 1985), but this distinction is of no relevance to the analysis that follows, which relies only on the condition (2.10).

If $\Phi_g(\mathbf{k})$ and $\Phi'_g(\mathbf{k})$ are equivalent phase functions, then we have

$$\begin{aligned}\rho(g\mathbf{k}) &= \exp[2\pi i\Phi_g(\mathbf{k})]\rho(\mathbf{k}), \\ \rho'(g\mathbf{k}) &= \exp[2\pi i\Phi'_g(\mathbf{k})]\rho'(\mathbf{k}).\end{aligned} \tag{2.11}$$

The second equation can be rewritten as

$$\begin{aligned}&\exp[2\pi i\chi(g\mathbf{k})]\rho(g\mathbf{k}) \\ &\quad = \exp[2\pi i\Phi'_g(\mathbf{k})]\exp[2\pi i\chi(\mathbf{k})]\rho(\mathbf{k}).\end{aligned} \tag{2.12}$$

Hence two sets of phase functions Φ_g and Φ'_g are equivalent if and only if there is a gauge function χ, independent of the group element g, such that

$$\Phi'_g(\mathbf{k}) - \Phi_g(\mathbf{k}) \equiv \chi(g\mathbf{k}) - \chi(\mathbf{k}) \tag{2.13}$$

for all wave vectors **k** in the diffraction pattern **D** and all elements g in the point group G.

We shall establish the equivalence of various phase functions by explicitly constructing the gauge functions which relate them. A gauge-invariant analysis will be presented elsewhere in the context of a discussion of three-dimensional space groups (Wright, Rokhsar & Mermin, in preparation). We shall, however, use below the fact that if a wave vector **k** is invariant under an operation g of the point group, $g\mathbf{k} = \mathbf{k}$, then $\Phi_g(\mathbf{k})$ is gauge invariant. This follows immediately from (2.13).

E. Extension of the phase conditions to the reciprocal lattice: extinction rules

Even though the phase functions are only defined on the diffraction pattern **D**, the reciprocal lattice **L** — the set of all sums of vectors in **D** — plays an important role in the determination of those phase functions. This is because any function $\Psi(\mathbf{k})$ defined for vectors in the diffraction pattern and satisfying a linearity condition like the conditions (2.5) or (2.10) obeyed by the phase functions or gauge functions can be uniquely extended from a linear function on the diffraction pattern **D** to a linear function on the entire reciprocal lattice **L**. (Since the phase functions are only defined to within an integer, by 'linear' we shall always mean 'linear modulo one'.)

To make this extension note first that if **k** is in **D** then so is $-\mathbf{k}$. Since **k** and $-\mathbf{k}$ sum to zero, the linearity condition gives

$$\Psi(-\mathbf{k}) \equiv -\Psi(\mathbf{k}). \tag{2.14}$$

Note next that any **k** in the lattice **L**(**D**) is of the form

$$\mathbf{k} = \mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_m, \tag{2.15}$$

where $\mathbf{k}_1, \ldots, \mathbf{k}_m$ are all in the diffraction pattern **D**. Given such an expression for **k** we *define* $\Psi(\mathbf{k})$ for vectors **k** that are in the lattice but *not* in the diffraction pattern by

$$\Psi(\mathbf{k}) \equiv \Psi(\mathbf{k}_1) + \Psi(\mathbf{k}_2) + \ldots + \Psi(\mathbf{k}_m). \qquad (2.16)$$

Evidently this definition will give a unique linear extension of Ψ from the diffraction pattern to the entire lattice, provided the value of $\Psi(\mathbf{k})$ does not depend on the particular way (2.15) in which **k** is represented as a sum of vectors in the diffraction pattern. But if $\mathbf{k}'_1 + \ldots + \mathbf{k}'_{m'}$ also gives **k**, then

$$\mathbf{k}_1 + \mathbf{k}_2 + \ldots + \mathbf{k}_m - \mathbf{k}'_1 - \mathbf{k}'_2 - \ldots - \mathbf{k}'_{m'} = 0. \qquad (2.17)$$

Independence of representation follows from the fact that every vector in (2.17) is in **D**, the fact that Ψ acting on vectors in **D** satisfies a linearity condition of the form (2.10), and the relation (2.14).

Thus the phase functions $\Phi_g(\mathbf{k})$ and gauge functions $\chi(\mathbf{k})$ have unique linear extensions to the entire lattice **L**. Since the pertinent conditions (2.5), (2.8), (2.10) and (2.13) are all linear relations among linear functions of **k**, we can apply those conditions to the entire lattice of wave vectors, even though as originally defined the functions $\Phi_g(\mathbf{k})$ and $\chi(\mathbf{k})$ only have meaning for wave vectors in the diffraction pattern **D**. From now on we therefore assume that the phase functions and gauge functions are defined on the entire lattice **L**.

Note that because of the linearity of χ on the lattice we can write the condition (2.13) for the equivalence of two sets of phase functions as

$$\Phi'_g(\mathbf{k}) - \Phi_g(\mathbf{k}) \equiv \chi[(g-1)\mathbf{k}], \qquad (2.18)$$

for all **k** in the reciprocal lattice **L**(**D**) and all g in the point group G.

We can now specify the source of systematic extinctions. If a vector **k** in the diffraction pattern **D** is invariant under a point-group operation g, then

$$\rho(g\mathbf{k}) = \rho(\mathbf{k}). \qquad (2.19)$$

The definition (2.4) of the phase function then implies that

$$\Phi_g(\mathbf{k}) \equiv 0, \qquad (2.20)$$

since vectors in the diffraction pattern have non-zero $\rho(\mathbf{k})$. Thus if a family of phase functions on the lattice contains some with $\Phi_g(\mathbf{k}) \not\equiv 0$ for a point-group element g and a wave vector **k** satisfying $g\mathbf{k} = \mathbf{k}$, then such wave vectors, though present in the lattice **L**, are forbidden by symmetry from appearing in the diffraction pattern **D**. This is the source of systematic extinctions. It is evident from (2.18) that this condition for systematic extinctions is gauge invariant.

F. Quasiperiodic vs incommensurate crystals: the condition of minimum rank

Thus far we have not placed any limitations on the complexity of the diffraction patterns and associated lattices that we are willing to consider, beyond the assumption that the diffraction pattern consists of well defined Bragg-like peaks. We now impose a further restriction on the diffraction patterns which limits the class of lattices we will consider below.

By the *rank* ν of a lattice **L**, we mean the smallest number of vectors $\mathbf{b}_1, \ldots, \mathbf{b}_\nu$ that can *generate* **L** over the integers, in the sense that every vector in **L** is a linear combination of the $\mathbf{b}_j$ with integral coefficients. We shall call such a set of vectors $\mathbf{b}_1, \ldots, \mathbf{b}_\nu$ an *integrally independent basis* for **L**.

For any point group G we define the *indexing dimension* of G to be the smallest rank that a lattice invariant under G can have. The crystallographic point groups are those with indexing dimension equal to the dimension of physical space; non-crystallographic point groups have indexing dimensions larger than the spatial dimension. We shall say that a lattice is crystallographic or quasicrystallographic if its rank is equal to the indexing dimension of its point group.

