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Cohomology for Anyone[1]

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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.

KEY WORDS: crystallography; space groups; cohomology; homology; algebraic topology.

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.[24]

Applying cohomology, we have proven certain theorems[8, 9, 28] in more generality than they were previously known, including to cases with 46-fold[26] and other exotic rotational symmetries. Our purpose here, using

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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, field theories routinely refer to scalars as "charges," and the Kosterlitz–Thouless treatment of two-dimensional phase transitions has given rise to the description of vorticity as "topological charge."[36] 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, 11, 13, 33]

Similarly, Fourier-space crystallography, as first formulated by Bienenstock and Ewald[4] and developed by Mermin and collaborators,[6, 18–20, 23–25, 30, 32] 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 can be described by a global translation. 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.[4] 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

[4] 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.[17] 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, Piunikhin alluded briefly to the same thing.[27] 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.

in diffraction.[5] Later, Mermin and König[14–16] 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[9] and have also found a third type of invariant corresponding to neither extinctions nor König–Mermin band sticking.[8]

1.1. Fourier-Space Crystallography

In order to establish notation, we briefly review the Rokhsar–Wright–Mermin formulation of crystallography in Fourier space; see Ref. 6 or 18 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.[6] 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, $\rho(\mathbf{k})$ and $\rho'(\mathbf{k})$, are indistinguishable if all their n-body correlation functions are the same; this is equivalent to the condition

$$\rho'(\mathbf{k}) = e^{2\pi i \chi(\mathbf{k})}\rho(\mathbf{k}), \tag{1.1}$$

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

$$\rho(g\mathbf{k}) = e^{2\pi i \Phi_g(\mathbf{k})}\rho(\mathbf{k}). \tag{1.2}$$

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 *group-compatibility condition* for $g, h \in G$,

$$\Phi_{gh}(\mathbf{k}) = \Phi_g(h\mathbf{k}) + \Phi_h(\mathbf{k}), \tag{1.3}$$

[5] The absence of systematic extinctions in these two space groups, $I2_12_12_1$ and $I2_13$, was well known. What was new was the description of an algebraic invariant that "detects" that these two groups are non-symmorphic.

[6] 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 reciprocal lattice.

while two phase functions, Φ and Φ', describe indistinguishable densities if they are related by a gauge function, χ,

$$\Phi'_g(\mathbf{k}) = \Phi_g(\mathbf{k}) + \chi(g\mathbf{k} - \mathbf{k}), \tag{1.4}$$

and so are identified. The lattice L, the action of the point group G, and the phase function Φ 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 Φ and Φ' in (1.4) will have different values when evaluated for generic g and $\mathbf{k}$. However, certain linear combinations of phase functions are independent of gauge. Immediately from (1.4), we see that if g leaves $\mathbf{k}$ invariant, then $\Phi_g(\mathbf{k})$ 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 $\rho(\mathbf{k}) = 0$, 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 $\hat{\mathbf{x}}$-axis; let L be the lattice generated by vectors a and b along the $\hat{\mathbf{x}}$- and $\hat{\mathbf{y}}$-axes. Then it is not hard to check that $\Phi_m(ia + jb) = \Phi_{rm}(ia + jb) = i\frac{1}{2}$, $\Phi_e(\mathbf{k}) = \Phi_r(\mathbf{k}) = 0$ 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.[7] For further discussion of this example, see Sec. 3.2.

[7] 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.

This is not the only kind of invariant. Of course any integral linear combination (such as $\Phi_{g_1}(\mathbf{k}_1)+\Phi_{g_2}(\mathbf{k}_2)$ where $g_i\,\mathbf{k}_i=\mathbf{k}_i$) 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

$$\Phi_g(\mathbf{k}_h)-\Phi_h(\mathbf{k}_g), \tag{2.1}$$

where g and h commute and where neither term alone is gauge invariant. König and Mermin[14–16] define the lattice vectors $\mathbf{k}_g$ and $\mathbf{k}_h$ in terms of a point $\mathbf{q}$ *not* in the reciprocal lattice but with the property that

$$\mathbf{k}_g \equiv \mathbf{q}-g\mathbf{q} \qquad \text{and} \qquad \mathbf{k}_h \equiv \mathbf{q}-h\mathbf{q} \tag{2.2}$$

are. The group operations g and h are then elements of the *little group* of $\mathbf{q}$. We refer the reader to their papers or to Ref. 28 for the proof that if the invariant (2.2) is non-zero, *any* electronic energy level at wavevector $\mathbf{q}$ must be at least two-fold degenerate.[8]

2.2. Topological Invariants[9]

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 simplices, 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, and a chain with zero boundary is called a cycle.

