Applications of group cohomology to the classification of quasicrystal symmetries

2003 J. Phys. A: Math. Gen. 36 10195

(http://iopscience.iop.org/0305-4470/36/40/005)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 10195–10214 PII: S0305-4470(03)64020-5

Applications of group cohomology to the classification of quasicrystal symmetries

Benji N Fisher[1] **and David A Rabson**[2]

[1] Mathematics Department, Boston College, Chestnut Hill, MA 02467, USA
[2] Physics Department, University of South Florida, 4202 E. Fowler Ave, Tampa, FL 33620, USA

E-mail: benji@member.AMS.org and davidra@ewald.cas.usf.edu

Received 28 May 2003, in final form 11 August 2003
Published 24 September 2003
Online at stacks.iop.org/JPhysA/36/10195

Abstract

In 1962, Bienenstock and Ewald described the classification of crystalline space groups algebraically in the dual, or Fourier, space. After the discovery of quasicrystals in 1984, Mermin and collaborators recognized in this description the principle of macroscopic indistinguishability and developed techniques that have since been applied to quasicrystals, including also periodic and incommensurately modulated structures. This paper phrases these techniques in terms of group cohomology. A *quasicrystal* is defined, along with its space group, without requiring that it come from a quasicrystal in real (direct) space. A certain cohomology group classifies the space groups associated to a given point group and lattice, and the dual homology group gives all gauge invariants. This duality is exploited to prove several results that were previously known only in special cases, including the classification of space groups (plane groups) for lattices of arbitrary rank in two dimensions. Extinctions in x-ray diffraction patterns and degeneracy of electronic levels are interpreted as physical manifestations of non-zero homology classes.

PACS numbers: 02.10.Hh, 61.50.Ah, 61.44.Br, 61.44.Fw
Mathematics Subject Classification: 20H15, 20J06

Introduction

Background

The Penrose tilings of the plane [1] have long-range order and are very symmetrical, but they are not periodic. A few years after the discovery of these tilings, physical quasicrystals were discovered [2–4]. These are solids with aperiodic structures that still have long-range order and interesting symmetries, properties that are most evident in Fourier space. In fact, the

x-ray diffraction patterns of some quasicrystals have five-fold symmetry, which is impossible for periodic crystals. Several mathematical models for quasicrystals have been proposed. A central question is how to classify the possible symmetries of a quasicrystal, analogously to the classification of crystallographic groups, which describe the symmetries of periodic crystals.

One approach to crystallography starts with the group $\mathcal{T}$ of translational symmetries of a crystal. If the crystal is periodic, then $\mathcal{T}$ is a lattice in $\mathbb{R}^3$ ('real space' or 'direct space'). The space group $\mathcal{G}$ is the group of all isometries that preserve the crystal, and it contains $\mathcal{T}$ as a normal, Abelian subgroup. The quotient $G = \mathcal{G}/\mathcal{T}$ is called the point group of the crystal, and it can be considered a subgroup of the orthogonal group O(3). A quasicrystal may have no translational symmetries, so this approach does not generalize directly. Instead, one can model a quasicrystal as the projection into $\mathbb{R}^3$ of a periodic crystal in a higher-dimensional space ('superspace') [5].

This paper takes a different approach to studying quasicrystals. In 1962, Bienenstock and Ewald [6] introduced the 'Fourier-space approach' to classifying symmetries of crystals. In this picture, a crystal is described by a periodic (electron or mass) density function on $\mathbb{R}^3$. The Fourier coefficients of this density function are thus defined on the dual lattice in the dual space $\mathbb{R}^{3*}$ ('Fourier space' or 'momentum space'). The symmetries of the crystal can then be described in terms of these Fourier coefficients, as discussed in section 1. Rokhsar, Wright and Mermin (RWM) [7] recognized in this formalism the principle that *indistinguishability* under group operations, rather than identity, underlies the symmetry of crystals. This approach has since been applied to quasicrystals and modulated crystals [8–16]; the only change is that one must relax the condition that the Fourier coefficients be defined on a (discrete) lattice in Fourier space.

The Fourier-space approach to crystallography had not been expressed explicitly in terms of group cohomology until [17], although the correspondence was pointed out by Mermin [10] and by Piunikhin [18]. (The direct-space approach has been expressed in this language by Ascher, Janner and others: [19–23].) The goal of this paper is to describe the Fourier-space approach in terms of group cohomology and to show how to take advantage of this well developed theory. Using this language, it is easy to prove and generalize results that other authors have obtained, often by laborious calculation. (In [15], these calculations are relegated to an appendix, and in [7], the reader is encouraged to skip them.) This paper gives several examples. Of course, some readers will still be sceptical that it is worth learning about *cocycles* and *coboundaries*. Such readers should be convinced by theorem 7.5, which classifies the space groups corresponding to a given point group in two dimensions and a Fourier-space lattice (or module) of arbitrary rank. Crystallographers interested in applying the cohomological language to quasicrystals are also referred to [17, 24].

For the reader familiar with the cohomological language, this should provide one more interesting application of several familiar definitions and theorems. The reader familiar with crystallography in Fourier space will recognize in section 1 a new set of names for several familiar ideas.

Previous work based on the RWM Fourier-space approach, but not using the cohomological language, has been limited to computations with lattices having explicit generators. Some results [12, 13] applied to only a few specific lattices at a time and others [9, 10] only to lattices equivalent to principal ideals in the ring of cyclotomic integers [25]. Very little was known about lattices having non-minimal ranks consistent with their rotational symmetry, for example, incommensurately modulated crystals. The techniques used in this paper lift these restrictions. The results presented here provide the theoretical framework for the first complete classifications of space groups in two and three dimensions [26].

Summary of results

The first three sections describe the ideas studied in this paper: quasicrystals, their space groups and their classification. For the most part, we follow the definitions and notation of Dräger and Mermin [27]. A *quasicrystal* $\hat{\rho}$ is defined as the coefficients of a formal Fourier series

$$\rho(x) = \sum_{k \in L} \hat{\rho}(k)\, \mathrm{e}^{2\pi \mathrm{i} k x} \tag{0.1}$$

where L is a lattice: a finitely generated additive group that spans $\mathbb{R}^{d*}$ but is not necessarily discrete. Briefly, one associates a triple $(G, L, \{\Phi\})$ to $\hat{\rho}$, where G is a subgroup of the orthogonal group $\mathrm{O}(d)$, L is a lattice in $\mathbb{R}^{d*}$ stable under G and $\{\Phi\}$ is a cohomology class in $H^1(G, \hat{L})$, $\hat{L} = \mathrm{Hom}(L, \mathbb{R}/\mathbb{Z})$. The 'point group' G can be thought of as the group of macroscopic symmetries of $\hat{\rho}$, and the triple $(G, L, \{\Phi\})$ describes all symmetries, so we call the triple the 'symmetry type' of $\hat{\rho}$. Section 1 gives these definitions in detail. Section 2 discusses these definitions from the point of view of the function ρ defined by the series (0.1), assuming that the series converges absolutely. This assumption is made to keep the analysis simple; a more comprehensive treatment of the relation between quasicrystals and functions ρ in direct space lies beyond the scope of this paper. Section 2 also discusses the relation between this and other models of quasicrystals and the classical definition of space groups and point groups. Section 3 explains a programme for classifying symmetry types that can be summarized by the phrase, 'G first, then L.' This provides a context for most of the results proved in the later sections. Other classifications first consider all lattices L of a given rank, and then consider what point groups G can be associated to these lattices. The approach used here is to fix the finite group G and then study the lattices symmetric under G.

The beauty of this programme is that, to classify d-dimensional symmetry types, there is no need to leave dimension d. If one takes the direct-space approach, the (super)space group of a quasicrystal is naturally a crystallographic group in a higher-dimensional superspace, with attendant complications. On the other hand, previous work using the Fourier-space approach, such as [7], concentrated too early on explicit generators of the lattice, and this led to unnecessary restrictions (such as requiring the lattice to be described by a principal ideal). Concentrating first on the group G makes it possible to calculate $H^1(G, \hat{L})$ for quite general two-dimensional lattices L. The authors are working on a paper that completes this programme in dimension 2 and hope, in future work, to do the same for dimension 3.

Each of the remaining sections illustrates the usefulness of the cohomological language by taking a standard result about group cohomology and applying it to crystallography. Many of the applications are already known, although in less generality. In effect, the literature of Fourier-space crystallography has been re-inventing the theory of group cohomology.

Perhaps the most significant result of the paper (even though it is a direct consequence of a standard result) is theorem 5.1, which states that the cohomology group $H^1(G, \hat{L})$ is dual to the homology group $H_1(G, L)$. There are two ways of thinking of this duality. One states that elements of H_1 describe functions on H^1 and so constitute 'fundamental gauge invariants' in the language introduced in section 1. In other words, this homology group classifies all possible 'gauge-invariant linear combinations of phases', the simplest of which have found physical manifestations. The opposite point of view thinks of a cohomology class, or a gauge-equivalence class of phase functions, as a linear function on the finite group $H_1(G, L)$. This homology group is simpler, both conceptually and computationally, than the cohomology group. In fact, as long as one works with $\hat{L}$, the Pontrjagin dual of the lattice in Fourier space, it is unclear to what extent one is really taking a Fourier-space approach. By concentrating on $H_1(G, L)$, we commit ourselves to this approach.

In the superspace approach to crystallography, the space group $\mathcal{G}$ is an extension of G by $\mathcal{T}$, so it is described by an element of $H^2(G, \mathcal{T})$. The two approaches are connected by making the identifications $\mathcal{T} = \mathrm{Hom}(L, \mathbb{Z})$ and $L = \mathrm{Hom}(\mathcal{T}, \mathbb{Z})$. From this point of view, theorem 5.1 states that $H^2(G, \mathcal{T})$ is dual to $H_1\big(G, \mathrm{Hom}(\mathcal{T}, \mathbb{Z})\big)$; see remark 5.3.

