COHOMOLOGY FOR ANYONE†

DAVID A. RABSON, JOHN F. HUESMAN, AND BENJI N. FISHER

ABSTRACT. Crystallography has proven a rich source of ideas over several centuries. Among the many ways of looking at space groups, N. David Mermin has pioneered the Fourier-space approach. Recently, we have supplemented this approach with methods borrowed from algebraic topology. We now show what topology, which studies global properties of manifolds, has to do with crystallography. No mathematics is assumed beyond what the typical physics or crystallography student will have seen of group theory; in particular, the reader need not have any prior exposure to topology or to cohomology of groups.

1. Introduction

Reviewing the Fourier-space formulation of crystallography, David Mermin wrote in 1992 that

More than one person has told me that what I am calculating here are cohomology groups. I have found this information less valuable than M. Jourdain found the news that he was speaking prose, but am too ignorant to state with confidence that this is not a useful point of view. [22]

Applying cohomology, we have proven certain theorems [26, 9, 8] in more generality than they were previously known, including to cases with 46-fold [24] and other exotic rotational symmetries. Our purpose here, using minimal jargon and mathematical machinery, is to explain just what the homological point of view is. Since this point of view represents, in some historical sense, a marriage between group theory and topology, and since most readers will already be familiar with the crystallographic implications of the former, we will display some easily appreciated topological analogues and offer a complete example space-group calculation, without shortcuts, employing some of the new tools.

Most concisely, topology is concerned with numbers that remain invariant under transformations; for example, the number of holes in a doughnut does not change under rotations, continuous stretching, or twisting. In physics, electric charge does not change under a gauge transformation. In the special case of a periodic crystal, this gauge transformation of vorticity has given rise to the description of vorticity as “topological charge” [34]. In the traditional, direct-space, formulation of crystallography, the space group of a structure does not depend on the choice of origin (“setting”), despite the fact that not all point-group elements need pass through the same point in a unit cell. There is a long history of the application of group cohomology to describe this invariance [2, 3, 31, 13, 11].

Similarly, Fourier-space crystallography, as first formulated by Bienenstock and Ewald [4] and developed by Mermin and collaborators [30, 28, 23, 22, 21, 6, 13], admits certain quantities invariant under a simpler analogue (to be defined below) of the electromagnetic gauge transformation. In the special case of a periodic crystal, this gauge transformation

†With apologies to N.D. Mermin, [19, 20].
can be described by a translation for each point-group symmetry. In the initial work on Fourier-space crystallography, tracking down these invariants was incidental to the main task of classifying space groups; most of the time, the invariant of a non-symmorphic space group corresponds to a necessary extinction in diffraction (something that clearly should not depend on the arbitrary choice of a gauge). Mermin first noticed that the invariants might not always be so simple in the very article alluding to the Bourgeois Gentleman.\footnote{Two of us were among those who suggested to David Mermin that Fourier-space crystallography could be described in the language of group cohomology; André LeClair was another \cite{LeClair}. As far as we can tell, the existence of this connection between Fourier-space crystallography and group cohomology was first mentioned in print in Mermin’s Molière reference; in the same year, P{"u}nkhin alluded briefly to the same thing \cite{Punikhin}. While it is perhaps interesting that results first formulated in one language can be recast in another, the correspondence becomes useful when it leads to new results.}

There, he noted that of the 157 non-symmorphic periodic space groups in three dimensions, and additionally of an important infinite class of quasiperiodic space groups that includes all the quasicrystals so far discovered, only two (both among the 157) had invariants that did not correspond to extinctions in diffraction.\footnote{The absence of systematic extinctions in these two space groups, \textit{I\textsubscript{2}\textsubscript{1}2\textsubscript{1}2\textsubscript{1}}\textsuperscript{1} and \textit{I\textsubscript{2}\textsubscript{1}3}, was well known. What was new was the description of an algebraic invariant that “detects” that these two groups are non-symmorphic.}

Later, Mermin and König \cite{Mermin1987a, König1987, König1987a} showed that the new kind of invariant had a different physical interpretation, that of electronic “band sticking.” The König-Mermin conditions on the invariant for band sticking were too restrictive; we have generalized them \cite{Rabson2019} and have also found a third type of invariant corresponding to neither extinctions nor König-Mermin band sticking \cite{Fisher2020}.

1.1. Fourier-Space Crystallography. In order to establish notation, we briefly review the Rokhsar-Wright-Mermin formulation of crystallography in Fourier space; see reference \cite{Rokhsar1983} or \cite{Wright1984} for a more careful development. We begin with the (reciprocal) lattice $L$, which consists of all integral linear combinations of a finite number of generating vectors.\footnote{The lattice of a periodic structure is discrete and generated by three vectors in three dimensions, while that of a quasiperiodic structure is not discrete and has more generators than dimensions. In Fourier-space crystallography, this is the only theoretical distinction between these two cases. Since we are not interested in the direct-space lattice (if it even exists), we shall use the term “lattice” for the the reciprocal lattice.}

The Fourier transform of a density (mass, electronic, etc.) has support on this lattice; we will refer to the Fourier transform as the density, since the direct-space density plays no role in the theory. Two densities, $\rho(k)$ and $\rho'(k)$, are indistinguishable if all their $n$-body correlation functions are the same; this is equivalent to the condition

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

where the \textit{gauge function} $\chi(k)$, defined modulo unity, is linear on the lattice. In case a point operation $g$ takes $\rho$ to $\rho'$, we write the special gauge function associated with $g$ as the \textit{phase function} $\Phi_g$; the point group $G$ consists of all $g$ such that

$$
\rho(gk) = e^{2\pi i \Phi_g(k)} \rho(k).
$$

The phase function is the central object of the Fourier formulation, and it is subject to a restriction and to an identification. As a consequence of the associativity of the group action on the lattice, the phase function must satisfy the \textit{group-compatibility condition} for $g, h \in G$,

$$
\Phi_{gh}(k) = \Phi_g(hk) + \Phi_h(k).
$$
while two phase functions, $\Phi$ and $\Phi'$, describe indistinguishable densities if they are related by a gauge function, $\chi$,

$$\Phi'_g(k) = \Phi_g(k) + \chi(gk - k),$$

and so are identified. The lattice $L$, the action of the point group $G$, and the phase function $\Phi$ determine the space group type of the crystal. Homology theory provides a convenient way of calculating all such functions, subject to the restriction (1.3) and the identification (1.4).

2. Invariants

We continue the review of Fourier-space crystallography, stressing the role played by gauge-invariant values of combinations of phase functions. We then switch context to elementary topology, where we define homology of loops drawn on two-dimensional surfaces in an intuitive way. Cohomology is introduced through a familiar example from vector calculus. Finally, we connect topology to crystallography by way of homology and cohomology of groups.

2.1. Invariants in Fourier-space Crystallography. Evidently, gauge-equivalent phase functions $\Phi$ and $\Phi'$ in (1.4) will have different values when evaluated for generic $g$ and $k$. However, certain linear combinations of phase functions are independent of gauge. Immediately from (1.4), we see that if $g$ leaves $k$ invariant, then $\Phi_g(k)$ is the same in any gauge; we call such a quantity a gauge invariant of the first kind. It follows from (1.2) that if a gauge invariant of the first kind is non-zero (always modulo the integers), then $\rho(k) = 0$, so there is an extinction in diffraction. For example, let $G = 2mm = \{e, r, m, rm\}$, where $e$ is the identity, $r$ denotes a 180° rotation, and $m$ is reflection in the $\hat{x}$-axis; let $L$ be the lattice generated by vectors $a$ and $b$ along the $\hat{x}$- and $\hat{y}$-axes. Then it is not hard to check that $\Phi_m(ia + jb) = \Phi_{rm}(ia + jb) = i^{1/2}$, $\Phi_e(k) = \Phi_r(k) = 0$ satisfies the group-compatibility condition (1.3). Thus $\Phi_m(a) = \frac{1}{2}$ is an invariant of the first kind, and the point $a$ is extinct in diffraction. For further discussion of this example, see §3.2 below.