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

[8] Expression (2.1) is a special case of what we refer to in Refs. 8 and 9 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.

[9] The elementary treatment of topology in this section draws on Alexandroff's slim introduction.[1]

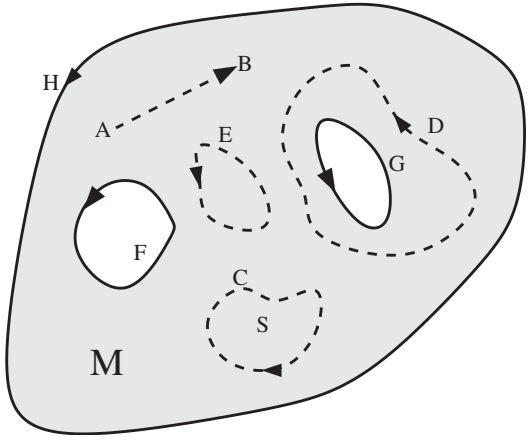


Fig. 1. The manifold M, containing two holes, illustrates a topological space. AB, C, D, E, F, G, and H are oriented 1-simplices; of these, all but AB are 1-cycles. The 1-cycles C and E are 1-boundaries. In particular, C is the boundary of submanifold S. The non-trivial cycles D and G are homologous to each other; they would not have been homologous (over $\mathbb{Z}$) if they had had opposite orientations.

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 $D = G+(D-G) \doteq G$, 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 *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[10] is $\mathbb{Z} \times \mathbb{Z}$.

[10] The homology group of these curves is called the first homology group; elsewhere[9, 28] 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.

The torus, T, of Fig. 2a (the surface of a doughnut, not the dough) cannot be deformed into the manifold of Fig. 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 Fig. 1, we start by describing a general method for calculating homology groups.

First we flatten the torus into the rectangle of Fig. 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) Δ and Γ. 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 Ref. 1 for theorems guaranteeing that the homology group is independent of these choices.

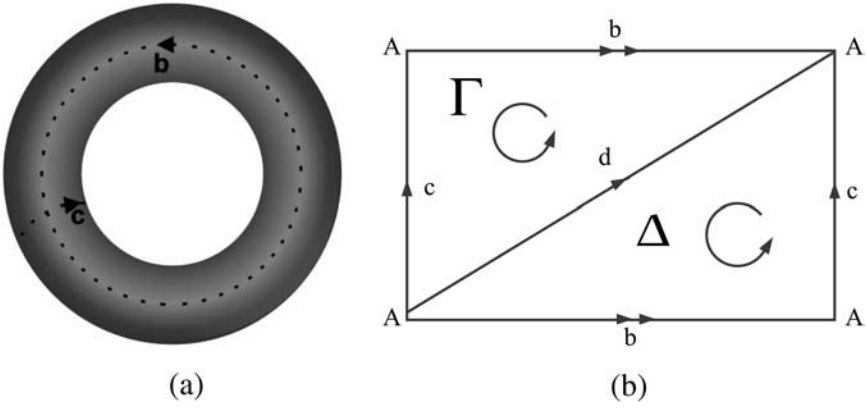


Fig. 2. Figure 2a illustrates the torus T (doughnut) embedded in Euclidean 3-space. Only the surface forms T. Figure 2b illustrates the same torus: the sides with double arrows are to be joined, generating a cylinder, and then the sides with single arrows. The triangulation consists of two 2-simplices, Δ and Γ, 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 Fig. 2a.