Sections 6 and 7 describe how the restriction-inflation sequence and the simple form of (co)homology of cyclic groups make the computation of $H_1(G, L)$ in dimensions 2 and 3 a tractable problem. As an application, theorem 7.5 gives a complete description of this homology group in the two-dimensional case. In physical terms, the result means that the only two-dimensional, non-symmorphic space groups are those whose point groups are dihedral, with cyclic subgroup of order $N = 2^e$. This generalizes, without all the computation, results already known in the restricted cases of lattices of minimal rank, corresponding to principal ideals. This theorem is closely related to that of Piunikhin: remark 7.6 discusses this further.

Another important part of crystallography is the description of the physical consequences of symmetry. Preliminary computations suggest that, in two and three dimensions, any homology group $H_1(G, L)$ is generated by cycles of a few simple types. If so, and if $\{\Phi\} \in H^1(G, \hat{L})$ is non-trivial, then $\langle \Phi, c \rangle \neq 0$ where c is one of these simple cycles. Non-vanishing gauge invariants tend to have physical implications, as described in section 8. One of these is described by König and Mermin [15], who suggest an approach that generalizes to quasicrystals some crystalline phenomena usually explained in terms of representation theory. Proposition 8.1 hints at how these ideas can be simplified and generalized using cohomology. Another subject the authors hope to consider in future work is to describe physical phenomena associated to each of the simple cycles.

Finally, we mention proposition 4.1, corollary 5.2 and proposition 5.5. The first two are results that were known only in cases where the gauge-equivalence (cohomology) classes had been calculated explicitly, and the third is a non-computational proof of the result in the appendix of [16].

This paper attempts to describe crystallography using group cohomology in a way that can be understood both by those familiar with crystallography and by those familiar with cohomology. The reader will judge how well it succeeds. In [17] the authors describe many of the same ideas explicitly in terms of cocycles, and in [24] they review the connection between crystallography and algebraic topology for those unfamiliar with the nomenclature of homological algebra.

Notation

d	coboundary map
∂	boundary map
ρ	formal sum of coefficients
$\hat{\rho}$	quasicrystal $L \to \mathbb{C}$
χ	gauge function $L \to \mathbb{R}/\mathbb{Z}$
Φ_g	element of $\hat{L}$ corresponding to g
Φ	phase function $G \to \hat{L}$
$\{\Phi\}$	gauge equivalence (cohomology) class of Φ in $H^1(G, \hat{L})$
G	point group of $\hat{\rho}$
G_L	point group (holohedry) of L
$\mathcal{G}$	space group of $\hat{\rho}$
L	lattice
L'	$\mathrm{Hom}(L, \mathbb{Q}/\mathbb{Z})$
$\hat{L}$	$\mathrm{Hom}(L, \mathbb{R}/\mathbb{Z})$, dual to L

M^G $\{x \mid gx = x, g \in G\}$
M_G $M/\langle\{kg - k \mid k \in M, g \in G\}\rangle$
N_g $1 + g + \cdots + g^{N-1}$ if $g^N = 1$
$\mathcal{T}$ lattice of direct-space or superspace translations

1. Definitions

This section defines quasicrystals and their symmetry types, the main objects of study in this paper. Unfortunately, the language of quasicrystals is far from being standardized. Definition 1.1 follows [27, 28] and several previous works, but some authors [29] prefer the term *quasilattice* for what we call a *lattice*, reserving the latter term for discrete sets. We avoid the former term, as it is sometimes used to describe instead a discrete set (not always closed under addition) of direct-space translations. Others refer to a lattice (in the sense used here) as a (generalized) lattice or (Fourier) module. This paper uses *quasicrystal* as the most general term, encompassing periodic and aperiodic crystals; some authors use the phrase (generalized) *crystal* for this, reserving the term *quasicrystal* for a particular kind of *aperiodic* crystal. We emphasize, however, that what we are studying is the formal Fourier density $\hat{\rho}$, without commitment to the convergence of the series (0.1), except in section 2, where we assume convergence explicitly. One might therefore think to call $\hat{\rho}$ a *Fourier quasicrystal* or even a *quasicrystal Fourier-density coefficient*, but such verbosity would seem churlish.

The rest of the definitions mostly follow Dräger and Mermin [27]. Section 2 explains these definitions in terms of quasicrystals in real space, again following [27].

Definition 1.1. *Let W be a Euclidean space. A lattice in W is a finitely generated, additive subgroup $L \subseteq W$ that spans W.*

It is well known that a lattice is discrete if and only if its rank is the same as the dimension of W. Since the lattice L is required to span W, the inequality $\operatorname{rank}(L) \geqslant \dim(W)$ always holds. In terms of physics, what we are describing is the *reciprocal lattice*. A periodic crystal additionally possesses a dual *direct-space lattice* of translations in the same number of dimensions, as discussed in section 2, and both lattices (reciprocal and direct) are discrete. It does not matter in the Fourier-space approach, for the purpose of classifying symmetries, whether a crystal is periodic or not. We do not consider here the possibility of an infinitely-generated lattice, nor do we consider singular-continuous spectra [30, 31].

Definition 1.2. *Let L be a lattice. A quasicrystal on L is a function $\hat{\rho} : L \to \mathbb{C}$ such that L is generated, as an Abelian group, by the values of k for which $\hat{\rho}(k) \neq 0$.*

The requirement that the support of $\hat{\rho}$ should generate L should be thought of as a condition on L, not on $\hat{\rho}$, since an arbitrary complex-valued function $\hat{\rho}$ on a lattice L_1 will be a quasicrystal on the lattice L generated by $\{k \mid \hat{\rho}(k) \neq 0\} \subseteq L_1$.

Definition 1.3. *Let L be a lattice. A gauge function on L is an element of the Pontrjagin dual*

$$\hat{L} = \operatorname{Hom}(L, \mathbb{R}/\mathbb{Z}). \tag{1.1}$$

Two quasicrystals $\hat{\rho}_1$ and $\hat{\rho}_2$ on L are indistinguishable if there is a gauge function $\chi \in \hat{L}$ such that

$$\hat{\rho}_2(k) = \mathrm{e}^{2\pi \mathrm{i} \chi(k)} \hat{\rho}_1(k) \qquad (\forall k \in L). \tag{1.2}$$

A quasicrystal on $L \subseteq W$ can be thought of as the formal Fourier series (0.1) where x is in the dual space of W. The motivation for these definitions comes from considering $\hat{\rho}$ as

the Fourier transform of the sum (if it exists) of such a series. If x is in the 'real space' $\mathbb{R}^d$ of column vectors, then the space spanned by L should be thought of as the dual space, so from now on identify W with the 'Fourier space' $\mathbb{R}^{d*}$ of row vectors[3]. Note that the orthogonal group $\mathrm{O}(d)$ acts naturally on the left on $\mathbb{R}^d$ and on the right on $\mathbb{R}^{d*}$.

This paper makes no attempt to characterize the functions ρ for which a series (0.1) can be defined, but section 2 explains, under restrictive analytic assumptions, what indistinguishability means in terms of the function ρ on real space. A symmetry of a quasicrystal is defined in terms of indistinguishability:

Definition 1.4. *Let L be a lattice in $\mathbb{R}^{d*}$, and let $\hat{\rho}$ be a quasicrystal on L. The holohedry group G_L is the subgroup of the orthogonal group $\mathrm{O}(d)$ consisting of all g such that $L \cdot g = L$. A symmetry of $\hat{\rho}$ is an element $g \in G_L$ such that $\hat{\rho} \circ g$ is indistinguishable from $\hat{\rho}$. In other words, there is a gauge function $\Phi_g \in \hat{L}$ such that*

$$\hat{\rho}(kg) = \mathrm{e}^{2\pi \mathrm{i} \Phi_g(k)} \hat{\rho}(k) \qquad (\forall k \in L). \tag{1.3}$$

The point group of $\hat{\rho}$ is the group G of all such symmetries. The map $\Phi : G \to \hat{L}$ is called a phase function.

Usually the individual functions Φ_g are also called phase functions. We avoid this usage in order to emphasize the fact that a phase function is a gauge function that depends on the parameter g in the point group. Note that, since $\hat{\rho}$ is required to be non-zero on a set of generators of L and Φ_g is linear on L, relation (1.3) determines $\Phi_g(k) \in \mathbb{R}/\mathbb{Z}$ for all $k \in L$. It is shown in [29, section 1.2] that, even in dimension $d = 2$, a lattice may be symmetric under a rotation of infinite order, so the holohedry group G_L is not always finite. This paper usually assumes that the point group of $\hat{\rho}$ is finite, but most results apply generally to any finite subgroup of the point group.

The condition $k(gh) = (kg)h$ leads to the *group-compatibility condition*:

$$\Phi_{gh}(k) = \Phi_h(kg) + \Phi_g(k). \tag{1.4}$$

The natural right action of $\mathrm{O}(d)$ on $\mathbb{R}^{d*}$ induces a left action of G on $\hat{L}$. In terms of this action, (1.4) reads $\Phi_{gh} = g\Phi_h + \Phi_g$. In other words, $\Phi : G \to \hat{L}$ is a *cocycle*[4] in $Z^1(G, \hat{L})$.

Now, let $\hat{\rho}_1$ and $\hat{\rho}_2$ be indistinguishable quasicrystals, and let χ be a gauge function as in (1.2). Then $\hat{\rho}_2$ has the same point group as $\hat{\rho}_1$, as can be seen by defining

$$\Phi_g^{(2)}(k) = \Phi_g^{(1)}(k) + \chi(kg - k). \tag{1.5}$$

Equation (1.5) is called a *gauge equivalence*. In terms of the left action of G on $\hat{L}$, it reads $\Phi_g^{(2)} - \Phi_g^{(1)} = g\chi - \chi$, which means that the difference of the two cocycles is the *coboundary*, or *gauge transformation*, $g\chi - \chi$. Since cohomologous cocycles (gauge-equivalent phase functions) express the same symmetry of indistinguishable quasicrystals, it is natural to associate to $\hat{\rho}$ (or to its equivalence class under indistinguishability) the *cohomology class* (or *gauge-equivalence class*) $\{\Phi\} \in H^1(G, \hat{L})$.