We develop a classification scheme only for crystallographic and quasicrystallographic lattices. A lattice with non-minimal rank can be viewed as the direct sum (*i.e.* the set of all sums of pairs of vectors, one from each lattice) of two or more lattices of minimal rank. In the crystallographic case such a direct sum is not viewed as a crystallographic lattice, but as a set of points appropriate for characterizing an incommensurately modulated structure. We impose the same organizing principle in the quasicrystallographic case, reserving the term 'quasicrystal' for structures whose lattices have minimal rank, and regarding more complicated structures as incommensurately modulated quasicrystals, which are most simply regarded as direct sums of ordinary ones.

Hereafter when we use the term 'lattice' we shall always mean crystallographic or quasicrystallographic lattices.

3. Two-dimensional lattices and cyclotomic integers

We now introduce some techniques that are special to the case of two dimensions. We shall be interested in quasicrystallographic patterns which have greater than sixfold symmetry, but our analysis will also include the crystallographic cases of four- and sixfold symmetry. (The crystallographic case of twofold symmetry is exceptional. Only in this case are there symmetry-preserving distortions of a two-dimensional lattice more general than isotropic changes of scale. Although this makes it in some respects the most complicated case it is, of course, entirely understood, and will not be considered here.)

A. The standard lattices

Consider a two-dimensional lattice with N-fold rotational symmetry (an *N-lattice*). If it contains a vector $\mathbf{b}_0$ and r is a rotation through $2\pi/N$, then rotational symmetry requires it to contain all the N vectors

$$\mathbf{b}_j = r^j \mathbf{b}_0 \tag{3.1}$$

given by rotating $\mathbf{b}_0$ through $2\pi j/N$, $j = 0, \ldots, N-1$. By the *standard lattice* we mean the set of all integral linear combinations of these N vectors. By construction it has N-fold rotational symmetry. We refer to the vectors $\mathbf{b}_j, j = 0, \ldots, N-1$ as *symmetric generating vectors* or as constituting a *symmetric basis* for the standard lattice. A symmetric basis is never integrally independent (since, among other relations, we have $\mathbf{b}_0 + \mathbf{b}_1 + \ldots + \mathbf{b}_{N-1} = 0$). Evidently any lattice with N-fold symmetry contains standard sublattices generated by any vector in the lattice and its rotations. Thus the rank of any N-lattice is at least the rank of the standard N-lattice, and therefore the indexing dimension for two-dimensional point groups with N-fold rotational symmetry is just the rank of the standard N-lattice. It is also easily shown that any lattice with N-fold symmetry, when properly scaled, is itself a sublattice of the standard lattice (Rokhsar, Mermin & Wright, 1987).

We say that two N-lattices are *equivalent* if they differ only by a scale factor and/or a rotation. It is a deep* theorem of algebraic number theory that for all even integers $2 < N < 46$, any N-lattice is equivalent to the standard N-lattice (Mermin, Rokhsar & Wright, 1987). For given $N \geq 46$ the number of inequivalent N-lattices is finite, but grows roughly exponentially with increasing N. (The excluded case $N = 2$ is pathological in that the definition of the standard lattice only yields a one-dimensional set of points.)

In this paper we shall only give a complete analysis of the simplest possible case: those space groups associated with diffraction patterns that give rise to standard lattices. We are nevertheless thereby giving the complete analysis of two-dimensional quasicrystallographic space groups for all lattices with $N < 46$ (and for $N = 48$, 50, 54, 60, 66, 70, 84 and 90 — the only other cases in which all lattices are equivalent to the standard one) (Mermin, Rokhsar & Wright, 1987).

Since N is even and since standard lattices have mirrorings, the standard lattice belongs to the holohedry *Nmm*. It is a surprising fact that for certain $N > 2$ there exist lattices without mirror symmetry. For example, when $N = 46$ there is an enantiomorphic pair of distinct non-standard lattices belonging to the holohedry N (Mermin, Rokhsar & Wright, 1987). In the rest of the paper we restrict our attention to standard lattices, though we shall call attention to those results that are more generally valid, as they emerge.

B. Standard lattices and cyclotomic integers

It is useful in understanding the properties of two-dimensional lattices and diffraction patterns (and essential if one wishes to extract pertinent information from the mathematics literature) to regard the two-dimensional wave vectors constituting such a lattice or diffraction pattern as points in the complex plane. A set of symmetric generating vectors [equation (3.1)] can be taken to be given by the Nth roots of unity,

$$\mathbf{b}_j \to \exp(2\pi ij/N) = \zeta_N^j, \quad \zeta_N = \exp 2\pi i/N, \quad j = 0, \ldots, N-1. \tag{3.2}$$

The standard N-lattice is simply the set Z_N of *all* integral linear combinations of the Nth roots of unity. This set is known as the *cyclotomic integers* of degree N.

From this point onward we shall find it convenient to abandon the geometric notation that uses vectors, and change to an algebraic notation that uses the complex numbers that represent those vectors in two dimensions. The algebraic notation is virtually indispensable in deriving the categories of lattices and space groups, and is more efficient for deriving intermediate results.

Two minor but important points arise.

(1) When N is odd, the cyclotomic integers of degree N are identical to the cyclotomic integers of degree $2N$. [This is because the set of all $2N$th roots of unity (for odd N) is just the set containing the Nth roots and their negatives. But $-\zeta_N^j$, as a trivial integral linear combination of the ζ_N^j, is already in Z_N.] In the mathematics literature the cyclotomic integers of odd degree N are always described as Z_N and the alternative name Z_{2N} is rarely used. We, however, wish to label the standard lattices by their rotational symmetry, which is always of even order. We therefore depart from the mathematical usage, using Z_{2N} for the cyclotomic integers of odd degree N. Since Z_{2N} is identical to Z_N this deviation from mathematical orthodoxy cannot lead to any ambiguity.

(2) The mapping of the standard N-lattice onto the cyclotomic integers of degree N reveals that the indexing dimension of quasicrystallographic diffraction patterns with N-fold symmetry (*i.e.* the rank of the standard N-lattice) is just the number of Nth roots of unity that are linearly independent over the integers. The particular value of this number does not

* We shall need on occasion to appeal to non-trivial results from the mathematics literature. In making such references we distinguish between results the proofs of which are relatively straightforward, but too lengthy to reproduce here, and results that are truly profound, requiring entire monographs for their derivation. The latter results we shall characterize as 'deep'.