This is not the only kind of invariant. Of course any integral linear combination (such as $\Phi_{g_1}(k_1) + \Phi_{g_2}(k_2)$ where $g_1 k_1 = k_1$) of gauge invariants of the first kind is still an invariant, but for two of the 157 periodic non-symmorphic space groups in three dimensions, the simplest gauge-invariant quantity one can construct takes the form

$$\Phi_g(k_h) - \Phi_h(k_g),$$

where $g$ and $h$ commute and where neither term alone is gauge invariant. König and Mermin [14, 15, 16] define the lattice vectors $k_g$ and $k_h$ in terms of a point $q$ not in the reciprocal lattice but with the property that

$$k_g \equiv q - gq \quad \text{and} \quad k_h \equiv q - hq$$

are. The group operations $g$ and $h$ are then elements of the little group of $q$. We refer the reader to their papers or to [26] for the proof that if the invariant (2.2) is non-zero, any electronic energy level at wavevector $q$ must be at least two-fold degenerate.\(^4\)

\(^4\)The point $a$ may also be extinct for the point group $4mm$ on the square lattice (and for analogous star lattices 8, 16, . . .). That there is no systematic extinction for $6mm$ on the triangular lattice, as a consequence of (1.3), demonstrates that the calculation of space groups is non-trivial.

\(^5\)Equation (2.1) is a special case of what we refer to in [9, 8] as an invariant of the second kind, which always leads to the electronic degeneracy; there also exists an invariant of the third kind, but we shall not need it here.
Figure 1. The manifold $M$, containing two holes, illustrates a topological space. $AB$, $C$, $D$, $E$, $F$, $G$, and $H$ are oriented 1-simplices; of these, all but $AB$ are 1-cycles. The 1-cycles $C$ and $E$ are 1-boundaries. In particular, $C$ is the boundary of sub-manifold $S$.

2.2. **Topological Invariants**\(^6\). Figure 1 offers a tour of some of the objects of topology. The shaded area represents a two-dimensional manifold $M$. The region $S$ is a submanifold; the other letters label various oriented curves. An oriented curve is called a 1-simplex. We have an intuitive idea, which we shall make formal shortly, of what it means for objects to bound one another. As examples, the 1-simplex $AB$ is bounded by the points $A$ and $B$, but the other labeled 1-simplices, which are closed, have no boundary points; such 1-simplices with no boundaries will be examples of 1-cycles. Cycles themselves may or may not bound submanifolds: the 1-cycle $C$ bounds $S$, but $D$ is not the boundary of any submanifold of $M$. To describe the boundary of $M$, we must exclude the two holes and so need a combination of cycles, which we shall see can be written as the sum $H - F - G$. Such a formal sum of 1-simplices is called a 1-chain; any sum, such as $C + C + AB = 2C + AB$, may be performed, although the result might not be very interesting.

The cycle $F$ encloses the left hole once, while cycles like $D$ and $G$ each enclose the right hole once. A cycle might enclose one or both holes an arbitrary number of times; we could draw a lemniscate (figure-eight) enclosing the left hole $-1$ times and the right hole $+1$ times.

Boundaries offer a way to identify cycles, such as $D$ and $G$, that enclose holes the same number of times. Since $D - G$ bounds the region between the two cycles, we shall write $D = G + (D - G) = G$, identifying the two cycles because they differ by the boundary $D - G$. Two cycles differing by a boundary will be called homologous; cycles $E$ and $C$ are also homologous to each other but not to $D$ and $G$. A set of homologous cycles forms a

\(^6\)The elementary treatment of topology in this section draws on Alexandroff’s slim introduction [1].
Figure 2. Figure 2a illustrates the torus $T$ (doughnut) embedded in Euclidean 3-space. Only the surface forms $T$. Figure 2b illustrates the same torus: the sides with double arrows are to be joined, generating a cylinder, and then the sides with single arrows. The triangulation consists of two 2-simplices, $\Delta$ and $\Gamma$, three 1-simplices, $b$, $c$, and $d$, and just a single 0-simplex (vertex), $A$. The 1-cycles $b$ and $c$ are also shown in Figure 2a.

homology class; the enumeration of classes of cycles identified by homology will have a direct analogue in the classification of phase functions identified by gauge transformation.

For this example, each homology class is labeled by two integers: one describing how many times each cycle in the class goes around the left hole and another describing how many times each cycle in the class goes around the right. Since cycles form an additive group, so do homology classes; the homology group of the figure\(^7\) is $\mathbb{Z} \times \mathbb{Z}$.

The torus, $T$, of Figure 2a (the surface of a doughnut, not the dough) cannot be deformed into the manifold of Figure 1, yet the two have the same homology group. This will follow from the fact that a cycle on the torus may enclose the hole any integer number of times and that it may enclose the dough (which is also a kind of hole) any integer number of times. Since this assertion is perhaps a little less transparent than the corresponding one for Figure 1, we start by describing a general method for calculating homology groups.

First we flatten the torus into the rectangle of Figure 2b. The arrows indicate that opposite sides are to be identified, or sealed together: after identifying the two sides with double arrows, one obtains a cylinder; identifying the other two sides then gives the torus. Figure 2b shows the torus with a diagonal added. In this triangulation, the torus $T$ consists of a single 0-simplex, or point, labeled $A$; the three 1-simplices $b$, $c$, and $d$; and the two 2-simplices (triangles) $\Delta$ and $\Gamma$. The straight arrows on the 1-simplices indicate their orientations; 2-simplices can be oriented as well, as indicated by the curly arrows. The orientations of the 2-simplices and their constituent 1-simplex sides bear no necessary relation. Neither the triangulation of $T$ nor the assignment of orientations is unique; we refer the reader to \(\text{[1]}\) for theorems guaranteeing that the homology group is independent of these choices.

\(^7\)The homology group of these curves is called the first homology group; elsewhere \([2, 26]\) we have had occasion to employ higher homology groups. We use the common mathematical notations $\mathbb{Z}$ for the integers, $\mathbb{R}$ for the real numbers.
According to (2.3), we have $(x_0, x_1) - (x_0, x_2) + (x_1, x_2) = -(x_1, x_0) + (x_1, x_2) + (x_2, x_0)$, in agreement with the orientations in the figure.

Labeling a 1-simplex by its endpoints (which may be the same point) and a 2-simplex (triangle) by its vertices,\(^8\) we define the **boundary operator** $\partial$ by

\[
\partial (x_0, x_1) = x_1 - x_0 \\
\text{and} \\
\partial (x_0, x_1, x_2) = (x_0, x_1) - (x_0, x_2) + (x_1, x_2).
\]

For example, in Figure 2a, $\partial b = \partial c = \partial d = 0$, and

\[
\partial \Gamma = -b - c + d \\
\partial \Delta = b + c - d.
\]

The definitions extend to 1-chains and 2-chains by linearity, and they agree with the intuitive notion of boundary. So the 1-simplex $(x_0, x_1)$ is a 1-cycle—that is, $\partial (x_0, x_1) = 0$—if and only if $x_0 = x_1$. The boundary of a triangle (Figure 3) $(x_0, x_1, x_2)$ is the sum of its sides, if we accept the convention that $(x_0, x_2) = -(x_2, x_0)$.

It follows from these definitions that the boundary of the boundary of a 2-chain vanishes. Since we may define the boundary of a point (a 0-simplex) as 0, the boundary of the boundary of a 1-chain also vanishes. In fact, in the general theory, $\partial \partial$ is identically zero.

The 1-chains whose boundaries are 0 form the group $Z_1$ of 1-*cycles*, while the 1-cycles that can themselves be written as boundaries of 2-chains constitute the group $B_1$ of 1-*boundaries*. Homology identifies 1-cycles that differ only by 1-boundaries: that is, we form the quotient

\[
H_1 = Z_1 / B_1,
\]

called the first homology group.

Applying these ideas to the triangulation of the torus, we first calculate the group $C_1$ of all 1-chains. Since there are exactly three 1-simplices, an arbitrary 1-chain takes the form $\ell b + mc + nd$, with $\ell, m, n \in \mathbb{Z}$; thus $C_1$ is a three-dimensional “space” (properly, module)

---

\(^8\)This labeling is not meant to suggest that a simplex is determined by its vertices. The *order* of the vertices does determine the orientation of the simplex.
over the integers. In this example, all three 1-simplices have vanishing boundaries, so the group of 1-cycles, $Z_1$, is the same as $C_1$:

$$Z_1 = \langle b, c, d \rangle,$$

where the angle brackets indicate the generators (over the integers). From (2.4), we see that the only 1-boundaries are integral multiples of $b + c - d$, so that $B_1 = \langle b + c - d \rangle$, a one-dimensional module. As a group, first homology with coefficients in the integers is given by

$$H_1(T, \mathbb{Z}) = \mathbb{Z}^3 / \mathbb{Z} = \mathbb{Z} \times \mathbb{Z}.$$

That is, any 1-cycle is homologous to a linear combination of $b$ (going once around the hole) and $c$ (going once around the dough), as we claimed above.