Definition 1.5. *Let L be a lattice in $\mathbb{R}^{d*}$, and let $\hat{\rho}$ be a quasicrystal on L. The symmetry type of $\hat{\rho}$ is the triple $(G, L, \{\Phi\})$, where G is the point group of $\hat{\rho}$ and $\{\Phi\}$ is the cohomology class described above. The space group of $\hat{\rho}$ is the extension of G by $\mathrm{Hom}(L, \mathbb{Z})$ corresponding to*

[3] These conventions are convenient for making the connection between direct and reciprocal space and for invoking well-known results in cohomology [32, 33]. In most other work in Fourier-space crystallography (e.g., [7, 27, 17, 24]), an element of Fourier space is thought of as a column vector with a left group action. As a consequence, some results here (e.g., (1.4)) will take slightly different, but entirely equivalent, forms.

[4] Readers unfamiliar with terms such as *cocycle* are referred to [17, 24] as well as the standard references [32, 33].

this cohomology class, as described in section 2 below. If the cohomology class is trivial, then $\hat{\rho}$, or its space group, is called symmorphic.

We use the term *space group* even if $d = 2$, where some authors might prefer *plane group*. Section 2 describes the space group from the real-space point of view. The symmorphic space group is simply the semidirect product $\mathrm{Hom}(L, \mathbb{Z}) \rtimes G$. If $\hat{\rho}$ is symmorphic, then there is some $\hat{\rho}_1$, indistinguishable from $\hat{\rho}$, such that the phase function of $\hat{\rho}_1$ is zero. Then (1.3) shows that $\hat{\rho}_1 \circ g = \hat{\rho}_1$ for all $g \in G$.

Definition 1.6. *Let L be a lattice in $\mathbb{R}^{d*}$, and let G be a subgroup of the holohedry group G_L. A gauge invariant of the pair (G, L) is a function $f : H^1(G, \hat{L}) \to \mathbb{C}$. If G is finite, then a fundamental gauge invariant is a homomorphism $f : H^1(G, \hat{L}) \to \mathbb{C}^\times$.*

Thus a gauge invariant assigns a number to each phase function, or to each quasicrystal $\hat{\rho}$ on L whose point group contains G, and that number depends only on the gauge-equivalence class. The set of all gauge invariants forms a vector space. Suppose that G is a finite group. It follows from theorem 5.1 that $H^1(G, \hat{L})$ is a finite Abelian group. Therefore, this vector space has finite dimension, and the set of characters $H^1(G, \hat{L}) \to \mathbb{C}^\times$ forms a basis. This explains the term *fundamental gauge invariant*. Any such character factors through the exponential map $\mathrm{e}^{2\pi i x} : \mathbb{Q}/\mathbb{Z} \to \mathbb{C}^\times$, so we also refer to any homomorphism $H^1(G, \hat{L}) \to \mathbb{Q}/\mathbb{Z}$ as a fundamental gauge invariant. In these terms, theorem 5.1 identifies the set of fundamental gauge invariants as the homology group $H_1(G, L)$.

2. Connections with real-space quasicrystals

For this section, assume that ρ is a function on $\mathbb{R}^d$ defined by an *absolutely convergent* series of the form (0.1). Other authors, such as de Bruijn [34] and Hof [35], have considered the general problem of associating Fourier series with quasicrystals, and work continues on this question. This paper deals with what to do *after* obtaining the function $\hat{\rho}$ on Fourier space, so the purpose of this section is to provide a simple analytic setting to illustrate this theory, not a comprehensive one. Of course, if the formal series (0.1) converges in any sense, then only finitely many terms can have absolute value greater than a given positive ε. Keeping only these terms gives a truncation of the series, or approximation of ρ, that is certainly absolutely convergent. Taking ε small enough, or taking sufficiently many terms, should give an approximation that has the same symmetry type as the original.

As in section 1, the terminology largely follows [27].

Definition 2.1. *A density function is any function $\rho : \mathbb{R}^d \to \mathbb{C}$ given by an absolutely convergent series (0.1), where $\hat{\rho}$ is a quasicrystal.*

Think of a density function as describing the electron density or mass density of a physical quasicrystal. One could also refer to ρ itself as a quasicrystal.

Under the hypothesis of absolute convergence, it is easy to see that the quasicrystal $\hat{\rho}$ can be recovered from the density function ρ. Let $C(r)$ denote the cube of side r, centred at the origin, in $\mathbb{R}^d$. Multiplying (0.1) by $\mathrm{e}^{-2\pi \mathrm{i} k' \cdot x}$, the series is still absolutely and uniformly convergent. Averaging over $C(r)$ gives

$$\frac{1}{r^d} \int_{C(r)} \rho(x)\, \mathrm{e}^{-2\pi \mathrm{i} k' \cdot x}\, \mathrm{d}x = \sum_{k \in L} \hat{\rho}(k)\, \frac{1}{r^d} \int_{C(r)} \mathrm{e}^{2\pi \mathrm{i}(k-k') \cdot x}\, \mathrm{d}x, \tag{2.1}$$

which converges absolutely and uniformly in r. Taking the limit as $r \to \infty$ gives $\hat{\rho}(k')$.

Define the positionally-averaged nth-order *autocorrelation function* of the density function ρ to be

$$\rho^{(n)}(x_1, \ldots, x_n) = \frac{1}{r^d} \int_{C(r)} \rho(x_1 - x) \cdots \rho(x_n - x)\, \mathrm{d}x. \tag{2.2}$$

Since the product of absolutely convergent series is absolutely convergent, $\rho(x_1 - x) \cdots \rho(x_n - x)$ is represented by an absolutely convergent series of the form (0.1), and the argument of the preceding paragraph shows that the same is true of the autocorrelation function:

$$\rho^{(n)}(x_1, \ldots, x_n) = \sum_{\substack{k_1, \ldots, k_n \in L \\ k_1 + \cdots + k_n = 0}} \hat{\rho}(k_1) \cdots \hat{\rho}(k_n)\, \mathrm{e}^{2\pi \mathrm{i}(k_1 \cdot x_1 + \cdots + k_n \cdot x_n)}. \tag{2.3}$$

Two density functions $\rho_1, \rho_2 : \mathbb{R}^d \to \mathbb{C}$ are called *indistinguishable* if their autocorrelation functions are the same. Mermin [36] and others have argued that using this criterion, rather than considering identity of density functions, is the most important theoretical difference between the Fourier-space approach and traditional crystallography. If two quasicrystals $\hat{\rho}_1$ and $\hat{\rho}_2$ are indistinguishable (as defined in section 1), then the corresponding density functions ρ_1 and ρ_2 are as well. It follows that a symmetry of $\hat{\rho}$ is a rotation g such that $\rho \circ g$ is indistinguishable from ρ, or a macroscopic symmetry of ρ. Define the point group of the density function ρ to be the same as the point group of the corresponding quasicrystal $\hat{\rho}$.

If the density function ρ describes a periodic crystal, then ρ is periodic with respect to a lattice $\mathcal{T} \subseteq \mathbb{R}^d$, and L is dual to $\mathcal{T}$ (assuming that $\mathcal{T}$ is the lattice of all periods of ρ). In this case, L is a discrete lattice, so a gauge function (an element of $\hat{L} = \mathrm{Hom}(L, \mathbb{R}/\mathbb{Z}) = \mathbb{R}^d/\mathcal{T}$) is determined by a translation on $\mathbb{R}^d$, and a symmetry of L is an orthogonal transformation of $\mathbb{R}^d$ that takes $\mathcal{T}$ to itself. In other words, the holohedry group G_L is the quotient of the *space group* $\mathcal{G}_\mathcal{T}$ of $\mathcal{T}$—the group of isometries that preserve $\mathcal{T}$—by the subgroup of translations corresponding to elements of $\mathcal{T}$. From this point of view, the action of G_L on $\mathcal{T}$ is induced by the conjugation action of $\mathcal{G}_\mathcal{T}$ on its subgroup of translations. The density function ρ can be thought of as an additional structure, or 'decoration', on the lattice $\mathcal{T}$. The space group of ρ is the group $\mathcal{G}$ of all isometries $\mathfrak{g}$ that respect this additional structure, $\rho \circ \mathfrak{g} = \rho$, and the point group $G = \mathcal{G}/\mathcal{T}$ is a subgroup of G_L.

Still in the periodic case, $\mathcal{G} \cong \mathcal{T} \times G$ as a set. The group structure of $\mathcal{G}$ can be recovered from the conjugation action of G on $\mathcal{T}$ and an element of $H^2(G, \mathcal{T})$ ([23], [19], [32, section IV.3] or [33, section 2]). As Hiller points out in [23], the boundary map of the long exact sequence associated to $0 \to \mathcal{T} \to \mathbb{R}^d \to \mathbb{R}^d/\mathcal{T} \to 0$ gives an isomorphism of $H^2(G, \mathcal{T})$ with $H^1(G, \mathbb{R}^d/\mathcal{T})$. Since $\mathbb{R}^d/\mathcal{T} \cong \mathrm{Hom}(L, \mathbb{R}/\mathbb{Z})$, this is the cohomology group considered in definition 1.5.

In the general case, turn these definitions around as in [27]. Start with the lattice $L \subseteq \mathbb{R}^{d*}$ and define $\mathcal{T} = \mathrm{Hom}(L, \mathbb{Z})$, naturally embedded in $V = \mathrm{Hom}(L, \mathbb{R})$. In the aperiodic case, $\dim V = \mathrm{rank}\, L > d$. This gives a coordinate-free description of the *superspace* V. In this context, the group $\mathcal{G}$ defined by the cohomology class $\{\Phi\} \in H^1(G, \hat{L}) \cong H^2(G, \mathcal{T})$ is often called a superspace group, but this paper uses the term *space group*.