Table 2. *Point groups with n-fold symmetry compatible with lattices of N-fold symmetry*

When the rotational symmetry n of the point group G is even, then the rotational symmetry N of the lattice is equal to n. The two point groups with even n and their generators are listed. When n is odd then $N = 2n$. There are again two point groups, but one of them, nm, can act on the complex numbers in two different ways, as indicated by the list of generators. As discussed in the text, the two ways in which nm acts on the *lattice* are only distinguishable when n is a power of an odd prime number.

n	Point group	Generators	Lattice
n even	nmm	$r: \alpha \to \zeta_n \alpha$; $m: \alpha \to \alpha^*$	Z_n
	n	$r: \alpha \to \zeta_n \alpha$	Z_n
n odd	$nm1$	$r: \alpha \to \zeta_n \alpha$; $m: \alpha \to \alpha^*$	Z_{2n}
	$n1m$	$r: \alpha \to \zeta_n \alpha$; $m: \alpha \to -\alpha^*$	Z_{2n}
	n	$r: \alpha \to \zeta_n \alpha$	Z_{2n}

play a major role in the analysis that follows. It is known as the Euler number of N, commonly denoted $\varphi(N)$. An easy way to compute $\varphi(N)$ is to list all the primes $p_1, p_2, \ldots$ that divide N; $\varphi(N)$ is then simply given by

$$\left[\left(\frac{p_1-1}{p_1}\right)\left(\frac{p_2-1}{p_2}\right)\cdots\right]N.$$

Thus 12 has prime factors 2 and 3, so $\varphi(12) = \frac{1}{2}\times\frac{2}{3}\times 12 = 4$ (primes that appear several times are counted only once).†

C. *The action of point groups on standard lattices*

The action of a two-dimensional point group on a set of cyclotomic integers can be conveniently represented in terms of familiar operations on the complex plane. Thus a rotation by $2\pi/n$ corresponds to multiplication by ζ_n, mirroring in the real axis corresponds to complex conjugation, and mirroring in the imaginary axis corresponds to complex conjugation followed by inversion (multiplication by -1). Table 2 lists the two-dimensional point groups G and their actions on cyclotomic integers.

The table displays the two ways in which mirror operations can be oriented with respect to the reciprocal lattice when n is odd (Fig. 1):

(1) In the case of $nm1$ there are n mirror lines (one of which is the real axis) each of which contains a pair of $(2n)$th roots of unity. In this case we define the operation m to be the mirror operation of complex conjugation (or mirroring in the real axis):

$$m\alpha = \alpha^* \quad (n \text{ odd}, G = nm1). \tag{3.3}$$

† The Euler number is also the number of integers less than N (including unity) that have no prime factors in common with N (Hardy & Wright, 1954).

(2) In the case of $n1m$ there are n mirror lines (one of which is the imaginary axis) which bisect the angles between neighboring $(2n)$th roots of unity [and therefore none of which contain $(2n)$th roots of unity]. In this case we define m to be a mirroring in the imaginary axis:

$$m\alpha = -\alpha^* \quad (n \text{ odd}, G = n1m). \tag{3.4}$$

When n is even the presence of either mirror (3.3) or (3.4) implies the presence of the other, so there is only a single improper point group, nmm.

In the crystallographic case of odd n (which occurs only for $N = 6$, $n = 3$) the two distinct subgroups of the symmetry group G_L of Z_6 give rise to two distinct space groups ($p3m1$ and $p31m$). One can distinguish the two possibilities in this case by checking whether the reciprocal-lattice vectors of minimum length do or do not lie on mirror lines. (Note that in the crystallographic case $3m1$ is the point group for which *real-space* symmetric basis vectors are *not* invariant under the mirroring, and therefore for which the reciprocal-lattice symmetric basis vectors *are* invariant.)

In generalizing the relationship beteen $nm1$ and $n1m$ to the quasicrystallographic case one must be careful, since there is no unique symmetric basis. We show in the next subsection (§ 3.*D*) that unless the odd integer n is a power of a prime number, these two ways of orienting the point group nm relative to the lattice Z_{2n} are in fact indistinguishable.

D. *Scale invariance of standard lattices and cyclotomic units*

A symmetric basis for the standard N-lattice Z_N is simply given by the Nth roots of unity, ζ_N^j, $j = 1, \ldots, N$. For the crystallographic cases $N = 4$ or 6, this symmetric basis is unique. For the non-crystallographic cases $N = 8, 10, \ldots$, the *scale* of the symmetric generating vectors may be altered without changing the lattice, reflecting an invariance of the entire quasicrystallographic lattice under such a change. This freedom to choose the scale of the symmetric generating vectors plays an important role in the classification of the quasicrystallographic space groups. The extent of the scale invariance is very simply characterized when the lattice is expressed in terms of the cyclotomic integers.

Any symmetric basis other than the Nth roots of unity can be viewed as consisting of a cyclotomic integer μ and its rotations $\zeta_N^j \mu$, or, equivalently, as the Nth roots of unity rescaled by $|\mu|$ and rotated by the phase of μ. If this second set is indeed a basis, then its integral linear combinations must give *all* the cyclotomic integers. In particular, there must be integers m_j such that the cyclotomic integer 1 is given by

$$1 = \sum_{j=0}^{N-1} m_j(\zeta_N^j \mu) = \mu \sum_{j=0}^{N-1} m_j \zeta_N^j. \tag{3.5}$$

Thus the cyclotomic integer μ has a multiplicative inverse among the cyclotomic integers: $\mu\lambda = 1$, with

$$\lambda = \sum_{j=0}^{N-1} m_j \zeta_N^j. \tag{3.6}$$

A cyclotomic integer whose inverse is also a cyclotomic integer is called a *unit.*

We have thus established that any symmetric basis for the cyclotomic integers is nothing but the Nth roots of unity, rescaled by a unit. The converse is also true: rescaling the Nth roots of unity by a unit λ yields a symmetric basis. Let μ be the cyclotomic integer with $\mu\lambda = 1$. If α is any cyclotomic integer, then $\mu\alpha$ is a cyclotomic integer and therefore has an expansion as an integral linear combination of the Nth roots of unity,

$$\mu\alpha = \sum_{j=0}^{N-1} m_j \zeta_N^j. \tag{3.7}$$

Multiplying this by λ we have

$$\alpha = \lambda \sum_{j=0}^{N-1} m_j \zeta_N^j = \sum_{j=0}^{N-1} m_j (\zeta_N^j \lambda), \tag{3.8}$$

which explicitly gives α as an integral linear combination of λ and its rotations.

When $N = 4$ or 6 it is easy to show that the only cyclotomic units are the Nth roots of unity, but for all greater values of N there are cyclotomic units with magnitudes different from unity. Since positive and negative powers of units are also units,* there will then be units of arbitrarily large and small magnitudes. The question of the magnitudes of the units in the cyclotomic integers of general degree N is a very difficult one, but the possible phases of units are completely understood (Washington, 1982).†

(*A*) If $\frac{1}{2}N$ is a prime power [*i.e.* $\frac{1}{2}N = p^s$ for some prime number p (including 2)] then all the units of Z_N lie on rays in the complex plane passing through the Nth roots of unity. Therefore all symmetric bases of Z_N are related by a (real) scale factor. Thus, when n is a power of an odd prime, the two subgroups $nm1$ and $n1m$ of G_L lead to distinguishable actions on the lattice Z_{2n}. (The issue does not arise when n is a power of 2.)

(*B*) If $\frac{1}{2}N$ is not a prime power, then the units lie either on the rays passing through the Nth roots of unity, or on a second set of rays that bisect the angles between adjacent rays in the first set. (The second set of units has a different scale from the first; in particular, unlike the first, which contains the Nth roots of unity, the second contains no points on the unit circle.) Thus when $\frac{1}{2}N$ is not a prime power there is a second family of symmetric bases along directions rotated from those in the first set by $\frac{1}{2}(2\pi/N) = \pi/N$. In this case it is impossible to distinguish the two types of mirror lines: whether the symmetric basis vectors lie on or between the mirror lines depends on how one chooses to pick those vectors: rotating the lattice Z_N by $2\pi/2N$ simply gives a scaled version of the (unrotated) lattice Z_N.