We have taken the coefficients of simplices to be integers, but we can use any additive group. One natural choice is the integers modulo two, $\mathbb{Z}_2 = \{0, 1\}$ with the addition rules $0 + 0 = 1 + 1 = 0$, $0 + 1 = 1 + 0 = 1$. Over $\mathbb{Z}_2$, twice any cycle vanishes. This corresponds to unoriented simplices: for example, if traversing the 1-simplex $C$ in Figure 1 once is identified with traversing the oppositely-oriented simplex once, we have $-C = -C + 2C = C$, so the coefficients are in $\mathbb{Z}_2$. If we use unoriented simplices, the homology groups of $M$ and $T$ are both two copies of the integers modulo 2:

$$H_1(M, \mathbb{Z}_2) = H_1(T, \mathbb{Z}_2) = \mathbb{Z}_2 \times \mathbb{Z}_2.$$

Before leaving the subject of manifolds, we consider the projective plane, $\mathbb{R}P^2$, which can be represented, like the torus, as a rectangle, but now opposite sides are identified in opposite directions, as in Figure 4.\footnote{Equivalently, it may be thought of as a disk with opposite points of the circumference identified or, via stereographic projection, as a Euclidean plane plus a line at infinity. Since each line contains a point at infinity, projection from the focal point $P$ to a line not passing through $P$ is defined on the entire plane except for $P$, hence the term projective plane.} The triangulation of the figure comprises the two 0-simplices $P$ and $Q$, three 1-simplices, $f$, $g$, and $h$, and two 2-simplices, $\Upsilon$ and $\Psi$. It is easy to see that all cycles are generated by $h$ and $f + g$. We determine the boundaries by

$$\partial \Upsilon = h - f - g$$
$$\partial \Psi = -h - f - g.$$

Thus $2h = \partial \Upsilon - \partial \Psi$ is a boundary, but the cycle $h$ is not. The other generating cycle, $f + g$, differs from $h$ by the boundary $\partial \Upsilon$; so there exists only a single cycle, which we may take to be $h$, modulo boundaries. The first homology group is

$$H_1(\mathbb{R}P^2, \mathbb{Z}) = H_1(\mathbb{R}P^2, \mathbb{Z}_2) = \mathbb{Z}_2.$$

The fact that any triangulation can be used to calculate the homology of a manifold is related to Euler’s formula:

$$V - E + F = 2,$$

where $V$, $E$, and $F$ denote the number of vertices, edges, and faces (or 0-, 1-, and 2-simplices) in a polyhedron. A polyhedron can be thought of as a polygonal dissection of the sphere; if we want, we can triangulate the faces and so obtain a triangulation of the sphere. The triangulation (or the polygonal dissection, if one takes the effort to define boundaries of faces
with more than three sides) can be used to compute the homology groups of the sphere $S$, and in particular the alternating sum

$$
\chi(S) = \text{rank } H_0(S) - \text{rank } H_1(S) + \text{rank } H_2(S),
$$

known as the *Euler Characteristic* of the sphere. It follows from elementary linear algebra that the alternating sum is the same whether one takes ranks of homology groups or of chain groups: that is, $\chi(S) = V - E + F$ is the same for any dissection of the sphere. From the triangulations above, it follows that the Euler characteristics of the torus and projective plane are 0 and 1.

### 2.3. From cycles to vector fields and de Rham cohomology

Homology of a manifold is closely connected to the question of which vector fields are conservative. Let $\mathbf{F} = P\hat{x} + Q\hat{y}$ be a vector field in the plane. If $\mathbf{F}$ is the gradient of a potential $\phi$, then the rules of vector calculus imply that $\nabla \times \mathbf{F} = \mathbf{0}$ and that the line integral of $\mathbf{F}$ over any contour vanishes. On the other hand, a curlless vector field may or may not be the gradient of a potential.

The standard counterexample is

$$
\mathbf{F} = \frac{x\hat{y} - y\hat{x}}{x^2 + y^2}.
$$

It is easy to verify that $\nabla \times \mathbf{F} = \mathbf{0}$ but that integrating counterclockwise around the unit circle $C$ gives $\oint_C \mathbf{F} \cdot d\mathbf{r} = 2\pi$. We could say that $\mathbf{F}$ has a $\delta$-function curl at the origin or, equivalently, we could cut the origin out of the plane, yielding a “punctured plane,” $M$. In the language of homology, the circle $C$ is a cycle in $M$ but not a boundary. If, instead of $C$, we consider the boundary $B$ of a region $R$ that does not contain the origin, then Green’s Theorem implies that $\oint_B \mathbf{F} \cdot d\mathbf{r} = 0$.

More generally, consider a vector field that is curlless on a plane punctured any number of times. Two cycles that differ by a boundary yield the same line integral, so homology naturally describes the classes of line integrals of a curlless vector field.
Table 1. Summary of some of the relations between homology and de Rham cohomology.

| 1-(co)chain          | sum of curves on $M$ | vector field, $\mathbf{F}$ |
|----------------------|----------------------|-----------------------------|
| 1-(co)cycle          | closed curves (contours for $\oint$) | $\nabla \times \mathbf{F} = 0$ on $M$ |
| 1-(co)boundary       | trivial: bounds region of $M$ | trivial: $\oint \mathbf{F} \cdot d\mathbf{r} = 0$ |

It is equally natural to fix a cycle and to consider different vector fields. Adding the gradient of a potential to $\mathbf{F}$ does not change any closed line integral, so we identify two vector fields that differ by a conservative field. The resulting vector space is the first de Rham cohomology group of the punctured plane, $M$, denoted $H^1_{\text{DR}}(M)$.

The condition (that $\mathbf{F}$ have no curl on $M$) and the identification (of vector fields differing by conservative fields) mirror the cycle and boundary conditions on contours, providing a natural duality between de Rham cohomology and $H_1(M, \mathbb{R})$, the homology of $M$ with real (not integral) coefficients. On the level of chains and vector fields, the duality is defined by the circulation integral, $\langle \mathbf{c}, \mathbf{F} \rangle = \oint \mathbf{c} \cdot d\mathbf{r}$. To see that this is well defined on (co)homology, it is enough to notice that $\oint \mathbf{c} \cdot d\mathbf{r} = 0$ if $\mathbf{c}$ is any cycle and $\mathbf{F}$ is conservative (fundamental theorem of calculus) or if $\mathbf{c}$ is a boundary and $\mathbf{F}$ is irrotational (Green’s Theorem).

The language of differential forms connects the gradient and the curl. In this language, $\omega \equiv \mathbf{F} \cdot d\mathbf{r} = P \, dx + Q \, dy$ is a differential 1-form. The differential of $\omega$, giving the curl, $d\omega = (\partial Q / \partial x - \partial P / \partial y) \, dx \, dy$, is a 2-form. The exterior derivative $d$ serves as the coboundary operator in this context; the vanishing of $d\omega$ makes $\omega$ a 1-cocycle. This resembles the cycle condition in homology, except that where $\partial$ demoted an $n$-chain to an $n-1$-chain, here $d$ promotes a 1-form into a 2-form. Similarly, a 0-form is a scalar-valued function, $\phi$, on the plane, and $d\phi = (\partial \phi / \partial x) \, dx + (\partial \phi / \partial y) \, dy$ is a 1-coboundary. De Rham cohomology is the space of cocycles modulo coboundaries, i.e., vector fields curlless on $M$ modulo conservative fields.

Table 1 summarizes some of the relations between homology and de Rham cohomology.

2.4. Crystallographic Invariants as Homology Elements. In the foregoing, we identified closed curves (cycles) differing only by boundaries. We then enumerated all the possible cycles, up to boundaries. We now describe a similar way to find all crystallographic invariants, demonstrating the method in the next section.