It is not needed in this paper, but one often considers $\mathcal{G}$ as a crystallographic group of isometries of V. In order to do so, one must define a Euclidean inner product on V, a point neglected in [27]. Since L spans $\mathbb{R}^{d*}$, the inclusion $L \subseteq \mathbb{R}^{d*}$ leads to a natural inclusion $\mathbb{R}^d \subseteq V$, compatible with the action of G. Take any positive-definite inner product on V that extends the standard one on $\mathbb{R}^d$, and average over G. This gives a G-invariant inner product on V that restricts to the usual one on $\mathbb{R}^d$, as required. Not all choices disappear during the averaging process: if one views the action of G on V as a group representation, each irreducible subrepresentation (outside $\mathbb{R}^d$) can be given an independent scale factor, and

isomorphic irreducible subrepresentations may or may not be orthogonal. Any such inner product on V leads to an orthogonal projection $V \to \mathbb{R}^d$, and the image of $\mathcal{T}$ under this projection will be a lattice.

Two other models of aperiodic quasicrystals start with a lattice $\mathcal{T} \subseteq V \cong \mathbb{R}^D$ and an embedding $\mathbb{R}^d \hookrightarrow V$ that meets $\mathcal{T}$ in at most one point. Taking $L = \mathrm{Hom}(\mathcal{T}, \mathbb{Z})$, one can think of these data in the terms described above. The 'cut-and-project' model takes a particular 'slice' $S \subset \mathcal{T}$ and a projection $p : V \to \mathbb{R}^d$; the set $p(S)$ is considered a quasicrystal. The other model takes a tiling of V, periodic with respect to $\mathcal{T}$, and intersects this tiling with $\mathbb{R}^d$. In this variant, the set of vertices of the resulting tiling of $\mathbb{R}^d$ is the model of a quasicrystal. In either case, a suitably general theory of the Fourier transform (see [37] or [38]) applied to the sum of delta functions at points of the quasicrystal leads to a set of Fourier coefficients $\hat{\rho}(k)$ for $k \in L$. The series $\sum_k |\hat{\rho}(k)|$ need not converge, so the results of this section do not apply, but the hypothesis of absolute convergence is not used in the rest of this paper.

3. Classification

The terminology in this section mostly follows [27]. In section 1, a symmetry type was defined to be a triple $(G, L, \{\Phi\})$, where G is a finite subgroup of the orthogonal group $\mathrm{O}(d)$, L is a lattice in $\mathbb{R}^{d*}$ symmetric under G and $\{\Phi\}$ is a cohomology class in $H^1(G, \hat{L})$. A symmetry type corresponds to a space group, although the (algebraic structure of the) space group determines only the algebraic structure of the lattice, not its embedding in $\mathbb{R}^{d*}$. This section defines when two symmetry types should be considered equivalent and describes a programme for classifying them. Since equivalent symmetry types have isomorphic space groups, we usually talk of classifying space groups.

Definition 3.1. *Two pairs (G_1, L_1) and (G_2, L_2) are in the same arithmetic crystal class if there is a proper rotation $r \in \mathrm{SO}(d)$ and an isomorphism $f : L_1 \to L_2$ as Abelian groups such that $G_2 = rG_1r^{-1}$ and $f(kg) = f(k)\, rgr^{-1}$ for all $k \in L_1$ and $g \in G_1$.*

Consider first the case $f(k) = kr^{-1}$. Requiring $r \in \mathrm{SO}(d)$ means that, in the case $d = 2$, mirror-image lattices are not necessarily in the same arithmetic crystal class [25]. Next suppose that r is the identity. Since f is not required to extend to a continuous map on $\mathbb{R}^{d*}$, this allows for continuous families of lattices all in the same arithmetic crystal class (see note 8 in [27]).

Definition 3.2. *Two symmetry types $(G_1, L_1, \{\Phi_1\})$ and $(G_2, L_2, \{\Phi_2\})$ are in the same space-group type if (G_1, L_1) and (G_2, L_2) are in the same arithmetic crystal class and it is possible to choose r and f as in definition 3.1 in such a way that $\{\Phi_2\} = \{f \circ \Phi_1 \circ c_r\} \in H^1(G_2, \widehat{L_2})$, where $c_r : G_2 \to G_1$ is the conjugation map $c_r(g) = r^{-1}gr$.*

One possibility, which does not occur with discrete lattices, is that $G_1 = G_2$, $L_1 = L_2$, and f is a non-trivial dilation. For example, identifying the complex plane with $\mathbb{R}^{2*}$, let $\zeta = \mathrm{e}^{2\pi \mathrm{i}/5}$ and $L = \mathbb{Z}[\zeta]$. Then $f(x) = (\zeta + \zeta^{-1})x$ gives an isomorphism of L onto itself, and $\zeta + \zeta^{-1} = (\sqrt{5} - 1)/2$ is a real number between 0 and 1. The identification of the symmetry types described by Φ and $f \circ \Phi$ is sometimes called *scale invariance* [8].

One of the main goals of crystallography is to classify the possible space-group types. This paper considers only the case where G is finite; see [29] for examples and further discussion of lattices with infinite holohedry groups. We propose the following classification programme:

(1) Find all finite groups $G \subseteq \mathrm{O}(d)$, up to conjugation by $\mathrm{SO}(d)$.
(2) For each point group G, classify the lattices L that are stable under G.

(3) Calculate the cohomology group $H^1(G, \hat{L})$.
(4) Consider the action of automorphisms of the pair (G, L) on this cohomology group. That is, consider f and r as above in the case $G_1 = G_2 = G$ and $L_1 = L_2 = L$.

The first step is well known in dimensions 2 and 3. If $d = 2$, such a group is either cyclic or dihedral; in the latter case, one can take the x-axis as one of the mirror lines. If $d = 3$, see, for example, (39, appendices A and B). In two dimensions, step 2 can be done using ideas from integer representation theory, especially the theory of twisted group algebras: see [28, section 28] and [40]. The authors are working on a paper that explains these ideas in simpler terms. The results of the current paper are useful for the third step. Sections 6 and 7 compute $H^1(G, \hat{L})$ in the case $d = 2$. The authors hope to study the case $d = 3$ in future work. The final step of the classification is actually quite controversial; perhaps it is safest to say that, for some applications, it is appropriate to identify the cohomology class of Φ with that of $f \circ \Phi \circ c_r$. In any event, this step will depend on the solution of step 2.

We summarize this approach to classification with the phrase, 'G first, then L'. We feel this is appropriate in the Fourier-space approach to quasicrystals, since the symmetry of an x-ray diffraction pattern is more apparent than the rank of the lattice. (The diffraction pattern may have more symmetries than the point group.) Perhaps more significantly, arbitrary lattices are much more varied than discrete lattices, so it is helpful to impose some order by first specifying the point group, as in the first step of the classification programme. For these reasons, definition 3.1 differs from the definition in [27]: Dräger and Mermin say that two quasicrystals are in the same arithmetic crystal class only if the holohedry groups G_{L_1} and G_{L_2} as well as the point groups G_1 and G_2 are related by the proper rotation r in definition 3.1 (although note 8 in [27] partially contradicts this). In a sense, the 'G first' approach is not really new: several papers, such as [7], assume that the lattice L has minimal rank consistent with its rotational symmetry, which is very natural from this point of view.

Sometimes the 'G first' approach requires very minor adjustments. For example, [7, 9] discuss the two-dimensional lattice L of equilateral triangles, symmetric under a six-fold rotation. Fixing the lattice, there are two distinct copies of the dihedral group D_3 (or $3m$ in international crystallographic notation) inside the holohedry group G_L: one contains mirror lines through the shortest vectors, and the other contains mirror lines between the shortest vectors. In the 'G first' approach, one instead fixes the dihedral group D_3 containing the reflection in the x-axis. There are then two types of lattice, one with its shortest vectors along the mirror lines and one with its shortest vectors between the mirror lines. Evidently, these are two different ways of describing the same situation.

A more significant difference between the two approaches emerges when considering the square lattice. Here, if the lattice is fixed, then there is only one dihedral group D_4, with mirror lines both through and between the shortest vectors. However, if the group is fixed, and one of the mirror lines is identified with the x-axis, then there are two square lattices to consider: one with a shortest vector along the x-axis and one with shortest vector along the 45° line. In our classification programme, these two lattices are considered distinct until the final step. This distinction is essential when classifying lattices of non-minimal rank, as discussed in [26]. Similar remarks apply when considering D_N where N is any higher power of 2.

4. Higher cohomology is torsion

In this section, assume that G is a finite group acting on the right on a free Abelian group L of finite rank. Let

$$N = \#G. \tag{4.1}$$

A standard theorem ([32, section VI.5] or [33, section 6, corollary 2]) states that the Tate cohomology groups $\hat{H}^i(G, M)$ are torsion, killed by N. In particular, the homology group $H_1(G, M) = \hat{H}^{-2}(G, M)$ and the cohomology group $H^1(G, M) = \hat{H}^1(G, M)$ are killed by N. In the crystallographic literature so far, the following consequence has been noted only in the cases where the cohomology group has been explicitly calculated [7, 9, 10]. Give the Pontrjagin dual $\hat{L} = \mathrm{Hom}(L, \mathbb{R}/\mathbb{Z})$ the standard left G-action, $(g\chi)(k) = \chi(kg)$.

Proposition 4.1. *Given a cohomology class in $H^1(G, \hat{L})$, one can choose a representative cocycle Φ so that*

$$\Phi_g(k) \in \left(\frac{1}{N}\mathbb{Z}\right)\Big/\mathbb{Z} \qquad (g \in G, k \in L).$$

That is, with a suitable choice of gauge, any phase function takes values in $\left(\frac{1}{N}\mathbb{Z}\right)/\mathbb{Z}$.