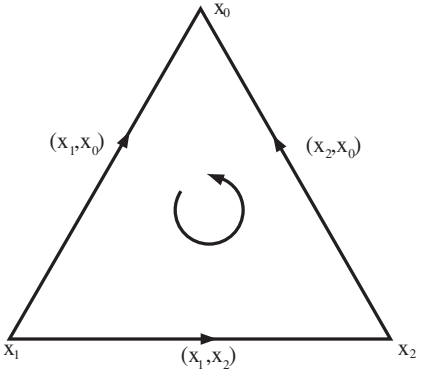


Fig. 3. The boundary of a 2-simplex (triangle) is the sum of its sides. According to (2.3), we have $\partial(x_0, x_1, x_2) = (x_0, x_1) - (x_0, x_2) + (x_1, x_2) = -(x_1, x_0) + (x_1, x_2) + (x_2, x_0)$, in agreement with the orientations in the figure.

Labeling a 1-simplex by its endpoints (which may be the same point) and a 2-simplex (triangle) by its vertices,[11] we define the *boundary operator* ∂ by

$$\begin{aligned} \partial(x_0, x_1) &= x_1 - x_0 \qquad \text{and} \\ \partial(x_0, x_1, x_2) &= (x_0, x_1) - (x_0, x_2) + (x_1, x_2). \end{aligned} \tag{2.3}$$

For example, in Fig. 2b, $\partial b = \partial c = \partial d = 0$, and

$$\begin{aligned} \partial \Gamma &= -b - c + d, \\ \partial \Delta &= b + c - d. \end{aligned} \tag{2.4}$$

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 (Fig. 3) (x_0, x_1, x_2) is the sum of its sides, if we accept the convention that $(x_0, x_2) \doteq -(x_2, x_0)$.

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.

[11] 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.

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

$$H_1 = Z_1 / B_1, \tag{2.5}$$

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) 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:

$$Z_1 = \langle b, c, d \rangle, \tag{2.6}$$

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

$$H_1(T, \mathbb{Z}) = \mathbb{Z}^3 / \mathbb{Z} = \mathbb{Z} \times \mathbb{Z}. \tag{2.7}$$

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 D in Fig. 1 once is identified with traversing the oppositely-oriented simplex once, we have $-D \doteq -D + 2D = D$, 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:

$$H_1(M, \mathbb{Z}_2) = H_1(T, \mathbb{Z}_2) = \mathbb{Z}_2 \times \mathbb{Z}_2. \tag{2.8}$$

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

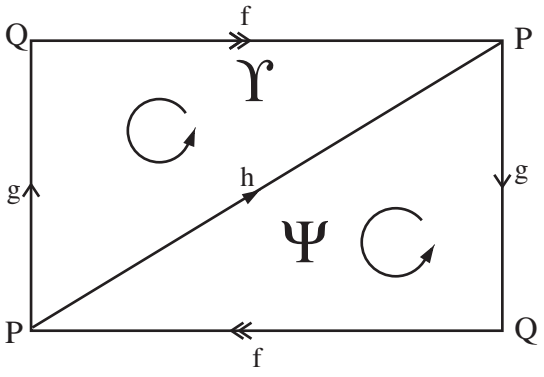


Fig. 4. The projective plane $\mathbb{R}P^2$ (compare Fig. 2b). Now, opposite sides are to be twisted before being glued together; we despair of showing what the result might look like in four dimensions. This triangulation consists of two 2-simplices, Ψ and Υ, three 1-simplices, f, g, and h, and two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

now opposite sides are identified in opposite directions, as in Fig. 4.[12] The triangulation of the figure comprises the two 0-simplices P and Q, three 1-simplices, f, g, and h, and two 2-simplices, Υ and Ψ. It is easy to see that all 1-cycles are generated by h and $f+g$. We determine the boundaries by

$$\begin{aligned} \partial\Upsilon &= h-f-g, \\ \partial\Psi &= -h-f-g. \end{aligned} \tag{2.9}$$

Thus $2h=\partial\Upsilon-\partial\Psi$ is a boundary, but the 1-cycle h is not. The other generating 1-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

$$H_1(\mathbb{R}P^2, \mathbb{Z}) = H_1(\mathbb{R}P^2, \mathbb{Z}_2) = \mathbb{Z}_2. \tag{2.10}$$

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

$$V-E+F=2, \tag{2.11}$$

[12] 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*.

where V, E, and F denote the numbers 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

$$\chi(S) = \text{rank } H_0(S) - \text{rank } H_1(S) + \text{rank } H_2(S), \tag{2.12}$$

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 $\mathbf{F} = P\hat{\mathbf{x}} + Q\hat{\mathbf{y}}$ be a vector field in the plane. If $\mathbf{F}$ is the gradient of a potential ϕ, 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

$$\mathbf{F} = \frac{x\hat{\mathbf{y}} - y\hat{\mathbf{x}}}{x^2 + y^2}. \tag{2.13}$$

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 δ-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 I. Summary of Some of the Relations between Homology and de Rham Cohomology

	homology	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 $H^1_{\mathrm{DR}}(M)$.