First, instead of thinking of a collection of functions $\Phi_g$, one for each element of the point group, think of the phase function $\Phi$ as acting on a pair consisting of a point-group element $g$ and a lattice vector $\mathbf{k}$. We will write this pair as $\mathbf{k}[g]$; such an object is an example of a 1-chain. The phase function acts on this 1-chain in the obvious way: $\Phi(\mathbf{k}[g]) = \Phi_g(\mathbf{k})$.

Addition is defined on 1-chains as though the various elements of the point group $G$ were independent basis vectors in a vector space and with the reciprocal lattice playing the role of numeric coefficients. Since the phase function is linear on the lattice, it acts distributively over addition. Thus, for example,

$$\Phi(a[g] + b[g] + c[h]) = \Phi((a+b)[g] + c[h]) = \Phi_g(a+b) + \Phi_h(c).$$

We note that this same example has an equivalent interpretation with contour integrals over functions that are analytic in the complex plane except at simple poles.

Since the lattice is not a field, the 1-chains form a module instead of a vector space.
Define the boundary operator on a 1-chain by analogy to (2.3):

\begin{equation}
\partial k[g] = gk - k
\end{equation}

so that for a general 1-chain \( c = \sum_i k_i[g_i] \),

\begin{equation}
\partial c = \sum_i g_i k_i - k_i .
\end{equation}

A 1-chain \( c \) is a 1-cycle if \( \partial c = 0 \). Considering the gauge transformation of (1.4), we have for the difference between phase functions \( \Phi \) and \( \Phi' \) evaluated on the 1-cycle \( c \)

\begin{equation}
\Phi'(c) - \Phi(c) = \chi \left( \sum_i g_i k_i - k_i \right) = 0 .
\end{equation}

Thus cycles are gauge invariants, and since \( \chi \) is an arbitrary linear function (from the lattice to the real numbers modulo unity), any gauge invariant is a cycle.

Certain gauge invariants are trivial. Applying (2.15), we establish that any 1-chain of the form

\begin{equation}
b = h k[g] - k[gh] + k[h]
\end{equation}

is a 1-cycle. However, any phase function \( \Phi \) evaluated at \( b \) must vanish by the group-compatibility condition (1.3). Adding \( b \) to any 1-cycle \( z \) yields another 1-cycle, \( z + b \), but in enumerating gauge invariants, we should not count \( z \) and \( z + b \) separately. Thus \( b \) acts very much like the 1-boundary considered in topology. In fact, (2.18) is exactly the definition of the boundary of the 2-chain \( k[g|h] \):

\begin{equation}
\partial k[g|h] \equiv h k[g] - k[gh] + k[h] .
\end{equation}

Thus, to determine all non-trivial gauge invariants of a group acting on a lattice, we calculate the group of 1-cycles and divide by the group of boundaries of 2-chains; the quotient group is called \( H_1(G, L) \) (\( G \) is the point group, \( L \) the lattice). As we have noted [26], this is less elegant than Mermin’s method but, obviating the need for a clever choice of gauge, has proven useful in establishing theorems and generalizing results to modulated crystals. Moreover, the systematic way in which gauge invariants fall out of this formulation has enabled us to find a new type, not previously noted [8].

A comparison to the definition of the boundary of the 2-simplex in the second line of (2.3) reveals nearly the same formal structure under the replacement \( g \to (x_0, x_1) \), \( h \to (x_1, x_2) \), \( gh \to (x_0, x_2) \), the difference being that we considered topological chains over integers, while the coefficients in crystallography lie instead in the lattice, on which the group acts non-trivially: hence the \( h k \) in the first term on the right instead of just \( k \).

There is a way of visualizing 1-chains in group homology that emphasizes the analogy with 1-cycles in topology: picture the 1-chain \( k[g] \) as a vector going from \( k \) to \( gk \). If \( g \) is a rotation, it is suggestive to draw the vector along a circular arc, as in Figure 5, in which \( r \) denotes a 90° rotation. This visualization is consistent with the definition (2.15) of the boundary of a 1-chain. The formula (2.19) for a 1-boundary can be written in the form \( k[gh] \doteq k[h] + (hk)[g] \), where \( \doteq \) denotes homology as in §2.2. This is also consistent with the vector picture: for example, Figure 5 illustrates the fact that \( a[r^3] \doteq a[r] + (ra)[r^2] \). One shortcoming of this method is that it does not illustrate linearity relations, such as \( (a + b)[g] = a[g] + b[g] \) and \( (-a)[g] = -(a[g]) \).
Figure 5. It may help to elucidate chains to think of them geometrically; a chain \( k[g] \) can be pictured as a circular arc pointing from \( k \) to \( gk \). The boundary \( \partial a[r^2] = \partial a[r^{-1}] = a[r] + (ra)[r^2] \), as suggested by the three arcs.

3. An Example of Calculating Space (Plane) Groups

To illustrate the homological method, we will calculate the homology group \( H_1(G, L) \) where the primitive rectangular lattice \( L \) is generated by a vector \( a \) in the \( \hat{x} \) direction and a vector \( b \) of different length in the \( \hat{y} \) direction and where the point group \( G = \{ e, r, m, rm \} \) is generated by a 180° rotation \( r \) and the mirror \( m \) that leaves \( a \) invariant (\( e \) is the identity). According to the International Tables for Crystallography [10], the possible plane groups are \( p2mm, p2gg, \) and \( p2mg \). We shall verify this result in the next subsection; we concentrate first on calculating the possible invariants.

Since our goal is to illustrate a general method as simply as possible, we avoid the shortcuts we used in the more complicated example of section 7 of [26]. In section 4.1, we show how the entire calculation can be automated in the symbolic-algebra program, Mathematica [36], for arbitrary examples.

3.1. Invariants of the Point Group 2mm on the Primitive Rectangular Lattice.

There are four elements of \( G \), and the lattice is generated by two vectors. To find all the cycles, we therefore take boundaries of the eight 1-chains \( k[g] \) where \( k \) is a lattice generator. (Any other 1-chain is an integral linear combination of these.)

\[
\begin{align*}
\partial a[e] &= 0 & \partial b[e] &= 0 \\
\partial a[m] &= 0 & \partial b[m] &= -2b \\
\partial a[rm] &= -2a & \partial b[rm] &= 0 \\
\partial a[r] &= -2a & \partial b[r] &= -2b
\end{align*}
\]

(3.1)
Second, for each possibility, a phase function exists. Invariant in $H$.

First, two phase functions not related by a gauge differ in their values on at least one gauge. Therefore, there are four possible gauge-invariant values for the phase function, given in Table 2.

3.2. Connection between invariants and space groups (cohomology). Now we’re ready to classify plane groups. According to the Rokhsar-Wright-Mermin specification, we need to find all functions $\Phi$, linear modulo unity on the lattice, satisfying (1.3). Since $2z_3$ and $2z_5$ are boundaries, we must have $2\Phi(z_3) = 2\Phi(z_5) = 0$ (all modulo unity), so that there are four possible gauge-invariant values for the phase function, given in Table 2.

We now make two assertions, the proof of which is the main content of reference [26]. First, two phase functions not related by a gauge differ in their values on at least one gauge invariant in $H_1(G, L)$. Thus, there are no more than four space groups in the example. Second, for each possibility, a phase function exists.

\[ Z_1(G, L) = \langle z_1, z_2, z_3, z_4, z_5, z_6 \rangle \]

where

\[ z_1 = b[e], \quad z_4 = a[e] \]
\[ z_2 = -b[r] + b[m], \quad z_5 = a[m] \]
\[ z_3 = b[rm], \quad z_6 = a[rm] - a[r] . \]

Now, we write down the 32 generators $k[g/h]$ ($k = a, b$ and $g, h$ in the point group) of all 2-chains, and calculate their boundaries:

\[ b_1 \equiv \partial a[e] = a[e] \]
\[ b_2 \equiv \partial b[e] = b[e] \]
\[ b_3 \equiv \partial a[r] = a[r] + a[m] - a[rm] \]
\[ b_4 \equiv \partial a[m] = a[r] - a[m] - a[rm] \]
\[ b_5 \equiv \partial b[r] = -b[r] + b[m] - b[rm] \]
\[ b_6 \equiv \partial b[m] = b[r] - b[m] - b[rm] . \]

All of the remaining boundaries are linear combinations of these six boundaries. Furthermore, it is evident that the six boundaries in (3.4) are integrally linearly independent, so\(^{12}\)

\[ B_1(G, L) = \langle b_1, b_2, b_3, b_4, b_5, b_6 \rangle . \]