Proof. Since the cohomology class of Φ is killed by N, $N\Phi$ is a coboundary. In other words, there is a $\chi \in \hat{L}$ such that $N\Phi = d\chi$, where d is the coboundary operator. Since $\hat{L} \cong (\mathbb{R}/\mathbb{Z})^{\mathrm{rank}(L)}$, one can choose $\chi_1 \in \hat{L}$ such that $N\chi_1 = \chi$. Let $\Phi^{(1)} = \Phi - d\chi_1$. Then $\Phi^{(1)}$ is in the same cohomology class as Φ, and $N\Phi^{(1)} = N\Phi - d\chi = 0$. In terms of $g \in G$ and $k \in L$, this means that $N\Phi_g^{(1)}(k) = 0 \in \mathbb{R}/\mathbb{Z}$, or $\Phi_g^{(1)}(k) \in \left(\frac{1}{N}\mathbb{Z}\right)/\mathbb{Z}$. □

Notation 4.2. If A is any Abelian group, denote the dual of A by

$$A' = \mathrm{Hom}(A, \mathbb{Q}/\mathbb{Z}).$$

If A is a right G-module, then give A' the standard left G-module structure: for $g \in G$, $\phi \in A'$ and any $a \in A$, $g\phi$ is defined by $(g\phi)(a) = \phi(ag)$. If A is a left G-module, then $g\phi$ is defined by $(g\phi)(a) = \phi(g^{-1}a)$, or $(g\phi)(ga) = \phi(a)$.

Proposition 4.3. *There is a natural isomorphism $H^1(G, L') \xrightarrow{\sim} H^1(G, \hat{L})$.*

Proof. Since L is a finitely generated free Abelian group, the short exact sequence $0 \to \mathbb{Q}/\mathbb{Z} \to \mathbb{R}/\mathbb{Z} \to \mathbb{R}/\mathbb{Q} \to 0$ leads to the short exact sequence

$$0 \to L' \to \hat{L} \to \mathrm{Hom}(L, \mathbb{R}/\mathbb{Q}) \to 0, \tag{4.2}$$

and $\mathrm{Hom}(L, \mathbb{R}/\mathbb{Q}) \cong (\mathbb{R}/\mathbb{Q})^r$, with $r = \mathrm{rank}(L)$. Since $\mathbb{R}/\mathbb{Q}$ is uniquely divisible, its Tate cohomology groups vanish, so the long exact sequence of Tate cohomology gives

$$0 = \hat{H}^0(G, \mathrm{Hom}(L, \mathbb{R}/\mathbb{Q})) \to H^1(G, L') \to H^1(G, \hat{L}) \to 0. \tag{4.3}$$

□

We need this proposition to apply the duality theorem we quote in section 5, which is stated in terms of L'. Note that surjectivity in proposition 4.3, but not injectivity, also follows from proposition 4.1.

Remark 4.4. If ρ_1 and ρ_2 are indistinguishable quasicrystals, then definition 1.3 requires $\hat{\rho}_2(k) = \mathrm{e}^{2\pi\mathrm{i}\chi(k)}\hat{\rho}_1(k)$, where $\chi \in \hat{L}$. This implies that $\chi(k) \in \mathbb{R}/\mathbb{Z}$, so that $|\hat{\rho}_1(k)| = |\hat{\rho}_2(k)|$. If one were to relax this condition, one would take $\chi : L \to \mathbb{C}/\mathbb{Z}$, so that $\mathrm{e}^{2\pi\mathrm{i}\chi(k)}$ could be any non-zero complex number. Making the corresponding change in definition 1.4, one would consider cohomology with coefficients in $\mathrm{Hom}(L, \mathbb{C}/\mathbb{Z})$ instead of $\hat{L}$. The analogues of propositions 4.1 and 4.3 would still hold, so $H^1(G, \mathrm{Hom}(L, \mathbb{C}/\mathbb{Z})) \cong H^1(G, \hat{L})$. In other words, the alternative definition of indistinguishability does not lead to any new symmetry types, and a quasicrystal $\hat{\rho}_1$ with point group G under the alternative definition is indistinguishable (in the alternative sense) from a quasicrystal $\hat{\rho}_2$ that has point group G using either definition.

5. Cohomology is dual to homology

In this section, assume that G is a finite group acting on the right on a finitely generated Abelian group L. In particular, this implies that $H_1(G, L)$ is finite.

In section 1, we observed that any gauge invariant $f : H^1(G, \hat{L}) \to \mathbb{C}$ can be expressed in terms of the fundamental gauge invariants, the homomorphisms $H^1(G, \hat{L}) \to \mathbb{Q}/\mathbb{Z}$. According to proposition 4.3, the set of fundamental gauge invariants is $H^1(G, L')'$ (cf notation 4.2). We now interpret this set as a homology group. If M is a right G-module then write 1-chains, or elements of $M \otimes \mathbb{Z}G$, as $c = \sum_g m_g[g]$, where $g \in G$ and $m_g \in M$. The boundary map is defined by

$$\partial(m[g]) = mg - m. \tag{5.1}$$

For details, see [32, section III.1] or [33, section 3].

Theorem 5.1. *Let G be a finite group, and let L be a finitely generated Abelian group on which G acts. Let $\hat{L}$, $H_1(G, L)^\wedge$ and $H^1(G, \hat{L})^\wedge$ denote the Pontrjagin duals as in (1.1). There are natural isomorphisms $H_1(G, L) \xrightarrow{\sim} H^1(G, \hat{L})^\wedge$ and $H^1(G, \hat{L}) \xrightarrow{\sim} H_1(G, L)^\wedge$, induced by the duality pairing*

$$\begin{aligned} H^1(G, \hat{L}) \times H_1(G, L) &\to \mathbb{R}/\mathbb{Z} \\ (\{\Phi\}, \{c\}) &\mapsto \langle \Phi, c\rangle = \sum_{g \in G} \Phi_g(k_g), \end{aligned} \tag{5.2}$$

where $c = \sum_g k_g[g]$.

Proof. According to proposition 4.3, the natural map from $H^1(G, L')$ to $H^1(G, \hat{L})$ is an isomorphism, where $L' = \mathrm{Hom}(L, \mathbb{Q}/\mathbb{Z})$ as in notation 4.2. The finiteness hypotheses on G and L imply that $H_1(G, L)$ is a finite group. It follows that the pairing in the theorem takes values in $\mathbb{Q}/\mathbb{Z}$ and that $H_1(G, L)^\wedge = H_1(G, L)'$. Roughly speaking, the finiteness hypotheses imply that one can replace $\mathbb{R}/\mathbb{Z}$ with $\mathbb{Q}/\mathbb{Z}$ throughout.

According to (32 proposition VI.7.1), there is a duality pairing between $H^1(G, L')$ and $H_1(G, L)$ that identifies each with the dual of the other (in the sense of notation 4.2). Up to a sign, this pairing agrees with that in the statement of the theorem by [32, section V.3] and [32, section III.1, example 3]. In particular, this shows that $H^1(G, L')$ is a finite group, so $H^1(G, \hat{L})^\wedge = H^1(G, L')^\wedge = H^1(G, L')'$. Thus the duality of the theorem is just a restatement of the duality between $H^1(G, L')$ and $H_1(G, L)$. □

Corollary 5.2. *The gauge-equivalence class of the phase function Φ is determined by the gauge-invariant rational numbers $\langle \Phi, c\rangle$ for $c \in H_1(G, L)$.*

Proof. This is simply a restatement of the injectivity of the map $H^1(G, \hat{L}) \to H_1(G, L)^\wedge$. □

Remark 5.3. As noted in section 2, the view from superspace is that the class $\{\Phi\}$ in $H^1(G, \hat{L}) \cong H^2(G, \mathcal{T})$ describes the space group $\mathcal{G}$, an extension of G by $\mathcal{T} = \mathrm{Hom}(L, \mathbb{Z})$. Recall that $\hat{L} \cong V/\mathcal{T}$, where V denotes the superspace $V = \mathcal{T} \otimes \mathbb{R}$. As described in [23], $\Phi_g \in V/\mathcal{T}$ is the coset of $\mathcal{T}$ consisting of all translations that can be combined with g to give an element of the space group $\mathcal{G}$. Theorem 5.1 still applies, so $H^1(G, V/\mathcal{T})$ is dual to $H_1(G, L) = H_1(G, \mathrm{Hom}(\mathcal{T}, \mathbb{Z}))$.

Let us make this duality pairing explicit. Let $c = \sum_g k_g[g]$ be a cycle, with coefficients $k_g \in \mathrm{Hom}(\mathcal{T}, \mathbb{Z})$, and let Φ be a cocycle as above. Choose a basis $t_1, \ldots, t_n$ of $\mathcal{T}$ over $\mathbb{Z}$; it is also an $\mathbb{R}$-basis of V. If $v = v_1 t_1 + \cdots + v_n t_n \in V$ and $k \in \mathrm{Hom}(\mathcal{T}, \mathbb{Z})$, define

$\langle v, k\rangle = v_1 k(t_1) + \cdots + v_n k(t_n) \in \mathbb{R}$. Similarly, define $\langle \bar{v}, k\rangle \in \mathbb{R}/\mathbb{Z}$ if $\bar{v} \in V/\mathcal{T}$. Then the duality pairing is defined by $\langle \Phi, c\rangle = \sum_g \langle \Phi_g, k_g\rangle$.

Remark 5.4. The simplest example of a 1-chain is $c = k[g]$, with $k \in L$ and $g \in G$. By (5.1), this chain is a cycle if and only if $kg = k$, and in this case the corresponding gauge invariant is simply $\Phi_g(k)$. However, the homology group $H_1(G, L)$ is not always generated by cycles of this form. In other words, it is possible for two gauge-inequivalent cocycles $\Phi^{(1)}$ and $\Phi^{(2)}$ to have the same 'obvious' gauge invariants: $\Phi^{(1)}_g(k) = \Phi^{(2)}_g(k)$ whenever $kg = k$. In fact, of the 230 classical space groups, there are two non-symmorphic ones, denoted by $I2_12_12_1$ and $I2_13$ in international crystallographic notation, for which all cycles of the form $c = k[g]$ are boundaries [10, 15]. Since these space groups are non-symmorphic, theorem 5.1 shows that $H_1(G, L) \neq 0$, so there must be other cycles. What is the next simplest cycle one can construct? Since $H_1(G, L)$ is killed by $N = \#G$, any cycle becomes trivial in $H_1\big(G, \frac{1}{N}L\big)$, so it is natural to consider the boundary of a 2-chain with values in $\frac{1}{N}L$: if the result happens to have coefficients in L, it is a 1-cycle in $H_1(G, L)$. In the notation of [32, section III.1, example 3], the boundary of the 2-chain $q[g|h]$ (where $q \in \frac{1}{N}L$ and $g, h \in G$) is given by

$$\partial(q[g|h]) = (qg)[h] - q[gh] + q[g]. \tag{5.3}$$

This cannot give a non-trivial homology class in $H_1(G, L)$ by itself. Perhaps the simplest combination that can is

$$\partial(q[g|h] - q[h|g]) = (qg - q)[h] - q([gh] - [hg]) + (q - qh)[g], \tag{5.4}$$

which will have values in $L \otimes \mathbb{Z}G$ provided that $qg - q$, $qh - q \in L$ and $gh = hg$. It is a simple exercise to calculate the homology groups corresponding to the two exceptional space groups $I2_12_12_1$ and $I2_13$. (See [17] for one of the two cases.) In both cases, the homology group is cyclic of order 2, generated by the class of such a cycle.