As a consequence of this it is only pertinent to distinguish between $nm1$ and $n1m$ when n is a power of an odd prime number; for other odd n there is only the single case nm.

4. Quasicrystallographic space groups in two dimensions for the standard lattices

In this section we construct all the two-dimensional quasicrystallographic space groups for standard lattices. The procedure is as follows.

The elements of various two-dimensional point groups are either all powers of the rotation r (a *proper* point group) or products of powers of r and powers of the mirror m (an *improper* point group). Thus a specification of Φ_r for proper point groups, or Φ_r and Φ_m for improper point groups, completely determines the corresponding space groups since the phase functions for all other point-group elements can be constructed in terms of these two by use of (2.8).

In § 4.*A* we prove that for any two-dimensional point group, a gauge can always be found in which the rotation phase function Φ_r is equal to zero. This completely solves the phase-function problem for all proper two-dimensional point groups. For such point groups all phase functions can be chosen to vanish; the only possible space group is the symmorphic one, *pn.* The solution does not require the lattice to be the standard lattice Z_N, so for any proper point group and any compatible lattice the only space group is the symmorphic one.

The non-trivial part of the two dimensional problem arises when the point group is improper. This is dealt with in §§ 4.*B*–*E*.

Section 4.*B* derives some preliminary results. We show that in the gauge in which the rotation phase function Φ_r vanishes, the group conditions on the mirror phase function Φ_m reduce to two simple conditions [equations (4.12) below]. We also state and prove two elementary lemmas that are useful in the sections that follow, which divide into cases depending on whether n is or is not a prime power.

In § 4.*C* we prove that when the rotational order n of G is not a prime power, then in any gauge giving $\Phi_r \equiv 0$, we must also have $\Phi_m \equiv 0$. This result is easily established in a manner that is independent of whether or not the lattice is standard. Because there is only one way of orienting the point group relative to the standard lattice when n is not a prime power

* This follows directly from the definition of units: if $\alpha\beta = 1$ then $1 = (\alpha\beta)^j = \alpha^j\beta^j$.

† We refer the reader to Washington's book for the (non-deep but non-trivial) proofs of the assertions that follow. See Corollary 4.13, page 34 (the meaning of which non-experts can deduce from the last line of the statement of Theorem 4.12, page 34).

Table 3. *Two-dimensional space groups for the standard lattices*

The space groups for the standard lattices are classified by the rotational symmetry n of their point groups, which is subdivided into two cases (n even and n odd). Rows with additional entries in the first column are restricted to the cases specified by those entries (p is any odd prime). The last two columns give the values of the phase functions Φ_r and (when mirrorings are present) Φ_m on the symmetric basis vectors using the gauge functions developed in the text. (Note, however, that the one non-zero entry is gauge invariant.) When n is less than 23 these are the only two-dimensional quasicrystallographic space groups, since when N is less than 46 there are no non-standard lattices.

	Point group	Lattice	Space group	$\Phi_r(\zeta_n^j)$	$\Phi_m(\zeta_n^j)$
n even	n	Z_n	pn	0	—
	nmm	Z_n	$pnmm$	0	0
$n=2^s$	nmm	Z_n	$pngm$	0	$\frac{1}{2}$
n odd	n	Z_{2n}	pn	0	—
$n\neq p^s$	nm	Z_{2n}	pnm	0	0
$n=p^s$	$nm1$	Z_{2n}	$pnm1$	0	0
$n=p^s$	$n1m$	Z_{2n}	$pn1m$	0	0

(§ 3.*D*), there is again only the symmorphic space group for a given point group with the standard lattice, *pnmm* for the point group *nmm*, and *pnm* for the point group *nm*.

The remaining case of an improper point group of rotational order n that *is* a prime power is dealt with in §§ 4.*D* and *E*, depending on whether n is odd or even.

Section 4.*D* establishes that when n is an *odd* prime power, there is enough freedom within the family of gauge functions giving $\Phi_r \equiv 0$ to pick one that also gives $\Phi_m \equiv 0$. This result depends in detail on the lattice being the standard one. It is straightforwardly established for $G = nm1$, but requires a rather more intricate argument for $n1m$. Thus when n is an odd prime power, the standard lattice has just two space groups, $pn1m$ and $pnm1$, both of them symmorphic.

Section 4.*E* establishes that when n is a power of 2 there are two inequivalent families of phase functions. In this case (and only in this case) there are non-trivial phase-function solutions to (2.5) and (2.8) on the standard lattice. The space groups are the symmorphic space group *pnmm* and the non-symmorphic space group *pngm*. In the latter case the mirror phase function on the symmetric generating set is $\Phi_m(\zeta_n^j) \equiv \frac{1}{2}$. Following the crystallographic nomenclature, we call such a space-group element (reflection and an associated gauge-invariant phase change) a *glide* operation.

These results are summarized in Table 3. The crystallographic space groups for n equal to 3, 4 or 6 provide specimens of most of these categories: $n=6$ and $n=4$ give the two varieties of even number, and $n=3$ is an odd prime power. Only when n is odd but not a prime power (which first happens for $n=15$) does something distinctly novel emerge. There is only the space group $p[15]m$: the two apparently different space groups $p[15]m1$ and $p[15]1m$ are actually indistinguishable, because of the non-trivial scale invariance of the lattice Z_{15}.

The reader who is not interested in the mathematical details of the derivation of the space groups is encouraged to skip ahead to § 5, which shows how to construct patterns with a given space-group symmetry and how to obtain the rules for systematic extinctions.

A. The rotation phase function Φ_r

We show that if the point group G has an n-fold axis then we can always pick the gauge χ so that the phase function Φ_r of the rotation r through $2\pi/n$ is zero. It will then follow by repeated application of the group compatibility condition (2.8) that the phase function associated with any power of r must be zero. Representing rotations r^j by multiplication by ζ_n^j, we construct gauge functions that reduce Φ_r to zero as follows.

Given a phase function Φ_r, we show that it is equivalent to zero by defining the gauge function χ to be

$$\chi(\alpha) \equiv \frac{1}{n}\,\Phi_r\left(\frac{n}{1-\zeta_n}\,\alpha\right). \tag{4.1}$$

It is important to note that since Φ_r is only defined for lattice vectors, if χ is to be defined for all lattice vectors it is essential that the operation of multiplication by $n/(1-\zeta_n)$ takes lattice vectors (*i.e.* cyclotomic integers) into lattice vectors. This is made explicit by the following argument, which shows that multiplication by $n/(1-\zeta_n)$ takes any cyclotomic integer α into an integral linear combination of itself and its rotations through multiples of $2\pi/n$:

Note first that since every power of ζ_n is an nth root of unity, the polynomial z^n-1 has the factorization

$$z^n-1=(z-1)(z-\zeta_n)(z-\zeta_n^2)\ldots(z-\zeta_n^{n-1}). \tag{4.2}$$

Dividing both sides of (4.2) by $z-1$ we have

$$z^{n-1}+z^{n-2}+\ldots+z+1 = (z-\zeta_n)(z-\zeta_n^2)\ldots(z-\zeta_n^{n-1}). \tag{4.3}$$

Setting z equal to 1 we then have

$$n/(1-\zeta_n)=(1-\zeta_n^2)(1-\zeta_n^3)\ldots(1-\zeta_n^{n-1}). \tag{4.4}$$

Since the right-hand side of (4.4) can be multiplied out to yield a linear combination of powers of ζ_n, multiplying both sides by α demonstrates that $n\alpha/(1-\zeta_n)$ is indeed a lattice vector.