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, $\langle c, \mathbf{F} \rangle = \oint_c \mathbf{F} \cdot d\mathbf{r}$. To see that this is well defined on (co)homology, it is enough to notice that $\oint_c \mathbf{F} \cdot d\mathbf{r} = 0$ if c is any cycle and $\mathbf{F}$ is conservative (fundamental theorem of calculus) or if c is a boundary and $\mathbf{F}$ is irrotational (Green's Theorem).

The language of differential forms[35] 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 ω, 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 ω a 1-*cocycle*. This resembles the cycle condition in homology, except that where ∂ 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, ϕ, 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.[13] Table I 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.

[13] 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.

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 Φ_g, one for each element of the point group, think of the phase function Φ 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.[14] Since the phase function is linear on the lattice, it acts distributively over addition. Thus, for example,

$$\Phi(\mathbf{a}[g]+\mathbf{b}[g]+\mathbf{c}[h]) = \Phi((\mathbf{a}+\mathbf{b})[g]+\mathbf{c}[h]) = \Phi_g(\mathbf{a}+\mathbf{b})+\Phi_h(\mathbf{c}). \quad (2.14)$$

Define the boundary operator on a 1-chain by analogy to (2.3):

$$\partial\mathbf{k}[g] = g\mathbf{k}-\mathbf{k}, \quad (2.15)$$

so that for a general 1-chain $c = \sum_i \mathbf{k}_i[g_i]$,

$$\partial c = \sum_i g_i\mathbf{k}_i - \mathbf{k}_i. \quad (2.16)$$

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 Φ and Φ' evaluated on the 1-cycle c,

$$\Phi'(c)-\Phi(c) = \chi\left(\sum_i g\mathbf{k}_i - \mathbf{k}_i\right) = 0. \quad (2.17)$$

Thus cycles are gauge invariants, and since χ 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

$$b = h\mathbf{k}[g]-\mathbf{k}[gh]+\mathbf{k}[h] \quad (2.18)$$

is a 1-cycle. However, *any* phase function Φ 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

[14] Since the lattice is not a field, the 1-chains form a module instead of a vector space.

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 $\mathbf{k}[g\,|\,h]$:

$$\partial\mathbf{k}[g\,|\,h] \equiv h\mathbf{k}[g] - \mathbf{k}[gh] + \mathbf{k}[h]. \tag{2.19}$$

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,[28] 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 $h\mathbf{k}$ in the first term on the right instead of just $\mathbf{k}$.

There is a way of visualizing 1-chains in group homology that emphasizes the analogy with 1-cycles in topology: picture the 1-chain $\mathbf{k}[g]$ as a vector going from $\mathbf{k}$ to $g\mathbf{k}$. If g is a rotation, it is suggestive to draw the vector along a circular arc, as in Fig. 5, in which r denotes a 90° rotation.

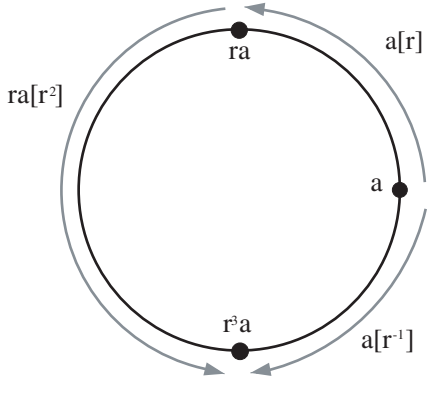


Fig. 5. It may help to elucidate chains to think of them geometrically; a chain $\mathbf{k}[g]$ can be pictured as a circular arc pointing from $\mathbf{k}$ to $g\mathbf{k}$. The 1-chain $\mathbf{a}[r^3] = \mathbf{a}[r^{-1}]$ is equivalent to $\mathbf{a}[r] + (r\mathbf{a})[r^2]$, as suggested by the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