Gauge invariants are considered again in section 8. We conclude this section with a new proof of the result in the appendix of [16]. This states that if the 'obvious' gauge invariants of Φ corresponding to a single $g \in G$ vanish, then (up to gauge equivalence) Φ_g is trivial. The examples cited above show that one cannot necessarily find a gauge in which $\Phi_g = 0$ simultaneously for all $g \in G$, even if all these gauge invariants vanish.

Proposition 5.5. *Let $g \in G$, and let $\{\Phi\} \in H^1(G, \hat{L})$. If one choice of Φ satisfies $\Phi_g = 0$ on $L^g = \{k \in L \mid kg = k\}$, then one can choose Φ such that $\Phi_g(k) = 0$ for all $k \in L$.*

Proof. Let $\langle g\rangle = \{1, g, \ldots, g^{N-1}\}$ denote the subgroup of G generated by g. We claim that Φ is trivial in $H^1(\langle g\rangle, \hat{L})$. By corollary 5.2, it suffices to show that $\langle \Phi, c\rangle = 0$ for all $c \in H_1(\langle g\rangle, L)$. According to (6.5), $H_1(\langle g\rangle, L) = L^g/N_g L$, where $N_g = 1 + g + \cdots + g^{N-1}$. Therefore the hypothesis $\Phi_g(L^g) = 0$ justifies the claim.

Since Φ is trivial in $H^1(\langle g\rangle, \hat{L})$, there is some $\chi \in \hat{L}$ for which $\Phi_g = (d\chi)_g = g\chi - \chi$. Then $\Phi^{(1)} = \Phi - d\chi$ represents the same class in $H^1(G, \hat{L})$, and $\Phi^{(1)}_g = 0$. □

6. Homology and cohomology of cyclic groups

This section and the following one classify the space groups corresponding to the finite point group G and the lattice L in two dimensions. This section discusses cyclic groups, and the next deals with dihedral groups. The classification applies to 'non-standard' [25] as well as to 'standard' lattices and applies whether or not the rank of L is minimal given that L is symmetric under G. Work in progress [26] classifies the lattices of non-minimal rank symmetric under G.

Let G be a finite cyclic group, say

$$G = \langle r \rangle = \{1, r, \ldots, r^{N-1}\}. \tag{6.1}$$

(If G is a subgroup of O(2) or O(3), then the generating element r might be a rotation or, for $N = 2$, it might be a mirror.) If M is any left G-module, then think of $r - 1$ and the norm element

$$N_r = 1 + r + \cdots + r^{N-1} \tag{6.2}$$

in terms of their actions on M: $(r - 1)x = rx - x$ and $N_r x = x + rx + \cdots + r^{N-1}x$. According to [32, section III.1] or [33, section 8], the Tate cohomology groups can, in this case, be computed as the cohomology of the complex

$$\cdots \stackrel{N_r}{\to} M \stackrel{r-1}{\to} M \stackrel{N_r}{\to} M \stackrel{r-1}{\to} M \stackrel{N_r}{\to} \cdots. \tag{6.3}$$

In particular,

$$H^1(G, M) = \hat{H}^1(G, M) = \ker(N_r)/(r - 1)M; \tag{6.4}$$

$$H_1(G, M) = \hat{H}^{-2}(G, M) = \ker(r - 1)/N_r M. \tag{6.5}$$

Note that the kernel of $r - 1$ is $M^r = \{x \in M \mid rx = x\}$.

In traditional crystallography, this description of the (co)homology groups is of limited interest since a two- or three-dimensional rotation that stabilizes a discrete lattice can only have order 1, 2, 3, 4 or 6. Quasicrystals can be symmetric under rotations of any order, so these results become much more useful.

The following proposition shows that if a two-dimensional point group is cyclic (of order $N > 1$) then the only corresponding space group is the symmorphic one. Note that this analysis applies uniformly to any two-dimensional lattice. The case where $L \cong \mathbb{Z}[e^{2\pi i/N}]$ is treated in [7].

Proposition 6.1. *Let $L \subseteq \mathbb{R}^{2*}$ be a lattice invariant under $G = \langle r \rangle$, where r is a rotation of order $N > 1$. Then $H^1(G, \hat{L}) = 0$.*

Proof. It is easier to work with homology of L than the cohomology of $\hat{L}$, so consider $H_1(G, L)$. The only vector in $\mathbb{R}^{2*}$ fixed by a non-trivial rotation is the zero vector. According to (6.5), this shows that $H_1(G, L) = 0$. The result now follows from theorem 5.1. □

7. The restriction-inflation sequence

For this section, let G be a finite group, let $H \lhd G$ be a normal subgroup and let

$$Q = G/H \tag{7.1}$$

denote the quotient. For any left G-module M, the inflation map $H^1(Q, M^H) \to H^1(G, M)$ and the restriction map $H^1(G, M) \to H^1(H, M)$ fit together to give an exact sequence [33, section 5]

$$0 \to H^1(Q, M^H) \to H^1(G, M) \to H^1(H, M). \tag{7.2}$$

This can be viewed as a consequence of the Hochschild–Serre spectral sequence, as can its homological version [32, theorem VII.6.3]:

$$H_1(H, M) \to H_1(G, M) \to H_1(Q, M_H) \to 0, \tag{7.3}$$

where M is now a right G-module and M_H denotes the quotient of M by the H-submodule generated by $\{xh - x \mid x \in M, h \in H\}$.

Let $G \subseteq \mathrm{O}(3)$ be a finite group. By the classification of such groups (appendices A and B in [39]), there are several infinite families of such G and finitely many sporadic ones, which must be dealt with on a case-by-case basis. Letting G be in one of the infinite families, it contains a normal, cyclic subgroup H, generated by a rotation or a roto-inversion, for which the quotient group $Q = G/H$ has order 1, 2 or 4. Since H is cyclic, the homology group $H_1(H, L)$ can be computed using (6.5). In the simplest case, H is generated by a roto-inversion, so $H_1(H, L) = 0$, and $H_1(G, L) = H_1(Q, L_H)$ by (7.3). We now apply this approach to the two-dimensional case.

Notation 7.1. For the rest of this section, let $L \subseteq \mathbb{R}^{2*}$ be a lattice invariant under the dihedral group with $2N$ elements:

$$G = D_N = \langle r, m \rangle \subseteq \mathrm{O}(2), \tag{7.4}$$

where r is a rotation of order $N > 1$ and m is a reflection. Let

$$H = C_N = \langle r \rangle, \qquad D_1 = D_N/H = \{e, \tilde{m}\} \tag{7.5}$$

denote the cyclic subgroup of D_N and the quotient group. Let

$$\zeta = \zeta_N = \mathrm{e}^{2\pi \mathrm{i}/N}, \tag{7.6}$$

so that L is a module over the ring of cyclotomic integers $\mathbb{Z}[\zeta]$, and note that $L_H = L/(1-\zeta)L$. Let

$$\mathbb{F}_2 = \mathbb{Z}/2\mathbb{Z} \tag{7.7}$$

denote the field with two elements.

The results that follow show that $H^1(D_N, \hat{L}) = 0$, so every space group corresponding to D_N and L is symmorphic, unless N is a power of 2. If $N = 2^e$, then theorem 7.5 states that $H^1(D_N, \hat{L})$ is a vector space over the field with two elements and counts its dimension. In other words, still assuming $N = 2^e$, the fundamental invariants all take the values 0 and $1/2$ (modulo 1). In particular, if L has rank 1 as a $\mathbb{Z}[\zeta]$-module, then the cohomology group has exactly two elements: one corresponds to the symmorphic space group, and the other corresponds to a non-symmorphic group. These results were obtained in [7] under the more restrictive assumption that $L \cong \mathbb{Z}[\zeta]$ as a $\mathbb{Z}[\zeta]$-module.

Proposition 7.2. *If N is not a power of 2, then $H^1(D_N, \hat{L}) = 0$. If N is a power of 2, then L_H is a vector space over $\mathbb{F}_2$.*

Proof. By theorem 5.1, it suffices to compute $H_1(D_N, L)$. By proposition 6.1, $H_1(H, L) = 0$. Then (7.3) implies that $H_1(D_N, L) \xrightarrow{\sim} H_1(D_1, L_H)$. According to lemma 7.3, $1 - \zeta$ is a unit unless $N = p^e$ is a prime power, in which case its norm is p. Thus $L_H = 0$, and $H_1(D_N, L) = 0$, unless $N = p^e$.

Suppose now that $N = p^e$. Then L_H is a vector space over $\mathbb{Z}[\zeta]/(1 - \zeta) \cong \mathbb{F}_p$, the field with p elements. If $p = 2$, this justifies the last claim in the statement. Now assume that p is odd. Decompose L_H into eigenspaces for $\tilde{m}$: $L_H = {L_H}^+ \oplus {L_H}^-$. On ${L_H}^+$, $N_{\tilde{m}} = 1 + \tilde{m} = 2$, so $N_{\tilde{m}} {L_H}^+ = 2{L_H}^+ = {L_H}^+$ (since multiplication by 2 is an isomorphism on an $\mathbb{F}_p$-vector space when p is odd), and $H_1\big(D_1, {L_H}^+\big) = 0$ by (6.5). On the other hand, $({L_H}^-)^{\tilde{m}} = 0$, so $H_1(D_1, {L_H}^-) = 0$ as well. Therefore, $H_1(D_1, L_H) = H_1\big(D_1, {L_H}^+\big) \oplus H_1(D_1, {L_H}^-) = 0$. □

The following lemma is not original, but we do not know a convenient reference for it.