We expect and verify that every boundary in (3.5) can be written as an integral linear combination of the cycles in (3.3) (since all boundaries are cycles). However, the cycles $z_1$ and $z_4$ are actually boundaries, so we throw them out. Furthermore, $z_5 - z_6 = b_3$, which is a boundary, so we write $z_5 = z_6$ (equality up to boundaries); similarly, $z_2 = z_3$. This leaves only two cycles, $z_3$ and $z_5$, which are obviously linearly independent and not boundaries. Finally, we note that $2z_3 = -(b_5 + b_6)$ and $2z_5 = b_3 - b_4$ are boundaries. Thus there are only four invariants:

\[ H_1(G, L) = \{0, z_3, z_5, z_3 + z_5\} . \]

12 In 4.2 we prove that $Z_1$ and $B_1$ always have the same rank.
The four sets of gauge-invariant values a phase function might take for the point group $2mm$ on the primitive-rectangular lattice. These correspond to the plane groups $p2mm$, $p2mg$, $p2gm$ (which is just a different setting of $p2mg$), and $p2gg$.

| possibility | $\Phi(z_3) = \Phi_{rm}(b)$ | $\Phi(z_5) = \Phi_m(a)$ |
|-------------|----------------------------|--------------------------|
| 1           | 0                          | 0                        |
| 2           | $1/2$                      | 0                        |
| 3           | 0                          | $1/2$                    |
| 4           | $1/2$                      | $1/2$                    |

Table 2. The four sets of gauge-invariant values a phase function might take for the point group $2mm$ on the primitive-rectangular lattice. These correspond to the plane groups $p2mm$, $p2mg$, $p2gm$ (which is just a different setting of $p2mg$), and $p2gg$.

| homology          | cohomology                      |
|-------------------|---------------------------------|
| 1-(co)chain       | $\sum_i k_i[g_i]$               |
| 1-(co)cycle       | gauge invariant                 |
| 1-(co)boundary    | trivial by group compatibility  |

Table 3. Summary of the application of group homology and cohomology to Fourier-space crystallography. (For additional applications and higher-order (co)homology, see [26][9].) Symbols: $k_i$ are reciprocal-lattice vectors and $g_i$ point-group elements. $\Phi$ is a phase function. Compare Table 1.

The proof in [26] rests on the duality of homology and cohomology, in which $\Phi$ plays the same role with respect to a chain $\sum k_i[g_i]$ as the vector field $F$ played with respect to a contour in subsection 2.3. Think of $\Phi$ as acting on $g$ to give $\Phi_g$; $\Phi_g$ acts linearly on $k \in L$ to give the number $\Phi_g(k)$, modulo unity as always. The 1-cochains form a group under addition. A 1-cochain is a 1-cocycle if its coboundary, defined by

$$ (d\Phi)(g, h) = \Phi_g \circ h - \Phi_{gh} + \Phi_h, $$

vanishes: this is simply the group-compatibility condition on $\Phi$, so we are clearly interested in 1-cocycles. Note that where the boundary operator $\partial$ decreased the number of group arguments, the coboundary operator $d$ increases it. A linear function $\chi$ on the lattice is called a 0-cochain; its coboundary is given by

$$ (d\chi)(g) = \chi \circ g - \chi. $$

Two different 1-cochains $\Phi$ and $\Phi'$ that differ by a coboundary of the form of (3.8) are related by a gauge function, according to (1.4), so we identify them. The group of 1-cocycles modulo 1-coboundaries, or first cohomology, is labeled $H^1(G, \hat{L})$, where $\hat{L}$ denotes the group of linear maps from $L$ to $\mathbb{R}/\mathbb{Z}$; if $\chi$ is an element of $\hat{L}$, then $2\pi i \chi(k)$ is a choice of phase for each $k$ among a generating set for the lattice $L$. Table 3 summarizes homology and cohomology; note the similarity between the requirement for homology and triviality for cohomology, and vice-versa.

The task of classifying space groups, then, comes down to calculating the cohomology group of cocycles modulo coboundaries, and this group is dual to the homology group of cycles modulo boundaries. Thus, the four possibilities in Table 2 above are exactly the four possible space groups for this example.
However, there are only three space groups for $2mm$ on the primitive rectangular lattice: $p2mm$, $p2mg$, and $p2gg$. Possibilities 2 and 3 in the table simply exchange the $\hat{x}$ and $\hat{y}$ directions.\textsuperscript{13}

### 3.3. Comparison to torus and lemniscate.

Table 2 shows that the homology (or cohomology) group of the point group $2mm$ acting on the primitive-rectangular lattice is isomorphic to $\mathbb{Z}_2 \times \mathbb{Z}_2$, the same homology group we considered in two examples in section \textsuperscript{2.2}\textsuperscript{14} The topological examples contained two holes in the sense of closed curves that did not bound: Figure 1 without orientation has two literal holes, while the doughnut has the hole in the center and the fried dough (which is not part of the surface and so is no different from a hole). In each case, exchanging the two holes reduces the number of combinations from four to three. The close analogies tell us that we can consider crystallography, as well, in terms of topological spaces. A point group and lattice admitting no non-symmorphic space groups is a trivial space, in which every closed curve can be collapsed to a point, while non-symmorphic space groups are non-zero cohomology classes in spaces with one or more holes. We shall show in section \textsuperscript{4.1} that in every case, the invariants correspond to some number of holes, each of which can be lassoed by a cycle a finite number of times before it vanishes. (More prosaically, the (co)homology group is isomorphic to the direct product of some number of cyclic groups of varying order.)

## 4. Generalizing the calculation

### 4.1. Automation of calculation in Mathematica.

The algorithm of section \textsuperscript{3.1} requiring no clever choices of gauge or anything specific to the point group or lattice, is easily automated. Our Mathematica implementation, available at the preprint archive, \texttt{cond-mat/0301601} takes only 13 lines of substantive code. A quick tour of the algorithm may assist those trying to do the calculation by hand as well as users of computer-algebra packages.

1. The point-group generators and their actions (to the right) on the lattice are specified by square matrices of dimension equal to the rank of the lattice. For example, the two-fold rotation $r$ and mirror $m$ in section \textsuperscript{5.1} are the matrices

\begin{equation}
\begin{align*}
    r &= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} ; \\
    m &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\end{align*}
\end{equation}

acting on the column vectors $a = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $b = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

2. The group $C_1$ of all 1-chains is generated by the combinations $k[g]$, where $k$ is a lattice generator and $g \in G$. The computer stores all these combinations in the list $c$. Think of this list, say $c = (c_1, \ldots, c_r)$, as a column vector.

3. Take the boundary (2.16) of each $c_i$. The \texttt{NullSpace[]} function in Mathematica, applied to the list of boundaries, gives a matrix $z$ that expresses generators $z_i$ of the

\textsuperscript{13}Once cohomology has been calculated, it is still necessary to consider rotations and (in quasiperiodic cases) scale invariance of the lattice. See \texttt{6, 12} for a full accounting of Bravais class, arithmetic crystal class, and space-group type.

\textsuperscript{14}To the manifold with two holes and the torus, each with coefficients in $\mathbb{Z}_2$, we may add $\mathbb{R}P^2 \times \mathbb{R}P^2$ with coefficients in $\mathbb{Z}$. 
cycle group $Z_1$ in terms of $c$:

$$
\begin{pmatrix}
  z_1 \\
  : \\
  z_s
\end{pmatrix} = Z
\begin{pmatrix}
  c_1 \\
  : \\
  c_r
\end{pmatrix}. 
$$

(4.2)

(4) The group $C_2$ of all 2-chains is generated by the combinations $k[gh]$, where $k$ is a lattice generator and $g, h \in G$. The boundaries $b_i$ of these 2-chains generate the group $B_1$ of 1-boundaries. Express these generators in terms of $c$:

$$
\begin{pmatrix}
  b_1 \\
  : \\
  b_n
\end{pmatrix} = bz3
\begin{pmatrix}
  c_1 \\
  : \\
  c_r
\end{pmatrix}. 
$$

(4.3)

(5) Find a rational transformation $z2$ that transforms a cycle from the basis of $C_1$ into the basis of $Z_1$. Our package uses $\text{PseudoInverse}[]$.