It is important to realize that although Φ_r is linear on the lattice, the n in (4.1) in the argument of Φ_r cannot be taken outside to cancel the $1/n$ in front, because in general the vector $\alpha/(1-\zeta_n)$ will *not* be in the lattice.

To see that the gauge function (4.1) does indeed reduce $\Phi_r(\alpha)$ to zero, note that in terms of cyclotomic integers, the general relation (2.18) between equivalent phase functions assumes the form

$$\Delta\Phi_r(\alpha) \equiv \Phi'_r(\alpha) - \Phi_r(\alpha) \equiv \chi[(\zeta_n - 1)\alpha]. \quad (4.5)$$

When the gauge function χ is given by (4.1), this gives

$$\Phi'_r(\alpha) \equiv \Phi_r(\alpha) + \frac{1}{n}\Phi_r\left[(\zeta_n - 1)n\frac{\alpha}{1-\zeta_n}\right]$$

$$\equiv \Phi_r(\alpha) - \frac{1}{n}\Phi_r(n\alpha) \equiv 0. \quad (4.6)$$

The last equality follows from the fact that α *is* in the lattice, and therefore we *can* extract the n from within the argument of the linear function Φ_r.

Thus within the class of equivalent phase functions comprising a given space group, it is always possible to choose a gauge function χ such that the phase function associated with the rotation r satisfies $\Phi_r(\alpha) \equiv 0$ for all vectors α in the lattice. (This is one of the major simplifying features of the two-dimensional problem; in three dimensions, phase functions associated with rotations cannot in general be reduced to zero by the proper choice of gauge.) Our subsequent analysis will be carried out in such a gauge.

When the point group G is n, there is therefore only one space group, which we denote by the symbol *pn*. In deriving this conclusion we nowhere used the fact that **L** was a standard lattice, so this conclusion remains more generally valid. If the lattice is non-standard the space-group symbol would remain the same, except that the '*p*' (for 'primitive') would be replaced by a specification of the lattice.

In discussing the phase functions Φ_m associated with mirrorings, we shall find it useful to take advantage of the freedom that remains in choosing a gauge function from among those giving $\Phi_r \equiv 0$. Note, therefore, that if Θ is linear on the lattice and assumes values that are integral multiples of $1/n$, then Φ_r is unaffected by a further gauge transformation of the form

$$\chi'(\alpha) \equiv \Theta\left(\frac{n\alpha}{\zeta_n - 1}\right), \quad (4.7)$$

since (4.5) gives for the corresponding change in Φ_r,

$$\chi'[(\zeta_n - 1)\alpha] \equiv \Theta(n\alpha) \equiv n\Theta(\alpha) \equiv 0. \quad (4.8)$$

B. The mirror phase function Φ_m

The non-trivial part of the two-dimensional problem lies in determining the phase function $\Phi_m(\alpha)$. It is easy to show that for point groups with both a rotation r and a mirroring m, the entire multiplication table can be constructed out of applications of the two relations

$$m^2 = e, \quad rmr = m. \quad (4.9)$$

Therefore it is enough to find phase functions that obey the group compatibility condition (2.8) for both of these relations.

Since the phase function associated with the identity e necessarily satisfies $\Phi_e(\alpha) \equiv 0$, condition (2.8) applied to the first of the relations (4.9) gives

$$0 \equiv \Phi_{m^2}(\alpha) = \Phi_m(m\alpha) + \Phi_m(\alpha). \quad (4.10)$$

A further application of (2.8) to the second relation (4.9) gives

$$\Phi_m(\alpha) \equiv \Phi_{rmr}(\alpha)$$
$$\equiv \Phi_r(m\zeta_n\alpha) + \Phi_m(\zeta_n\alpha) + \Phi_r(\alpha)$$
$$\equiv \Phi_m(\zeta_n\alpha), \quad (4.11)$$

since the phase function Φ_r vanishes. We therefore have two conditions on the phase function Φ_m:

$$\Phi_m(m\alpha) \equiv -\Phi_m(\alpha), \quad \Phi_m(\zeta_n\alpha) \equiv \Phi_m(\alpha), \quad (4.12)$$

for arbitrary lattice vectors α.

Before classifying the distinct solutions of (4.12), we first establish two simple but useful results.

Lemma A. If n is the order of the rotation r, *i.e.* $r^n = e$, and if the integer a is a proper divisor of n, then $a\Phi_m(\alpha) \equiv 0$ for all α.

This follows from the fact that if n can be factored as $n = ab$, then ζ_n^b is an ath root of unity. Thus, for any vector α,

$$\zeta_n^b\alpha + \zeta_n^{2b}\alpha + \ldots + \zeta_n^{ab}\alpha = 0. \quad (4.13)$$

Using the linearity of the phase function Φ_m and the second of equations (4.12) (repeatedly), we conclude that

$$a\Phi_m(\alpha) \equiv 0, \quad (4.14)$$

as was to be shown.

Lemma B. If $a\Psi$ and $b\Psi$ are both integers for two relatively prime integers a and b, then Ψ itself is an integer.

For Ψ is then simultaneously c/a and c'/b for some integers c and c', so that $cb = c'a$. But since a and b are relatively prime, this is only possible if a divides c, and b divides c', which means that Ψ is an integer.

As a result of Lemma *A*, the classification of the solutions of (4.12) divides naturally into two cases: (1) the order n of r is *not* a prime power and (2) the order n of r *is* a prime power.

C. The mirror phase function Φ_m when the order n of r is not a prime power

If the order n of the rotational symmetry of the point group G has at least two distinct prime factors — *i.e.* if n is not simply a power of a single prime number — then it is easy to establish that phase functions Φ_m satisfying the second of equations (4.12) must be equivalent to zero.

If n is not a prime power, then it can be written as the product of two integers a and b which have no common prime factors. Lemma A then requires that

$$a\Phi_m(\alpha)\equiv 0 \quad \text{and} \quad b\Phi_m(\alpha)\equiv 0, \tag{4.15}$$

and Lemma B requires $\Phi_m(\alpha)$ to be an integer - *i.e.* $\Phi_m(\alpha)\equiv 0$.

We can apply this result to improper point groups G in two cases.

(1) If n is even and not a prime power, then G is the entire point group nmm of the lattice, G_L. All phase functions are equivalent to the simple choice $\Phi_r\equiv\Phi_m\equiv 0$, and therefore there is a unique space group, which we denote by the space-group symbol *pnmm*. In this case the conclusion that there is a single space group with all phase functions equal to zero also remains valid even when the lattice is not a standard lattice.