Lemma 7.3. *Let $N > 1$, $\zeta = \zeta_N = e^{2\pi i/N}$, and let $N_{\mathbb{Q}(\zeta)}$ denote the norm from $\mathbb{Q}(\zeta)$ to $\mathbb{Q}$. If $N = p^e$ is a prime power, then $N_{\mathbb{Q}(\zeta)}(1-\zeta) = p$; otherwise, $N_{\mathbb{Q}(\zeta)}(1-\zeta) = 1$.*

Proof. Let $F_N(x)$ denote the cyclotomic polynomial of order N. That is, $F_N(x)$ is the monic, irreducible polynomial whose roots are the primitive Nth roots of unity[5]. Since these are exactly the conjugates of ζ over $\mathbb{Q}$, it follows that

$$F_N(1) = \prod_{F_N(\alpha)=0} (1-\alpha) = N_{\mathbb{Q}(\zeta)}(1-\zeta).$$

Since the roots of $x^N - 1$ are all the Nth roots of unity, $x^N - 1 = \prod_{d|N} F_d(x)$. Dividing by $x - 1$ and setting $x = 1$ leads to $N = \prod_{1<d|N} F_d(1)$. The lemma now follows by induction on N. □

Notation 7.4. Let M be an $n \times n$ matrix over $\mathbb{F}_2$ such that $M^2 = I_n$. The Jordan normal form of M consists of 1×1 and 2×2 blocks only, with the number 1 the only possible eigenvalue. For example, the Jordan normal form of the standard 2×2 reflection matrix $\left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right]$ is $\left[\begin{smallmatrix} 1 & 0 \\ 1 & 1 \end{smallmatrix}\right]$. Let $j_1(M)$ denote the number of 1×1 Jordan blocks and $j_2(M)$ denote the number of (defective) 2×2 Jordan blocks in the Jordan normal form of M. Then $j_1(M) + 2j_2(M) = n$, and $j_1(M) + j_2(M) = n - j_2(M)$ is the dimension of the 1-eigenspace of M.

Theorem 7.5. *Let $L \subseteq \mathbb{R}^{2*}$ be a lattice invariant under $G = C_N$ or D_N. Then $H^1(G, \hat{L}) = 0$ unless $G = D_N$ and $N = 2^e$, with $e \geqslant 1$. In this case, let M be the matrix of $\tilde{m}$ acting on the $\mathbb{F}_2$-vector space L_H. Then $H^1(D_N, \hat{L})$ is an $\mathbb{F}_2$-vector space of dimension $j_1(M)$.*

Proof. The case $G = C_N$ is considered in proposition 6.1, so assume that $G = D_N$. Proposition 7.2 shows that the cohomology group vanishes if N is not a power of 2, so assume now that $N = 2^e$. By theorem 5.1, $H^1(D_N, \hat{L})$ is dual to $H_1(D_N, L)$, so it suffices to show that this homology group has the stated form. By proposition 6.1 and the exact sequence (7.3), $H_1(D_N, L) \cong H_1(D_1, L_H)$.

Since $D_1 = \{e, \tilde{m}\}$, it follows from (6.5) that $H_1(D_1, L_H) \cong (L_H)^{\tilde{m}}/(1+\tilde{m})L_H$. Note that, although m is antilinear, $\tilde{m}$ is linear as a map on L_H, so notation 7.4 applies. An easy calculation shows that each 1×1 Jordan block contributes a one-dimensional space to $H_1(D_1, L_H)$ and that each 2×2 Jordan block contributes nothing. □

Remark 7.6. Piunikhin [18] recognized the cohomological interpretation of phase functions and noted that $H^1(G, \hat{L})$ describes an extension $1 \to \mathrm{Hom}(L, \mathbb{Z}) \to \mathcal{G} \to G \to 1$. Piunikhin implicitly assumes that $\mathrm{Hom}(L, \mathbb{Z})$ is a lattice if L is. We do not see a natural way to regard $\mathrm{Hom}(L, \mathbb{Z})$ as a lattice, but as we described in section 2 there are many ways to do so, all in the same arithmetic crystal class. Given this, $\mathcal{G}$ is a quasicrystallographic group in the sense of Novikov', and Piunikhin's classification [41] of such groups (with finite point group G) in two dimensions answers the same question as theorem 7.5 here. Our proof is different, and the description here of the dimension of $H^1(G, \hat{L})$ is simpler than Piunikhin's: he describes the classification in terms of an anti-linear involution on L, while theorem 7.5 uses linear algebra over $\mathbb{F}_2$.

This is a good place to point out a misstatement in [41]. Let T denote a lattice in $\mathbb{R}^2$, invariant under D_N with N even. Then T can be thought of as a $\mathbb{Z}[\zeta]$-module. Let I denote the anti-linear involution of T corresponding to a mirror reflection $m \in D_N$. Piunikhin describes the correspondence between isomorphism classes of such pairs (T, I) and arithmetic crystal classes of such lattices as being 2-to-1, since (T, I) and $(T, \zeta I)$ are not isomorphic as

[5] The usual notation for this polynomial is $\Phi_N(x)$. In this paper, Φ is used to denote a phase function.

modules with involution. This is not true in general: for example, consider $T = \mathbb{Z}[\zeta_{2N}]$ as a $\mathbb{Z}[\zeta]$-module, and let I be complex conjugation.

8. Cohomology products and physical implications

This section uses the notation and hypotheses of sections 1 and 2. For physical applications, work in dimension $d = 3$. In particular, G is a finite subgroup of the orthogonal group O(3), $\hat{\rho}$ is a quasicrystal on the lattice $L \subseteq \mathbb{R}^{3*}$ and Φ is the corresponding phase function, or cocycle, representing a cohomology class in $H^1(G, \hat{L})$. So far, we have considered only geometric aspects of crystallography. This section discusses some physical implications. We show that the language of group cohomology, especially the cup and cap products, provides a convenient framework for making connections between phase functions and group representations.

Given a map $M \otimes_{\mathbb{Z}} N \to P$ of G-modules, one constructs the cup product

$$H^m(G, M) \times H^n(G, N) \xrightarrow{\cup} H^{m+n}(G, P) \tag{8.1}$$

and, if $m \leqslant n$, the cap product

$$H^m(G, M) \times H_n(G, N) \xrightarrow{\cap} H_{n-m}(G, P) \tag{8.2}$$

as in [32, section V.3] or [33, section 7]. If $m = n$ and $M = N'$, then (up to a sign) the cap product is the same as the duality pairing of section 5, with $H_0(G, P) = H_0(G, \mathbb{Q}/\mathbb{Z}) = \mathbb{Q}/\mathbb{Z}$. Among the various properties enjoyed by these two products are two associative laws: $(\alpha \cup \beta) \cup \gamma = \alpha \cup (\beta \cup \gamma)$ and $(\alpha \cup \beta) \cap c = \alpha \cap (\beta \cap c)$ if $\alpha, \beta, \gamma \in H^*$, $c \in H_*$ and the coefficients are chosen compatibly.

Recall from sections 1 and 5 that elements of $H^1(G, \hat{L})$ describe symmetry types of quasicrystals and that $H_1(G, L)$ is the set of fundamental gauge invariants. These are related to several other (co)homology groups by the cup and cap products, and these groups also have important interpretations.

Consider $H^1(G, L)$. If $q \in \mathbb{R}^{3*}$ satisfies $qg - q \in L$ for all $g \in G$, then $\sigma(g) = qg^{-1} - q$ is a cocycle with values in L. From the long exact sequence [32, proposition 0.4] or [33, theorem 1] associated to $0 \to L \to \mathbb{R}^{3*} \to \mathbb{R}^{3*}/L \to 0$, it follows that any class in $H^1(G, L)$ is represented by such a cocycle.

Next, recall the interpretation of the cohomology group $H^2(G, \mathbb{Q}/\mathbb{Z})$. A *projective representation*, or *ray representation*, of G is a homomorphism into the projective linear group PGL(n), just as an ordinary representation is a homomorphism into the general linear group GL(n). One associates to each projective representation a 2-cocycle, or *factor system*, with values in $\mathbb{C}^\times$; the factor system depends on additional choices, but its cohomology class in the *Schur multiplier* $H^2(G, \mathbb{C}^\times)$ depends only on the representation. One standard reference is [28, section 11.E]. In fact, this theory is one of the main precursors of group cohomology. Since G is a finite group, the exponential map $\mathbb{Q}/\mathbb{Z} \to \mathbb{C}^\times$ gives an isomorphism $H^2(G, \mathbb{Q}/\mathbb{Z}) \xrightarrow{\sim} H^2(G, \mathbb{C}^\times)$ (cf section 4). The same duality theorem (32, proposition VI.7.1) cited in the proof of theorem 5.1 shows that $H_2(G, \mathbb{Z})$ is dual to $H^2(G, \mathbb{Q}/\mathbb{Z})$, so 2-cycles with integer coefficients can be thought of as invariants of factor systems.

We are now ready to discuss physical applications. Let $\Phi \in H^1(G, \hat{L})$ be non-trivial, so that it represents a non-symmorphic space group. By theorem 5.1, there is some $c \in H_1(G, L)$ such that $\langle \Phi, c \rangle \neq 0$. It is reasonable to hope that there is a physical way to distinguish a non-symmorphic quasicrystal from a symmorphic one, so one expects such a non-trivial gauge invariant to have physical implications. If c is represented by a cycle of the form $k[g]$ (with $k \in L$, $g \in G$ and $kg = k$), then this is well known. If $\hat{\rho} : L \to \mathbb{R}$ is any function transforming

as in (1.3) and $\Phi_g(k) = \langle \Phi, k[g] \rangle \neq 0$, then $\hat{\rho}(k) = 0$. This is observed as a dark spot in the x-ray-diffraction pattern and is called a *systematic extinction*.