(6) From steps 4 and 5, the product $bz3.z2$ expresses the generators $b_i$ of $B_1$ in the basis of $Z_1$. We call $\text{LatticeReduce}[]$ to find the smallest set of rows that will generate $B_1$ over the integers, yielding the matrix $b$. Thus

$$
\begin{pmatrix}
  b_1 \\
  : \\
  b_s
\end{pmatrix} = b
\begin{pmatrix}
  z_1 \\
  : \\
  z_s
\end{pmatrix}
$$

(4.4)

gives a minimal set of generators for $B_1$. We explain in 122 below that $B_1$ and $Z_1$ have the same rank, so that $b$ is a square matrix. We can calculate the first homology group $H_1 = Z_1/B_1$ as follows. The Smith normal form [32, Thm. 25.26], [12] of the matrix $b$ is a diagonal matrix $d$ such that there are invertible integral transformations $p$ and $q$ with

$$
d = p b q
$$

(4.5)

Thus $q$ and $p$ describe new bases for $Z_1$ and $B_1$, say $\{z'_1\}$ and $\{b'_i\}$. In these new bases, $b'_i = d_i z'_i$; in other words, $d_i$ times cycle $z'_i$ is a boundary. Thus the homology group $H_1$ can be described as all linear combinations of $z'_1, \ldots, z'_s$, where the coefficient of $z'_i$ lies between 0 and $d_i - 1$, and there are no relations other than $d_i z'_i = 0$.

(7) Our function $\text{SpacegroupH1Full[]}[]$ returns the matrices $c, z, b, d, p,$ and $q$ above.

Returning again to the example of section 3.1 we find

$$
d = \text{diag}(1, 1, 1, 1, 2, 2)
$$

(4.6)

The module $Z_1$ has dimension six, as in 3.3. The four unit entries indicate that the corresponding cycles are boundaries, while the two entries of 2 tell us that two, $z'_5$ and $z'_6$, are not, although $2z'_5$ and $2z'_6$ are. We invert the Smith transformation to solve for $z'_5$ and $z'_6$:

$$
p^{-1} \text{diag}(0, 0, 0, 0, 1, 1) q^{-1}
$$

(4.7)

This yields a matrix with two non-zero rows, $(0, -1, 0, 0, 0, 0)$ and $(0, 0, 0, 0, 0, 1)$, giving $z'_5 = -z_2$ and $z'_6 = z_6$. The $z$ matrix converts the $Z_1$ basis into the basis of $C_1$, which we
decode with the help of the list c to compare with the results of section 3.1

\begin{equation}
\begin{align*}
 z'_0 &= -z_2 = z_3 \\
 z'_6 &= z_6 = z_5
\end{align*}
\end{equation}

We admit this algorithm to be inelegant: like direct-space formulations, it requires the construction of matrices of dimension equal to the rank of the lattice. Unlike the Rokhsar-Wright-Mermin method, it cannot treat related point groups, e.g., $2^j\text{mm} = \{4\text{mm}, 8\text{mm}, (16)\text{mm} \ldots\}$, all at once but rather requires a separate calculation for each. However, we find it useful in those cases (such as 46-fold symmetry and modulated lattices) where discovering a good choice of gauge, requisite to Rokhsar-Wright-Mermin, seems too difficult.

### 4.2. Finite number of Space Groups

When applying the Rokhsar-Wright-Mermin approach to quasicrystals, there are a few surprises. One is that, even in two dimensions, a finitely-generated lattice that is not discrete may have an infinite point group \[35\]. Assume, as we have been doing implicitly so far, that the point group is finite. Happily, this is enough to guarantee that there are only finitely many space groups associated to the point group $G$ and the lattice $L$. As explained in \[3.2\], this amounts to saying that the homology group $H_1(G, L)$ is finite. In any example, this can be checked by verifying that the matrices $b$ and $d$ of \[4.1\] have the same rank as the cycle group $Z_1$.

In order to prove generally that $H_1(G, L)$ is finite, it suffices to show that $Nz$ is a boundary for any 1-cycle $z$, where $N$ is the order of the point group $G$. Grant this for the moment. There are then finitely many 1-cycles, say $z_1, z_2, \ldots, z_s$, (where $M$ is the rank of the cycle group $Z_1$) that generate all the others: any 1-cycle $z$ can be written as a linear combination of the generators $z_i$. In order to represent all homology classes, it suffices to take coefficients between 1 and $N$, since $Nz_i$ is a boundary. Thus there are only finitely many homology
classes. We can also explain this in terms of matrices: if \( N z_i \) is a boundary for each generator \( z_i \), then \( b' b = N I_M \) for some integer matrix \( b' \), where \( I_s \) denotes the \( s \times s \) identity matrix. This implies that \( b \) has rank \( s \).

It remains to explain why \( N \) times a cycle is a boundary. Let \( z = \sum_h k_h[h] \) be a cycle, where \( h \) runs through the point group. According to (2.16), the cycle condition \( \partial z = 0 \) can be written in the form

\[
\sum_h h k_h = \sum_h k_h.
\]

(4.9)

Construct a 2-chain \( c \) such that \( \partial c = N z \) using the fundamental technique of averaging over the group: let

\[
c = \sum_{g, h} k_h[g|h].
\]

(4.10)

According to (2.19),

\[
\partial c = \sum_{g, h} (h k_h)[g] - \sum_{g, h} k_h[gh] + \sum_{g, h} k_h[h].
\]

(4.11)

The first two terms in (4.11) cancel: to see this, fix \( g \) and apply the cycle condition (4.9) in the first term; and fix \( h \) and replace \( g \) with \( gh^{-1} \) in the second term. The summand in the third term in (4.11) is independent of \( g \), so the third term is simply \( N z \).

4.3. From Real Space to Fourier Space. So far, we have described the Fourier-space approach to crystallography in the language of (co)homology, explained how this language lends itself to explicit calculations, and pointed out the analogy with topological (co)homology. The real advantage of adopting this framework comes from applying the theorems developed over the years for homological algebra in general and group cohomology in particular. The duality between phase functions and crystallographic invariants (§2.4) is a special case of one such theorem, the duality between homology and cohomology. The calculation of invariants (§§3.1 and 4.1) is one example of a standard technique. The finiteness result (§4.2) is another.

In this subsection, we summarize the connection between the real-space and Fourier-space approaches to crystallography, using the common language of group cohomology. Each step in this comparison involves a standard result, explained in textbooks such as [1], but we will not try to reproduce these explanations. At the end, we illustrate these generalities by returning to the example of the point group 2\( mm \).

In real-space crystallography, one considers a crystal and its space group \( G \). For a periodic, \( d \)-dimensional crystal, the space group consists of all isometries of \( \mathbb{R}^d \) that preserve the crystal. If we are interested in a quasiperiodic crystal, we construct a periodic crystal in a higher-dimensional space, say \( \mathbb{R}^D \), that projects to the quasiperiodic one; for this discussion, \( G \) will be the space group of the higher-dimensional, periodic crystal.\(^{15}\) (In the periodic case, take \( D = d \).) Let \( \mathcal{T} \) denote the lattice of pure real-space translations in \( G \).

In group-theoretic terms, the point group is the quotient \( G = \mathcal{G}/\mathcal{T} \). It can be thought of as the group of “macroscopic symmetries”: think of all translations as “microscopic,” and so identify any two elements of the space group if they differ by a translation. Both \( G \) and \( \mathcal{T} \)

\(^{15}\)Different choices of the periodic \( D \)-dimensional crystal may lead to different \( D \)-dimensional space groups [29].
are fairly easy to describe: \( G \) is a finite subgroup of the orthogonal group,\(^{16}\) and \( \mathcal{T} \) consists of all integral linear combinations of \( D \) generating vectors. These two groups are also fairly easy to determine experimentally. It remains to describe the space group \( \mathcal{G} \) in terms of these two simpler groups. One possibility is that the point group is contained in \( \mathcal{G} \), and the space group is generated by \( G \) and \( \mathcal{T} \). In this case, the space group is called *symmorphic* in crystallographic terminology, or a *semidirect product* in the language of group theory.

Not all space groups are symmorphic. A standard result of group theory states that the space groups corresponding to \( G \) and \( \mathcal{T} \) are classified by the cohomology group\(^{17}\) \( H^2(G, \mathcal{T}) \). Using the Long Exact Sequence of cohomology (cf. the last Remark in §5 of [14]), this is isomorphic to \( H^1(G, \mathbb{R}^D/\mathcal{T}) \).