(2) If n is odd and not a prime power, then as established in § 3.*D*, even though nm appears as two distinct subgroups of the lattice point group $[2n]mm$, the relations of the two subgroups to the lattice are interchanged by a simple rescaling.* (This is *not* the case when n *is* a prime power.) Since all choices of the phase functions are equivalent to the choice $\Phi_r\equiv\Phi_m\equiv 0$, there is again a unique space group which we denote by the symbol *pnm*.

It remains to discuss the case when n *is* a power of a single prime number. We subdivide this into two cases, depending on whether or not the prime is 2.

D. The mirror phase function Φ_m when the order n of r is an odd prime power

When n is an odd prime power ($n=p^s$, p an odd prime), then the rank ν of the lattice Z_{2n} (see §§ 2.*F* and 3.*B*) is just

$$\nu=(p-1)p^{s-1}=(p-1)q, \tag{4.16}$$

where we have defined

$$q=p^{s-1} \tag{4.17}$$

to avoid having to write exponents within exponents. We can take as a set of integrally independent generating vectors the following ν nth roots of unity:

$$\zeta_n^0,\zeta_n^1,\ldots,\zeta_n^{\nu-2},\zeta_n^{\nu-1}. \tag{4.18}$$

This set is indeed a basis. To see this note that since ζ_n^q is a pth root of unity, we have

$$\zeta_n^\nu=\zeta_n^{(p-1)q}=-(1+\zeta_n^q+\zeta_n^{2q}+\ldots+\zeta_n^{(p-2)q}). \tag{4.19}$$

This tells us how to express the q vectors, $\zeta_n^\nu,\ldots\zeta_n^{n-1}$ in terms of the vectors (4.18): equation (4.19) directly gives ζ_n^ν as a linear combination of the vectors (4.18), and the remaining higher powers of ζ_n are given in terms of the vectors (4.18) simply by multiplying (4.19) successively by $\zeta_n,\zeta_n^2,\ldots,\zeta_n^{q-1}$. The $2n$ vectors $\pm\zeta_n^0,\ldots,\pm\zeta_n^{n-1}$ constitute a symmetric basis for the lattice Z_{2n}.

Since p is a factor of n Lemma A gives

$$p\Phi_m(\alpha)\equiv 0. \tag{4.20}$$

We examine the consequences of this in two cases.

Case 1. $G=nm1$. There is then a mirroring in G that leaves one of the generating vectors (4.18) fixed.† In this case m leaves $\zeta_n^0=1$ invariant [equation (3.3)]. The first of equations (4.12) then requires that

$$2\Phi_m(\zeta_n^0)\equiv 0. \tag{4.21}$$

Since $p\neq 2$, in conjunction with Lemma B, (4.20) and (4.21) require $\Phi_m(\zeta_n^0)$ to be an integer, *i.e.* $\Phi_m(\zeta_n^0)\equiv 0$. The second of equations (4.12) then gives $\Phi_m(\zeta_n^j)\equiv 0$ for all the generating vectors. Since the standard lattice Z_{2n} consists of all integral linear combinations of these generating vectors (including the vectors themselves), the phase functions Φ_m can all be taken to be zero.

Therefore for the standard lattice Z_{2n} we have the unique space group $pnm1$ when n is a power of an odd prime, and the mirrorings in nm leave some units fixed.

Case 2. $G=n1m$. There is then no mirroring in G that leaves any of the generating vectors (4.18) fixed.

Evidently (4.20) will hold for any vector α in the lattice if and only if it holds for the generating vectors (4.18).‡ Since the second of equations (4.12) requires $\Phi_m(\zeta_n^j)$ to be the same for all the generating vectors (to within an additive integer) we must have

$$\Phi_m(\zeta_n^j)\equiv c/p \tag{4.22}$$

for some single integer c, independent of j.

We now show that we can use the remaining freedom of choice in the gauge function χ [as expressed in (4.7)] to make c equal to 0. When χ has the general form (4.7) consistent with the vanishing of Φ_r, then (2.18) gives

$$\Delta\Phi_m(\alpha)\equiv\Theta\left[\frac{n}{\zeta_n-1}(m-1)\alpha\right], \tag{4.23}$$

where Θ is a linear function on the lattice whose values are multiples of $1/n=1/p^s$. We must show that it is possible to choose such a function Θ so that

$$\Delta\Phi_m(\zeta_n^j)\equiv -c/p. \tag{4.24}$$

Since the mirroring m takes α into $-\alpha^*$ [equation (3.4)], we have $(m-1)\alpha=-(\alpha+\alpha^*)$, and therefore,

* This is a property of the standard lattice, so our conclusions in this case cannot be taken over to non-standard lattices without further investigation.

† Here is a place where we require the standard lattice: it is essential for the argument that follows that the symmetric generating vectors are themselves in the lattice.

‡ This again requires the lattice to be standard.

in particular,

$$\Delta\Phi_m(\zeta_n^j) \equiv \Theta\left[\frac{n}{1-\zeta_n}(\zeta_n^j+\zeta_n^{-j})\right]. \quad (4.25)$$

We first show that $\Delta\Phi_m(\zeta_n^j)$ differs from $\Delta\Phi_m(\zeta_n^0)$ by an integer. It will then be enough to show that $\Delta\Phi_m(\zeta_n^0)$ can be made equivalent to $-c/p$. The linearity of Θ gives

$$\Delta\Phi_m(\zeta_n^j)-\Delta\Phi_m(\zeta_n^0) \equiv \Theta\left[\frac{n}{1-\zeta_n}(\zeta_n^j+\zeta_n^{-j}-2)\right]. \quad (4.26)$$

Because the values of Θ are integral multiples of $1/n$, the right-hand side of (4.26) will indeed be an integer provided we can show that $(\zeta_n^j+\zeta_n^{-j}-2)/(1-\zeta_n)$ is in the lattice. But this follows from the identity

$$\frac{\zeta_n^j+\zeta_n^{-j}-2}{1-\zeta_n} = \frac{\zeta_n^{-j}(1-\zeta_n^j)^2}{1-\zeta_n} = \zeta_n^{-j}(1-\zeta_n)(1+\zeta_n+\zeta_n^2+\ldots+\zeta_n^{j-1})^2, \quad (4.27)$$

since the right-hand side can be expanded to give an integral linear combination of nth roots of unity — *i.e.* a lattice vector.

It therefore remains only to show for any given integer c that we can choose a Θ that gives $\Delta\Phi_m(\zeta_n^0) = -c/p$. In the case $j=0$, (4.25) gives

$$\Delta\Phi_m(\zeta_n^0) \equiv \Theta\left(\frac{2p^s}{1-\zeta_n}\right). \quad (4.28)$$

But $p/(1-\zeta_n)$ is a lattice vector. This follows from the identity

$$\frac{p}{1-\zeta_n} = -(1+\zeta_n+\zeta_n^2+\ldots+\zeta_n^{q-1})\sum_{j=1}^{p-1} j\zeta_n^{qj}, \quad (4.29)$$

which is easily verified by multiplying both sides by $1-\zeta_n$, noting that a factor of $1-\zeta_n$ converts the first term on the right into $1-\zeta_n^q$, carrying out the expansion of the resulting polynomial in ζ_n^q, and using (4.19) to simplify the resulting expression.