Not every gauge invariant is of the above form. Suppose that $g, h \in G$ and $q \in \mathbb{R}^{3*}$ satisfy

(i) $gh = hg$;
(ii) $k_g = qg - q, k_h = qh - q \in L$;
(iii) $\Phi_g(k_h) - \Phi_h(k_g) \neq 0$.

Then $k_g[h] - k_h[g]$ represents a non-trivial homology class; cf (5.4). In this situation König and Mermin [15] describe a projective representation of $H = \langle g, h \rangle \subseteq G$ that commutes with the Hamiltonian h_q corresponding to the wave vector q and the potential of the crystal. Therefore, every eigenspace of the Hamiltonian is a projective subrepresentation, with the same factor system: $(g, h) \mapsto \Phi_h(qg - q)$. König and Mermin note that the quantity (iii) is gauge invariant and, since it does not vanish, this shows that the projective representation (on each eigenspace) is not equivalent to an ordinary representation. In particular, each eigenspace of the Hamiltonian has dimension greater than 1, since one-dimensional projective representations have trivial factor systems. This is expressed by saying that each energy level of h_q is degenerate, and the phenomenon is sometimes called *band sticking*.

We interpret part of this argument as follows. Let $H = \langle g, h \rangle$. Then (i) implies that $c = [g|h] - [h|g]$ is a 2-cycle with coefficients in $\mathbb{Z}$ (cf (5.4) and [32, section II.3, exercise 1]). Condition (ii) implies that $\sigma(g) = k_{g^{-1}} = qg^{-1} - q$ represents a class in $H^1(H, L)$, so $\sigma \cap c = k_g[h] - k_h[g]$ represents a class in $H_1(G, L)$. Thus (iii) means that $\langle \Phi, \sigma \cap c \rangle \neq 0$. Since $\Phi \cup \sigma$ is the 2-cocycle $(g, h) \mapsto \Phi_h(k_g)$, the following proposition applies.

Proposition 8.1. *Let H be a finite subgroup of* O(3) *and let $L \subseteq \mathbb{R}^{3*}$ be a lattice stable under H. Let $c \in H_2(H, \mathbb{Z})$, $\sigma \in H^1(H, L)$ and $\Phi \in H^1(H, \hat{L})$ be given. Then*

$$\langle \Phi, \sigma \cap c \rangle = \langle \Phi \cup \sigma, c \rangle.$$

In particular, if this quantity is non-zero, then Φ represents a non-symmorphic space group, and the factor system $\Phi \cup \sigma$ is non-trivial.

Proof. This follows from associativity of cup and cap products, as described above, and from the compatibility $\langle \alpha, \beta \rangle = -\alpha \cap \beta$ between the duality pairing and the cap product. □

Computations of $H_1(G, L)$ using the methods described in section 7 suggest that this homology group is usually generated by cycles of the form $\sigma \cap c$ as described in the proposition and those of the form $k[g]$ with $kg = k$. The hypotheses of the proposition are thus less restrictive than they seem at first glance. There are, however, examples where $H_1(G, L)$ is not generated by such cycles. It is not clear what, if any, physical consequences there are in such cases. The authors hope to return to both these points in future papers.

Acknowledgments

This work has been supported in part by the National Science Foundation through grants DMS-0204823 and DMS-0204845. DAR is a Cottrell Scholar of Research Corporation and is grateful to the Boston College mathematics department, whose hospitality in the summer of 2000 made this collaboration possible. Both authors sincerely thank the referee of a previous version of this paper, who provided several important references as well as making many suggestions for improvement.

References

[1] Penrose R 1979–80 Pentaplexity: a class of nonperiodic tilings of the plane *Math. Intelligencer* **2** 32–7

[2] Shechtman D, Blech I, Gratias D and Cahn J 1984 Metallic phase with long-range orientational order and no translational symmetry *Phys. Rev. Lett.* **53** 1951–3

[3] Janot C 1994 *Quasicrystals: A Primer* 2nd edn (Singapore: Clarendon)

[4] DiVincenzo D P and Steinhardt P J (ed) 1999 *Quasicrystals: The State of the Art* 2nd edn (River Edge, NJ: World Scientific)

[5] de Wolff P M, Janssen T and Janner A 1981 The superspace groups for incommensurate crystal structures with a one-dimensional modulation *Acta Crystallogr.* A **37** 625–36

[6] Bienenstock A and Ewald P P 1962 Symmetry of Fourier space *Acta Crystallogr.* **15** 1253–61

[7] Rokhsar D S, Wright D C and Mermin N D 1988 The two-dimensional quasicrystallographic space groups with rotational symmetries less than 23-fold *Acta Crystallogr.* A **44** 197–211

[8] Rokhsar D S, Wright D C and Mermin N D 1988 Scale equivalence of quasicrystallographic space groups *Phys. Rev.* B **37** 8145–9

[9] Rabson D A, Mermin N D, Rokhsar D S and Wright D C 1991 The space groups of axial crystals and quasicrystals *Rev. Mod. Phys.* **63** 699–733

[10] Mermin N D 1992 The space groups of icosahedral quasicrystals and cubic, orthorhombic, monoclinic, and triclinic crystals *Rev. Mod. Phys.* **64** 3–49

[11] Mermin N D and Lifshitz R 1992 Bravais classes for the simplest incommensurate crystal phases *Acta Crystallogr.* A **48** 515–32

[12] Lifshitz R and Mermin N D 1994 Bravais classes and space groups for trigonal and hexagonal quasiperiodic crystals of arbitrary finite rank *Acta Crystallogr.* A **50** 85–97

[13] Lifshitz R and Mermin N D 1994 Space groups of trigonal and hexagonal quasiperiodic crystals of rank 4 *Acta Crystallogr.* A **50** 72–85

[14] Lifshitz R 1997 Theory of color symmetry for periodic and quasiperiodic crystals *Rev. Mod. Phys.* **69** 1181–218

[15] König A and Mermin N D 1997 Electronic level degeneracy in nonsymmorphic periodic or aperiodic crystals *Phys. Rev.* B **56** 13607–10

[16] König A and Mermin N D 1999 Screw rotations and glide mirrors: crystallography in Fourier space *Proc. Natl. Acad. Sci. USA* **96** 3502–6

[17] Rabson D A and Fisher B N 2002 Fourier-space crystallography as group cohomology *Phys. Rev.* B **65** 024201

[18] Piunikhin S A 1992 The relationship between various definitions of quasicrystallographic groups *Mat. Zametki* **52** 74–80, 159
Piunikhin S A 1992–1993 *Math. Notes* **52** 1220–4 (Engl. Transl.) MR 94f:20095

[19] Ascher E and Janner A 1965 Algebraic aspects of crystallography. Space groups as extensions *Helv. Phys. Acta* **38** 551–72

[20] Ascher E and Janner A 1968–1969 Algebraic aspects of crystallography: II. Non-primitive translations in space groups *Commun. Math. Phys.* **11** 138–67

[21] Schwarzenberger R L E 1980 *n-dimensional crystallography* (Boston, MA: Pitman) (Advanced Publishing Program)

[22] Janssen T and Janner A 1984 Superspace groups and representations of ordinary space groups: alternative approaches to the symmetry of incommensurate crystal phases *Physica A* **126** 163–76

[23] Hiller H 1986 Crystallography and cohomology of groups *Am. Math. Monthly* **93** 765–79

[24] Rabson D A, Huesman J F and Fisher B N 2003 Cohomology for anyone *Foundations of Physics* **33** 1769–96

[25] Mermin N D, Rokhsar D S and Wright D C 1987 Beware of 46-fold symmetry: the classification of two-dimensional quasicrystallographic lattices *Phys. Rev. Lett.* **58** 2099–101

[26] Fisher B N and Rabson D A in preparation

[27] Dräger J and Mermin N D 1996 Superspace groups without the embedding: the link between superspace and Fourier-space crystallography *Phys. Rev. Lett.* **76** 1489–92

[28] Curtis C W and Reiner I 1981 *Methods of Representation Theory* vol I (New York: Wiley)

[29] Tkhang L T K, Piunikhin S A and Sadov V A 1993 The geometry of quasicrystals *Uspekhi Mat. Nauk* **48** 41–102 Translation in Russian Math. Surveys **48** (1993), no. 1, 37–100; MR 95a:52026

[30] Godrèche C and Luck J 1990 Multifractal analysis in reciprocal space and the nature of the Fourier transform of self-similar structures *J. Phys. A: Math. Gen.* **23** 3769–97

[31] Godrèche C and Luck J 1992 Indexing the diffraction spectrum of a non-pisot self-similar structure *Phys. Rev.* B **45** 176–85

[32] Brown K S 1982 Cohomology of Groups *Graduate Texts in Mathematics* vol 87 (New York: Springer)
[33] Atiyah M F and Wall C T C 1967 Cohomology of groups *Algebraic Number Theory* ed J W S Cassels and A Fröhlich (London: Academic) ch IV pp 94–127
[34] de Bruijn N G 1981 Algebraic theory of Penrose's nonperiodic tilings of the plane. I *Ned. Akad. Wetensch. Indag. Math.* **43** 39–52
[35] Hof A 1997 Diffraction by aperiodic structures *The Mathematics of Long-range Aperiodic Order (Waterloo, On, 1995)* (Dordrecht: Kluwer) pp 239–68
[36] Mermin N D 1992 Copernican crystallography *Phys. Rev. Lett.* **68** 1172–5
[37] de Bruijn N G 1986 Quasicrystals and their Fourier transform *Ned. Akad. Wetensch. Indag. Math.* **48** 123–52
[38] Hof A 1995 On diffraction by aperiodic structures *Commun. Math. Phys.* **169** 25–43
[39] Weyl H 1952 *Symmetry* (Princeton, NJ: Princeton University Press)
[40] Theohari-Apostolidi T 1985 On integral representations of twisted group rings *J. Algebra* **93** 413–7
[41] Piunikhin S A 1990 Quasicrystallographic groups in the sense of Novikov *Mat. Zametki* **47** 81–7, 159
Piunikhin S A 1990 *Math. Notes* **47** 478–82 (Engl. Transl.) MR 91h:20076