In the periodic case, the Fourier lattice \( \mathcal{L} \) is the dual of the translation group \( \mathcal{T} \). That is, the Fourier lattice consists of those vectors \( \mathbf{k} \) such that \( \mathbf{k} \cdot \mathbf{t} \) is integral for all \( \mathbf{t} \) in the direct lattice \( \mathcal{T} \). (Those who worry about where the factor of \( 2\pi \) went should refer to [11.1] and [11.2]). Dräger and Mermin [6] realized that this can be turned around in the quasiperiodic case: the translation group \( \mathcal{T} \) and the super-space \( \mathbb{R}^D \) can be described, without explicit coordinates, as duals of the Fourier lattice. Algebraically, this leads to the isomorphism \( \mathbb{R}^D/\mathcal{T} = \hat{\mathcal{L}} \), where \( \hat{\mathcal{L}} \) denotes the linear maps from \( L \) to \( \mathbb{R}/\mathbb{Z} \) as in \( \mathcal{L} \). Thus space groups are classified by the cohomology group \( H^1(G, \hat{\mathcal{L}}) \), which is exactly the set of phase functions (identifying those that differ by a gauge transformation) described in §§1.1 and 3.2.

We now return to the point group 2\textit{mm} as in §3.1. Let \( \mathcal{T} \) denote the lattice in \( \mathbb{R}^2 \) dual to the Fourier lattice \( \mathcal{L} \) generated by \( a \) and \( b \). We will use the terminology of cocycles and coboundaries introduced in §3.2 with \( \Phi \) replaced by \( \mathbf{t} \). We will also use the notation \( \{g|\mathbf{t}\} \) for elements of the space group, where \( g \) is in the point group and \( \mathbf{t} \) is a translation (not necessarily in \( \mathcal{T} \)): this acts on the vector \( \mathbf{x} \) by the formula \( \{g|\mathbf{t}\}\mathbf{x} = g\mathbf{x} + \mathbf{t} \). It follows that \( \{g_1|\mathbf{t}_1\} \cdot \{g_2|\mathbf{t}_2\} = \{g_1g_2|\mathbf{t}_1 + g_1(\mathbf{t}_2)\} \).

For each element \( g \) of \( G = \{e, r, m, rm\} \), choose a translation \( \mathbf{t}_g \) such that \( \{g|\mathbf{t}_g\} \) is in the space group. By choosing the origin appropriately, we can arrange it so that \( \mathbf{t}_m \) lies along the \( \hat{x} \)-axis and \( \mathbf{t}_{rm} \) lies along the \( \hat{y} \)-axis. For each of the glide reflections \( \{m|\mathbf{t}_m\} \) and \( \{rm|\mathbf{t}_{rm}\} \), there are two possibilities: the translational part can lie in \( \mathcal{T} \), or it can be half of a translation in \( \mathcal{T} \). Since \( m \) and \( rm \) generate the point group, the choice of \( \mathbf{t}_m \) and \( \mathbf{t}_{rm} \) determines the space group. We shall see that the different possible choices lead to the four possibilities in Table 2. We shall postpone the verification that each of the four choices actually leads to a space group with translation subgroup \( \mathcal{T} \) and point group \( G \).

The definition of multiplication in the space group shows that the combination (cf. [3.7])

\[
(4.12) \quad d\mathbf{t}(g, h) \equiv \mathbf{t}_g - \mathbf{t}_{gh} + g(\mathbf{t}_h)
\]

is the translational part of \( \{g|\mathbf{t}_g\}\{h|\mathbf{t}_h\}\{gh|\mathbf{t}_{gh}\}^{-1} \) and so lies in \( \mathcal{T} \). In fact, \( d\mathbf{t} \) is a 2-cocycle with values in \( \mathcal{T} \).\(^{18}\) The choice of origin, mentioned above, does not change the value of \( d\mathbf{t} \). Choosing a different translation \( \mathbf{t}_g \) for each \( g \) would change \( d\mathbf{t} \) by a 1-coboundary, so it

---

\(^{16}\)The real-space approach cannot be used to describe quasicrystals with infinite point groups, but it is not clear that these are physically interesting.

\(^{17}\)This result applies because \( \mathcal{T} \) is a normal, Abelian subgroup of \( \mathcal{G} \).

\(^{18}\)If we allow cochains with values in \( \mathbb{R}^2 \), then \( \mathbf{t}_g \) is a 1-cochain and \( d\mathbf{t} \) is its boundary. It is therefore automatically a cycle. However, \( d\mathbf{t} \) is not necessarily the boundary of a 1-cochain with values in \( \mathcal{T} \).
makes sense to identify cocycles that differ by a coboundary. Thus $dt$ determines a class in $H^2(G, \mathcal{T})$, and this cohomology class corresponds to the given space group.

Another point of view is that one should not choose a particular $t_g$ but should consider all possible choices at once. In other words, instead of the vector $t_g$, consider its coset $t_g = t_0 + \mathcal{T}$, as an element of the quotient group $\mathbb{R}^2/\mathcal{T}$. From this point of view, $t$ is a 1-cochain with values in $\mathbb{R}^2/\mathcal{T}$. The fact that $dt$ takes values in $\mathcal{T}$ means that $t$ is a cocycle. A different choice of origin changes this cocycle by a coboundary. Thus the space group is described by the class of $t$ in $H^1(G, \mathbb{R}^2/\mathcal{T})$. The relation between $\bar{t}$ and $dt$ illustrates the general isomorphism between $H^1(G, \mathbb{R}^D/\mathcal{T})$ and $H^2(G, \mathcal{T})$.

The phase function that describes the space group is simply $\Phi_g(k) = k \cdot t_g$, where the dot product defines the duality pairing between Fourier and real space. Note that changing $t_g$ by a translation in $\mathcal{T}$ changes the phase by an integer, which we always ignore. This illustrates the general isomorphism between $H^1(G, \mathbb{R}^D/\mathcal{T})$ and $H^1(G, \hat{L})$. As promised, the four possible choices of $t_m$ and $t_{rm}$ indeed correspond to the four possibilities in Table 2. From either the Fourier-space point of view or the real-space one, two of the four space groups are equivalent under exchanging and rescaling the axes.

We already know, from §3.2 that $H^1(G, \hat{L})$ contains exactly four elements. Therefore, the isomorphism between $H^2(G, \mathcal{T})$ (which classifies space groups from the direct-space point of view) and $H^1(G, \hat{L})$ (the group of phase functions up to gauge equivalence) gives a roundabout verification of the point we omitted above: all four ways of choosing the glide reflections $t_m$ and $t_{rm}$ actually lead to space groups with translation subgroup $\mathcal{T}$ and point group $G$.

4.4. Is there a topological space for every crystal class? We have offered an analogy between the classification of space groups by group cohomology and some topological problems on manifolds. One can ask how deep the connection really goes. We might wish to know whether, for a point group $G$ with its action on a lattice $L$, we could always find a topological manifold $M$ and coefficient group $C$ such that

$$H_n(G, L) \cong H_n(M, C)$$

for all integers $n \geq 0$. We do not know, in general, whether such a manifold exists. However, there does exist a general construction for a topological space so that (4.13) works for $n = 1$. Since $H_1(G, L)$ is isomorphic to a finite direct product of cyclic groups $\mathbb{Z}_N = H_1(L_N, \mathbb{Z})$, where $L_N$ denotes the lens space $\mathbb{I}$ §24.4, the corresponding direct product of lens spaces has the desired first homology group $\mathbb{I}$ Prop. 0.8].

The topological view provides a picture of what one is doing in the Rokhsar-Wright-Mermin formulation. There, the task of finding all gauge invariants is complicated first by the possibility that these gauge invariants may be linear combinations of phase functions, as in (2.1), and second by the need to find a clever choice of gauge to make all values that are not invariant, or derivable from them, vanish. Viewed cohomologically, the second point is no concern, since the gauge-invariant values completely determine the phase function $\mathbb{I}$. The first complication is also no concern in the homological approach; the fact that (2.1) is a linear combination of terms simply reflects an inopportune choice of basis vectors for the cycle group $\mathbb{Z}_1$. A more convenient basis would include an invariant like $k_h[g] - k_g[h]$, and each basis element can be thought of as corresponding to a hole in a topological space.