Because $p/(1-\zeta_n)$ is a lattice vector, we are allowed to remove a factor $2p^{s-1} = 2n/p$ from the linear function Θ in (4.28):

$$\Delta\Phi_m(\zeta_n^0) \equiv -\frac{2n}{p}\Theta\left[(1+\zeta_n+\zeta_n^2+\ldots+\zeta_n^{q-1}) \times \sum_{j=1}^{p-1} j\zeta_n^{qj}\right]. \quad (4.30)$$

We can specify the linear function Θ arbitrarily on any integrally independent set. We choose it to be zero for all vectors in the integrally independent generating set (4.18) except ζ_n^0. With the aid of (4.19) one can then verify that when the argument of Θ is expanded in the integrally independent generating vectors (4.18), ζ_n^0 occurs with the coefficient $1-p$. We therefore have simply

$$\Delta\Phi_m(\zeta_n^0) \equiv -\frac{2n}{p}\Theta(\zeta_n^0). \quad (4.31)$$

But $\Theta(\zeta_n^0)$ is of the form c'/n where c' is any integer. Since even integers can be found congruent to any integer, modulo the odd prime p, we can pick c' to give $\Delta\Phi_m(\zeta_n^0) = -c/p$ for any desired value of the integer c.

Thus $\Phi_m(\zeta_n^0)$ can be taken to be zero, and therefore $\Phi_m(\zeta_n^j)$ can be taken to be zero for any j. Since the ζ_n^j together constitute a basis the linear phase function Φ_m can be taken to be zero everywhere on the lattice. We conclude that when n is a power of an odd prime, and the mirrorings leave no unit fixed ($G = n1m$), we have a single space group $pn1m$.

F. The mirror phase function Φ_m when the order n of r is a power of 2

When $n = 2^s$, Lemma *A* requires that

$$2\Phi_m(\alpha) \equiv 0 \quad (4.32)$$

for all lattice vectors α. The second of equations (4.12) requires $\Phi_m(\alpha)$ to have the same value on all the generating vectors ζ_n^j, and (4.32) requires that value to be either 0 or $\frac{1}{2}$. In contrast to the other prime power cases, the value $\frac{1}{2}$ cannot be eliminated by a further gauge transformation. For when n is even ζ_n^0 is invariant under the mirroring m (see Table 2), and therefore $\Phi_m(\zeta_n^0)$ is gauge invariant, as an immediate consequence of (2.18).

Therefore when n is a power of 2 (and only then) there are two distinct choices for the phase functions. Setting all phase functions equal to zero gives the space group *pnmm*; setting all the $\Phi_r(\zeta_n^j)$ equal to 0 and all the $\Phi_m(\zeta_n^j)$ equal to $\frac{1}{2}$ gives the non-symmorphic space group *pngm*.

5. A simple quasicrystalline pattern with a non-symmorphic space group

Non-symmorphic space groups occur only when the point group is *nmm* with n a power of 2, in which case $\Phi_m(\zeta_n^j) = \frac{1}{2}$. In this section, we consider such cases, and construct a pattern with $p8gm$ symmetry.

As shown in § 2.*E*, a lattice vector α invariant under a point-group operation g cannot appear in the diffraction pattern if $\Phi_g(\alpha)$ is non-integral. Since a rotation in two dimensions leaves only the origin fixed, extinctions can only occur for vectors invariant under mirror operations. When the lattice is represented by the cyclotomic integers Z_n the two types of mirror operations for even n can be described as (1) reflections in a line through the origin and an nth root of unity and (2) reflections in a line through the

origin passing between two neighboring nth roots of unity.

Consider first the mirroring m which reflects in the real axis. The lattice vectors α invariant under m are simply those lattice vectors along the real axis:

$$\alpha = l_0 + l_1\{\zeta_n + \zeta_n^{-1}\} + l_2\{\zeta_n^2 + \zeta_n^{-2}\} + \ldots + l_{n/4-1}\{\zeta_n^{n/4-1} + \zeta_n^{-n/4+1}\}, \quad (5.1)$$

for arbitrary integers l_i and $n = 2^j \geq 8$. Using the linearity of the phase function, we find

$$\Phi_m(\alpha) \equiv \tfrac{1}{2}(l_0 + 2l_1 + 2l_2 + \ldots + 2l_{n/4-1}) \equiv \tfrac{1}{2}l_0, \quad (5.2)$$

so that vectors of the form (5.1) with l_0 odd cannot be present in the diffraction pattern. The mirrorings in the lines through the other nth roots of unity can each be analyzed in the same way.

Next consider an example of the second type of mirroring, m', which reflects in the line between 1 and ζ_n. In terms of the mirroring m and the rotation r, we have $m' = rm$. Application of (2.8) with $\Phi_r(\alpha) \equiv 0$ gives

$$\Phi_{m'}(\alpha) \equiv \Phi_m(\alpha), \quad (5.3)$$

so

$$\Phi_{m'}(\zeta_n^j) \equiv \tfrac{1}{2}. \quad (5.4)$$

The lattice vectors α in the invariant space of m' are along $1 + \zeta_n$:

$$\alpha = l_0\{1 + \zeta_n\} + l_1\{\zeta_n^{-1} + \zeta_n^2\} + \ldots + l_{n/4-1}\{\zeta_n^{1-n/4} + \zeta_n^{n/4}\}, \quad (5.5)$$

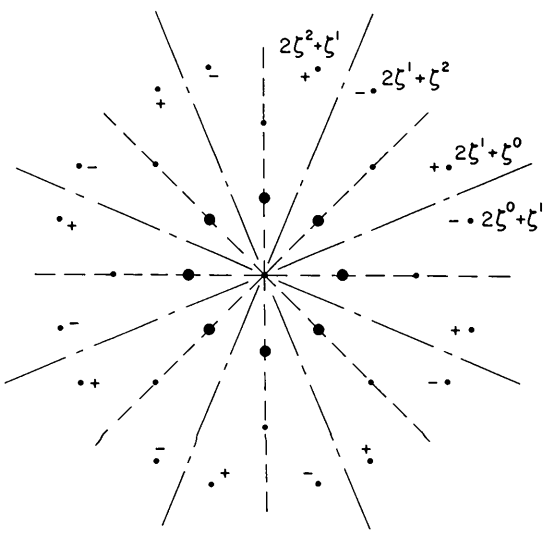

Fig. 2. The Fourier transform of a structure with $p8gm$ space-group symmetry. Large solid circles indicate a set of symmetric basis vectors for the reciprocal lattice Z_8; the diffraction peaks corresponding to these reciprocal-lattice vectors are forbidden by symmetry. The 16 reciprocal-lattice vectors $2\zeta^l + \zeta^{l\pm1}$ all have Fourier amplitudes with the same magnitude but with alternating sign, as indicated. Mirror lines are denoted by dashed lines. Under reflection in any of the eight mirror lines, the phases of the Fourier amplitudes for these reciprocal-lattice vectors each change by π.

for arbitrary l_i, and therefore it follows from (5.4) that

$$\Phi_{m'}(\alpha) \equiv \tfrac{1}{2}(2l_0 + 2l_1 + \ldots) \equiv 0. \quad (5.6)$$

Therefore none of the lattice vectors (5.5) are forbidden from appearing in the diffraction pattern. Again, the mirrorings through lines between other pairs of nth roots can be similarly analyzed, so no vectors invariant under the second kind of mirroring are forbidden.