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 $\mathbf{k}[gh] \doteq \mathbf{k}[h] + (h\mathbf{k})[g]$, where $\doteq$ denotes homology as in Sec. 2.2. This is also consistent with the vector picture: for example, Fig. 5 illustrates the fact that $\mathbf{a}[r^3] \doteq \mathbf{a}[r] + (r\mathbf{a})[r^2]$. One shortcoming of this method is that it does not illustrate linearity relations, such as $(\mathbf{a}+\mathbf{b})[g] = \mathbf{a}[g] + \mathbf{b}[g]$ and $(-\mathbf{a})[g] = -(\mathbf{a}[g])$.

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 $\hat{\mathbf{x}}$ direction and a vector b of different length in the $\hat{\mathbf{y}}$ 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 Sec. 7 of Ref. 28. In Sec. 4.1, we show how the entire calculation can be automated in the symbolic-algebra program, *Mathematica*,[38] 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 $\mathbf{k}[g]$ where $\mathbf{k}$ is a lattice generator. (Any other 1-chain is an integral linear combination of these.)

$$\begin{aligned} \partial a[e] &= 0, & \partial b[e] &= 0, \\ \partial a[m] &= 0, & \partial b[m] &= -2b, \\ \partial a[rm] &= -2a, & \partial b[rm] &= 0, \\ \partial a[r] &= -2a, & \partial b[r] &= -2b. \end{aligned} \tag{3.1}$$

From these eight values, we read off the generators of the additive group of cycles (the angle brackets mean "generated by"):

$$Z_1(G, L) = \langle z_1, z_2, z_3, z_4, z_5, z_6 \rangle, \tag{3.2}$$

where

$$\begin{aligned} z_1 &= b[e], & z_4 &= a[e], \\ z_2 &= -b[r]+b[m], & z_5 &= a[m], \\ z_3 &= b[rm], & z_6 &= a[rm]-a[r]. \end{aligned} \tag{3.3}$$

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

$$\begin{aligned} b_1 &\equiv \partial a[e\,|\,e] = a[e], \\ b_2 &\equiv \partial b[e\,|\,e] = b[e], \\ b_3 &\equiv \partial a[r\,|\,m] = a[r]+a[m]-a[rm], \\ b_4 &\equiv \partial a[m\,|\,r] = a[r]-a[m]-a[rm], \\ b_5 &\equiv \partial b[r\,|\,m] = -b[r]+b[m]-b[rm], \\ b_6 &\equiv \partial b[m\,|\,r] = b[r]-b[m]-b[rm]. \end{aligned} \tag{3.4}$$

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[15]

$$B_1(G, L) = \langle b_1, b_2, b_3, b_4, b_5, b_6 \rangle. \tag{3.5}$$

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 $z_5 \doteq z_6$ (equality up to boundaries); similarly, $z_2 \doteq z_3$. 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:

$$H_1(G, L) = \{0, z_3, z_5, z_3 + z_5\}. \tag{3.6}$$

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 Φ, linear

[15] In Sec. 4.2, we prove that Z_1 and B_1 always have the same rank.

Table II. The Four Sets of Gauge-Invariant Values a Phase Function Might Take for the Point Group 2*mm* on the Primitive-Rectangular Lattice. These Correspond to the Plane Groups *p*2*mm*, *p*2*mg*, *p*2*gm* (Which Is Just a Different Setting of *p*2*mg*), and *p*2*gg*

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

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 II.

We now make two assertions, the proof of which is the main content of Ref. 28. 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.