---

19That is, just that part of the classification that concerns families of gauge-equivalent phase functions $\mathbb{I}$.
We wish to thank Edwin Clark, Mohamed Elhamdadi, and Veit Elser for useful conversations. This work was supported by the National Science Foundation through grants DMS-0204823 and DMS-0204845. DAR is a Cottrell Scholar of Research Corporation.

REFERENCES

1. Paul Alexandroff, *Elementary concepts of topology*, Translated by Alan E. Farley, Dover Publications Inc., New York, 1961.
2. Edgar Ascher and Aloysio Janner, *Algebraic aspects of crystallography. Space groups as extensions*, Helv. Phys. Acta 38 (1965), 551–572.
3. , *Algebraic aspects of crystallography. II. Non-primitive translations in space groups*, Comm. Math. Phys. 11 (1968/1969), 138–167.
4. A. Bienenstock and P. P. Ewald, *Symmetry of Fourier space*, Acta Crystallographica 15 (1962), 1253–61.
5. Kenneth S. Brown, *Cohomology of groups*, Graduate Texts in Mathematics, vol. 87, Springer-Verlag, New York, 1982.
6. Jörg Dräger and N. David Mermin, *Superspace groups without the embedding: The link between superspace and Fourier-space crystallography*, Physical Review Letters 76 (1996), no. 9, 1489–1492.
7. B. A. Dubrovin, A. T. Fomenko, and S. P. Novikov, *Modern geometry—methods and applications. Part II*, Graduate Texts in Mathematics, vol. 104, Springer-Verlag, New York, 1985, The geometry and topology of manifolds, translated from the Russian by Robert G. Burns.
8. Benji N. Fisher and David A. Rabson, in preparation.
9. , *Applications of group cohomology to the classification of crystals and quasicrystals*, submitted for publication, 2003.
10. Theo Hahn (ed.), *International tables for crystallography. Vol. A*, second ed., Published for the International Union of Crystallography, Chester, 1987, Space-group symmetry.
11. Howard Hiller, *Crystallography and cohomology of groups*, Amer. Math. Monthly 93 (1986), no. 10, 765–779.
12. David Jabon, *IntegerSmithNormalForm*, http://library.wolfram.com/database/MathSource/682, 1994.
13. T. Janssen and A. Janner, *Superspace groups and representations of ordinary space groups: alternative approaches to the symmetry of incommensurate crystal phases*, Phys. A 126 (1984), no. 1-2, 163–176.
14. Anja König and N. David Mermin, *Electronic level degeneracy in nonsymmorphic periodic or aperiodic crystals*, Physical Review B 56 (1997), no. 21, 13607–13610.
15. , *Screw rotations and glide mirrors: Crystallography in Fourier space*, Proc. Nat. Acad. Sci. USA 96 (1999), 3502–3506.
16. , *Symmetry, extinctions, and band sticking*, American Journal of Physics 68 (2000), 525–530.
17. André LeClair, 1991, private communication.
18. R. Lifshitz, *The symmetry of quasiperiodic crystals*, Phys. A 232 (1996), no. 3-4, 633–647, The nature of crystalline states (Kudowa-Zdrój, 1995).
19. N. David Mermin, *Bringing home the atomic world: Quantum mysteries for anybody*, American Journal of Physics 49 (1981), 940–943.
20. , *Quantum mysteries for anyone*, Journal of Philosophy 78 (1981), 397–408.
21. , *Copernican crystallography*, Physical Review Letters 68 (1992), 1172–1175.
22. , *The space groups of icosahedral quasicrystals and cubic, orthorhombic, monoclinic, and triclinic crystals*, Rev. Modern Phys. 64 (1992), no. 1, 3–49.
23. N. David Mermin, David A. Rabson, Daniel S. Rokhsar, and David C. Wright, *Stacking quasicrystallographic lattices*, Phys. Rev. B (3) 41 (1990), no. 15, 10498–10502.
24. N. David Mermin and Daniel S. Rokhsar, *Beware of 46-fold symmetry: The classification of two-dimensional quasicrystallographic lattices*, Physical Review Letters 58 (1987), no. 20, 2099–2101.
25. S. A. Piumikhin, *The relationship between various definitions of quasicrystallographic groups*, Mat. Zametki 52 (1992), no. 6, 74–80, 159, Translation in Math. Notes 52 (1992), no. 5-6, 1220–1224 (1993) ; MR 94f:20095.
26. David A. Rabson and Benji N. Fisher, *Fourier-space crystallography as group cohomology*, Physical Review B 65 (2002), 024201.
27. David A. Rabson, Tin-Lun Ho, and N. David Mermin, *Space groups of quasicrystallographic tilings*, Acta Cryst. A 45 (1989), 538–547.

28. David A. Rabson, N. David Mermin, Daniel S. Rokhsar, and David C. Wright, *The space groups of axial crystals and quasicrystals*, Rev. Modern Phys. 63 (1991), no. 3, 699–733.

29. Daniel S. Rokhsar, David C. Wright, and N. David Mermin, *Scale equivalence of quasicrystallographic space groups*, Physical Review B 37 (1988), 8145–8149.

30. *The two-dimensional quasicrystallographic space groups with rotational symmetries less than 23-fold*, Acta Crystallographica A 44 (1988), no. 2, 197–211.

31. Rolf L. E. Schwarzenberger, *n-dimensional crystallography*, Pitman (Advanced Publishing Program), Boston, Mass., 1980.

32. Karlheinz Spindler, *Abstract Algebra with Applications, Volume I*, Marcel Dekker, New York, 1994.

33. Michael Spivak, *Calculus on manifolds. A modern approach to classical theorems of advanced calculus*, W. A. Benjamin, Inc., New York-Amsterdam, 1965.

34. David Thouless, *Topological considerations*, The Quantum Hall Effect, second edition (Steven M. Girvin Richard E. Prange, ed.), Springer-Verlag, 1990.

35. Le Ty Kuok Tkhang, S. A. Plunikhin, and V. A. Sadov, *The geometry of quasicrystals*, Uspekhi Mat. Nauk 48 (1993), no. 1(289), 41–102, Translation in Russian Math. Surveys 48 (1993), no. 1, 37–100; MR 95a:52026.

36. Wolfram Research Inc., *Mathematica, version 4*, 1999.
Figure Captions

Figure 1. The manifold $M$, containing two holes, illustrates a topological space. $AB$, $C$, $D$, $E$, $F$, $G$, and $H$ are oriented 1-simplices; of these, all but $AB$ are 1-cycles. The 1-cycles $C$ and $E$ are 1-boundaries. In particular, $C$ is the boundary of sub-manifold $S$.

Figure 2. Figure 2a illustrates the torus $T$ (doughnut) embedded in Euclidean 3-space. Only the surface forms $T$. Figure 2b illustrates the same torus: the sides with double arrows are to be joined, generating a cylinder, and then the sides with single arrows. The triangulation consists of two 2-simplices, $\Delta$ and $\Gamma$, three 1-simplices, $b$, $c$, and $d$, and just a single 0-simplex (vertex), $A$. The 1-cycles $b$ and $c$ are also shown in Figure 2a.

Figure 3. The boundary of a 2-simplex (triangle) is the sum of its sides. According to (2.3), we have $(x_0, x_1) - (x_0, x_2) + (x_1, x_2) = -(x_1, x_0) + (x_1, x_2) + (x_2, x_0)$, in agreement with the orientations in the figure.

Figure 4. The projective plane $\mathbb{R}P^2$ (compare Figure 2b). Now, opposite sides are to be twisted before being glued together; we despair of showing what the result might look like in four dimensions. This triangulation consists of two 2-simplices, $\Psi$ and $\Upsilon$, three 1-simplices, $f$, $g$, and $h$, and two 0-simplices, $P$ and $Q$. Twice $h$ is a boundary, and modulo boundaries, $h$ is the only cycle.

Figure 5. It may help to elucidate chains to think of them geometrically; a chain $k[g]$ can be pictured as a circular arc pointing from $k$ to $gk$. The boundary $\partial a[r^3] = \partial a[r^{-1}] = a[r] + (ra)[r^2]$, as suggested by the three arcs.
Figure 1.
Figure 2a.
Figure 2b.
Figure 3.
Figure 4.
Figure 5.