As an illustration of a non-symmorphic non-crystallographic space group, we construct a pattern with the simplest such space group, $p8gm$.

Let ζ be the eighth root of unity, $\zeta = \exp(2\pi i/8)$. A symmetric generating set is $\zeta^0, \ldots, \zeta^7$. We choose the Fourier coefficients in the density to vanish everywhere except at the 16 lattice vectors

$$2\zeta^j + \zeta^{j\pm1}, \quad j = 0, \ldots, 7, \quad (5.7)$$

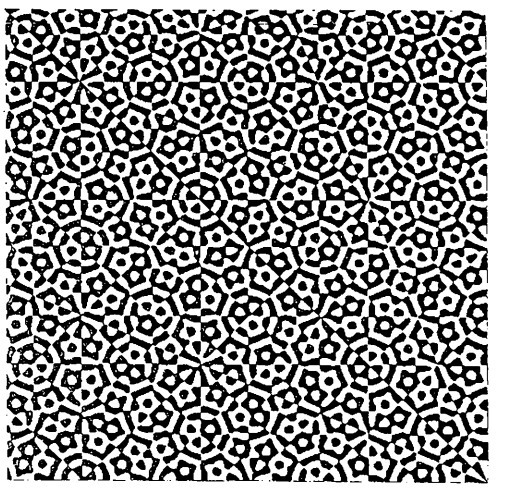

Fig. 3. The pattern with $p8gm$ symmetry described in § 5.

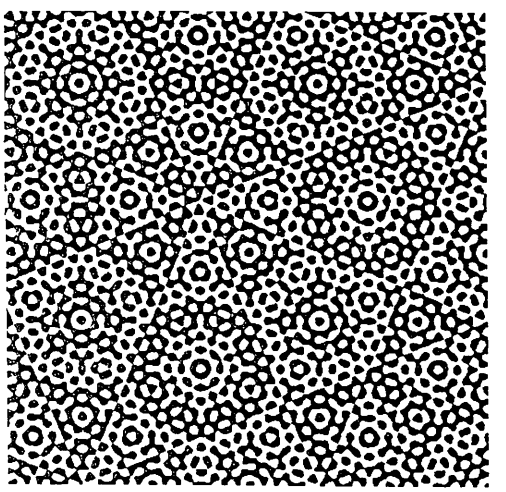

Fig. 4. A pattern with $p8mm$ symmetry, differing from that in Fig. 3 by the phases of the Fourier coefficients.

and, of course at the point 0, where the Fourier coefficient is the average density ρ_0.

The space group $p8gm$ has

$$\Phi_m(2\zeta^j+\zeta^{j\pm1})\equiv\tfrac{1}{2},\quad \Phi_r(2\zeta^j+\zeta^{j\pm1})\equiv 0. \qquad (5.8)$$

If we take the Fourier coefficients at the lattice vectors (5.7) to be given by

$$\rho(2\zeta^j+\zeta^{j\pm1})=\pm\rho_1,\quad j=0,\ldots,7, \qquad (5.9)$$

where ρ_1 is a constant overall amplitude, then it is evident from Fig. 2 and the defining relation (2.4) that mirrorings and rotations of (5.9) are indeed characterized by the phase functions (5.8).

The symmetry of the resulting real-space density is shown in Fig. 3, by coloring the plane black or white depending on the sign of $\rho-\rho_0$. To aid the reader in deciding to what extent 'quasi-glide lines' are present in this pattern, we display in Fig. 4 the corresponding symmorphic pattern with $p8mm$ symmetry given by taking all 16 Fourier coefficients in (5.9) to have the same sign.

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References

ALEXANDER, S. (1986). *J. Phys. (Paris)*, **47**, C3-143-151.
BAK, P. (1985*a*). *Phys. Rev. Lett.* **54**, 1517-1519.
BAK, P. (1985*b*). *Phys. Rev. B*, **32**, 5764-5772.
BAK, P. (1986). *J. Phys. (Paris)*, **47**, C3-135-141.
BIENENSTOCK, A. & EWALD, P. P. (1962). *Acta Cryst.* **15**, 1253-1261.
HARDY, G. H. & WRIGHT, E. M. (1954). *An Introduction to the Theory of Numbers.* Oxford Univ. Press.
JANNER, A. & JANSSEN, T. (1977). *Phys. Rev. B*, **15**, 643-658.
JANSSEN, T. (1986*a*). *J. Phys. (Paris)*, **47**, C3-85-94.
JANSSEN, T. (1986*b*). *Acta Cryst.* **A42**, 261-271.
LEVINE, D., LUBENSKY, T. C., OSTLUND, S., RAMASWAMY, S., STEINHARDT, P. J. & TONER, J. (1985). *Phys. Rev. Lett.* **54**, 1520-1523.
MERMIN, N. D., ROKHSAR, D. S. & WRIGHT, D. C. (1987). *Phys. Rev. Lett.* **58**, 2099-2101.
ROKHSAR, D. S., MERMIN, N. D. & WRIGHT, D. C. (1987). *Phys. Rev. B*, **35**, 5487-5495.
WASHINGTON, L. (1982). *Introduction to Cyclotomic Fields.* New York: Springer-Verlag.

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A Note on the Rotational Superposition Problem

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Abstract

A rotation axis vector with magnitude $\tan(\theta/2)$ for a rotation angle θ and a closely related unit vector of dimension 4 are used to show that: (i) the quadratic residual (weighted sum of squares of coordinate differences) that results when one vector set is rotated relative to another is a quadratic form of order 4, (ii) the stationary values of the residual are given by the eigenvalues of a matrix of order 4, (iii) the minimum residual is given by the largest eigenvalue, (iv) the rotations required to obtain such residuals are uniquely defined by the corresponding eigenvectors, and (v) the stationary values are related by the operations of 222 symmetry. No precautions against the generation of improper rotations are required. In addition, an equivalent solution based on a scalar iteration is presented, together with some relationships of general interest.

Introduction

The problem of the optimal superposition of one vector set on another by pure rotation arises notably in the comparison of parts of related protein molecules, and its solution has attracted the attention of a number of writers, notably McLachlan (1972, 1979, 1982), Kabsch (1976, 1978), Diamond (1976) and Lesk (1986).

McLachlan's earlier method is iterative and analogous to rotating one vector set about the axis of the prevailing couple to reduce that couple to zero, when the couple is supposed to be the sum of the moments arising from forces along the lines separating equivalent points in the two vector sets having magnitudes proportional to those separations. His later method is an eigenvalue/vector method using a symmetric matrix of order 6. Kabsch's method is an eigenvalue/vector method based on matrices of order

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