The proof in Ref. 28 rests on the duality of homology and cohomology, in which Φ plays the same role with respect to a chain $\sum \mathbf{k}[g]$ as the vector field $\mathbf{F}$ played with respect to a contour in Sec. 2.3. Think of Φ as acting on g to give Φ_g; Φ_g acts linearly on $\mathbf{k} \in L$ to give the number $\Phi_g(\mathbf{k})$, modulo unity as always. The 1-cochains form a group under addition. A 1-cochain is a 1-*cocycle* if its coboundary, defined by

$$(d\Phi)(g, h) = \Phi_g \circ h - \Phi_{gh} + \Phi_h, \tag{3.7}$$

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

$$(d\chi)(g) = \chi \circ g - \chi. \tag{3.8}$$

Two different 1-cochains Φ and Φ' 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 χ is an element of $\hat{L}$, then $2\pi i\chi(\mathbf{k})$ is a choice of phase for each

Table III. Summary of the Application of Group Homology and Cohomology to Fourier-Space Crystallography. (For additional applications and higher-order (co)homology, see Refs. 9 and 28.) Symbols: $\mathbf{k}_i$ Are Reciprocal-Lattice Vectors and g_i Point-Group Elements. Φ Is a Phase Function. Compare Table I

	homology	cohomology
1-(co)chain	$\sum_i \mathbf{k}_i[g_i]$	Φ
1-(co)cycle	gauge invariant	satisfies group compatibility
1-(co)boundary	trivial by group compatibility	trivial by gauge transformation

k among a generating set for the lattice L. Table III 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 II earlier are exactly the four possible space groups for this example.

However, there are only three space groups for 2*mm* on the primitive rectangular lattice: *p*2*mm*, *p*2*mg*, and *p*2*gg*. Possibilities 2 and 3 in the table simply exchange the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions.[16]

3.3. Comparison to Torus and Lemniscate

Table II shows that the homology (or cohomology) group of the point group 2*mm* 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 Sec. 2.2.[17] The topological examples contained two holes in the sense of closed curves that did not bound: Fig. 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

[16] Once cohomology has been calculated, it is still necessary to consider rotations and (in quasiperiodic cases) scale invariance of the lattice. See Refs. 6 and 18 for a full accounting of *Bravais class*, *arithmetic crystal class*, and *space-group type*.

[17] 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 $\mathbb{Z}$.

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 Sec. 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 Sec. 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, 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 Sec. 3.1 are the matrices

$$r = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad m = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.1}$$

   acting on the column vectors $a = \binom{1}{0}$ and $b = \binom{0}{1}$.
2. The group C_1 of all 1-chains is generated by the combinations $\mathbf{k}[g]$, where $\mathbf{k}$ is a lattice generator and $g \in G$. The computer stores all these combinations in the list c. Think of this list, say $\mathsf{c} = (c_1, \ldots, c_r)$, as a column vector.
3. Take the boundary (2.16) of each c_i. The inullspace[] function, applied to the list of boundaries, gives a matrix z that expresses generators z_i of the cycle group Z_1 in terms of c:

$$\begin{pmatrix} z_1 \\ \vdots \\ z_s \end{pmatrix} = \mathsf{z} \begin{pmatrix} c_1 \\ \vdots \\ c_r \end{pmatrix}. \tag{4.2}$$

4. The group C_2 of all 2-chains is generated by the combinations $\mathbf{k}[g\,|\,h]$, where $\mathbf{k}$ is a lattice generator and $g, h \in G$. The boundaries b_i of these 2-chains (2.19) generate the group B_1 of 1-boundaries. Express these generators in terms of c:

$$\begin{pmatrix} b_1 \\ \vdots \\ b_t \end{pmatrix} = \mathsf{bz3} \begin{pmatrix} c_1 \\ \vdots \\ c_r \end{pmatrix}. \tag{4.3}$$

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 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 LatticeReduce[] to find the smallest set of rows that will generate B_1 over the integers, yielding the matrix b. Thus

$$\begin{pmatrix} b_1 \\ \vdots \\ b_s \end{pmatrix} = \mathsf{b} \begin{pmatrix} z_1 \\ \vdots \\ z_s \end{pmatrix} \tag{4.4}$$

gives a minimal set of generators for B_1. We explain in Sec. 4.2 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 [Ref. 34, Thm. 25.26],[12] of the matrix b is a diagonal matrix d such that there are invertible integral transformations p and q with

$$\mathsf{d} = \mathsf{p}\,\mathsf{b}\,\mathsf{q}. \tag{4.5}$$

Thus q and p describe new bases for Z_1 and B_1, say $\{z_i'\}$ 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 $d_i z_i' \doteq 0$.

7. Our function SpacegroupH1Full[] returns the matrices c, z, b, d, p, and q above.

Returning again to the example of Sec. 3.1, we find

$$\mathsf{d} = \mathrm{diag}(1, 1, 1, 1, 2, 2). \tag{4.6}$$

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:

$$\mathsf{p}^{-1}\,\mathrm{diag}(0,\,0,\,0,\,0,\,1,\,1)\,\mathsf{q}^{-1}. \tag{4.7}$$

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 Sec. 3.1:

$$\begin{aligned} z'_5 &= -z_2 \doteq z_3, \\ z'_6 &= \;\; z_6 \;\; \doteq z_5. \end{aligned} \tag{4.8}$$

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., $2^j mm = \{4mm, 8mm, (16)mm, \ldots\}$, all at once[29] but rather requires a separate calculation for each. However, we find it useful in those cases (such as 46-fold symmetry and modulated

Table IV. The Substantive Lines of *Mathematica* Code Described in Sec. 4.1. The Circled Numbers Refer to the Steps Listed in the Text. The Full Version of the Code Is Available at the Preprint Archive, cond-mat/0301601. The inullspace[ ] Call Replaces the Built-in NullSpace[ ] Function which, Under Certain Circumstances, Returns for an Integer Matrix a Basis for the Null Space over the Rationals Rather than Over the Integers

```
        (* For g a list of matrices, return <g>, the group generated. *)
    groupgen[g_] := FixedPoint[Union[Flatten[Outer[Dot,#,g,1],1],#]&, g]
        (* Project a term of form (v1 y[g1]) onto elements of c1. *)
    c1proj[x_,c1_] := ( (x/.{y[g_] -> If[g==#[[2]],1,0]}).#[[1]] )& /@ c1
①   latnum = Dimensions[x[[1]][[1]]][[1]]; (* x = list of generators *)
    latgen = IdentityMatrix[latnum];
    group = groupgen[x];
②   c = Distribute[{latgen,group}, List];
③   z = inullspace[Transpose[(#[[2]].#[[1]] - #[[1]])& /@ c]];
④   c2 = Distribute[{latgen,group,group}, List];
    bz2 = Union[((#[[3]].#[[1]])y[#[[2]]] - #[[1]]y[#[[2]].#[[3]]]
        +#[[1]]y[#[[3]]])& /@ c2];
    bz3 = Union[(c1proj[#,c])& /@ bz2];
⑤   z2 = Chop[Rationalize[PseudoInverse[N[z]]]];
⑥   b = LatticeReduce[Rationalize[Chop[bz3.z2]]];
    {d,{p,q}} = ExtendedSmithForm[b];
```

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.[37] 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 Sec. 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 Sec. 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 s 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 Nz_i is a boundary for each generator z_i, then $\mathsf{b}'\mathsf{b} = NI_s$ 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 $z = \sum_h \mathbf{k}_h[h]$ 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

$$\sum_h h\mathbf{k}_h = \sum_h \mathbf{k}_h. \tag{4.9}$$

Construct a 2-chain c such that $\partial c = Nz$ using the fundamental technique of averaging over the group: let

$$c = \sum_{g,h} \mathbf{k}_h[g \mid h]. \tag{4.10}$$

According to (2.19),

$$\partial c = \sum_{g,h} (h\mathbf{k}_h)[g] - \sum_{g,h} \mathbf{k}_h[gh] + \sum_{g,h} \mathbf{k}_h[h]. \tag{4.11}$$

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 Nz.

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 (Sec. 2.4) is a special case of one such theorem, the duality between homology and cohomology. The calculation of invariants (Secs. 3.1 and 4.1) is one example of a standard technique. The finiteness result (Sec. 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 Ref. 5, 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 $2mm$.

In real-space crystallography, one considers a crystal and its *space group* $\mathcal{G}$. 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, $\mathcal{G}$ will be the space group of the higher-dimensional, periodic crystal.[18] (In the periodic case, take $D = d$.) Let $\mathcal{T}$ denote the lattice of pure real-space translations in $\mathcal{G}$.

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 $\mathcal{T}$ are fairly easy to describe: G is a finite subgroup of the orthogonal group,[19] and $\mathcal{T}$ consists of all integral linear combinations of D generating vectors. These two

[18] Different choices of the periodic D-dimensional crystal may lead to different D-dimensional space groups.[31]

[19] The real-space approach cannot be used to describe quasicrystals with infinite point groups, but it is not clear that these are physically interesting.

groups are also fairly easy to determine experimentally. It remains to describe the space group $\mathscr{G}$ in terms of these two simpler groups. One possibility is that the point group is contained in $\mathscr{G}$, and the space group is generated by G and $\mathscr{T}$. 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 $\mathscr{T}$ are classified by the cohomology group[20] $H^2(G, \mathscr{T})$. Using the Long Exact Sequence of cohomology (cf. the last remark in Sec. 5 of Ref. 11), this is isomorphic to $H^1(G, \mathbb{R}^D/\mathscr{T})$.

In the periodic case, the Fourier lattice L is the dual of the translation group $\mathscr{T}$. 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 $\mathscr{T}$. (Those who worry about where the factor of 2π went should refer to (1.1) and (1.2).) Dräger and Mermin[6] realized that this can be turned around in the quasiperiodic case: the translation group $\mathscr{T}$ 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 $\mathbb{R}^D/\mathscr{T} = \hat{L}$, where $\hat{L}$ denotes the linear maps from L to $\mathbb{R}/\mathbb{Z}$ as in Sec. 3.2. Thus space groups are classified by the cohomology group $H^1(G, \hat{L})$, which is exactly the set of phase functions (identifying those that differ by a gauge transformation) described in Secs. 1.1 and 3.2.

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

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

[20] This result applies because $\mathscr{T}$ is a normal, Abelian subgroup of $\mathscr{G}$.

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

$$d\mathbf{t}(g,h) \equiv \mathbf{t}_g - \mathbf{t}_{gh} + g(\mathbf{t}_h) \tag{4.12}$$

is the translational part of $\{g \mid \mathbf{t}_g\}\{h \mid \mathbf{t}_h\}\{gh \mid \mathbf{t}_{gh}\}^{-1}$ and so lies in $\mathscr{T}$. In fact, $d\mathbf{t}$ is a 2-cocycle with values in $\mathscr{T}$.[21] 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 makes sense to identify cocycles that differ by a coboundary. Thus $d\mathbf{t}$ determines a class in $H^2(G, \mathscr{T})$, and this cohomology class corresponds to the given space group.

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

The phase function that describes the space group is simply $\Phi_g(\mathbf{k}) = \mathbf{k} \cdot \mathbf{t}_g$, where the dot product defines the duality pairing between Fourier and real space. Note that changing $\mathbf{t}_g$ by a translation in $\mathscr{T}$ changes the phase by an integer, which we always ignore. This illustrates the general isomorphism between $H^1(G, \mathbb{R}^D/\mathscr{T})$ and $H^1(G, \hat{L})$. As promised, the four possible choices of $\mathbf{t}_m$ and $\mathbf{t}_{rm}$ indeed correspond to the four possibilities in Table II. 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 Sec. 3.2, that $H^1(G, \hat{L})$ contains exactly four elements. Therefore, the isomorphism between $H^2(G, \mathscr{T})$ (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 round-about verification of the point we omitted above: all four ways of choosing the glide reflections $\mathbf{t}_m$ and $\mathbf{t}_{rm}$ actually lead to space groups with translation subgroup $\mathscr{T}$ and point group G.

[21] If we allow cochains with values in $\mathbb{R}^2$, then $\mathbf{t}_g$ is a 1-cochain, and $d\mathbf{t}$ is its coboundary, which is therefore automatically a cocycle. However, $d\mathbf{t}$ is not necessarily the coboundary of a 1-cochain with values in $\mathscr{T}$.

4.4. Is There a Topological Space for Every Crystal Class?

We have offered an analogy between the classification of space groups[22] 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

$$H_n(G, L) \stackrel{?}{\cong} H_n(M, C) \tag{4.13}$$

for *all* integers $n \geqslant 0$. 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* [Ref. 7, Sec. 24.4], the corresponding direct product of lens spaces has the desired first homology group [Ref. 5, 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 invariants, or derivable from them, vanish. Viewed cohomologically, the second point is no concern, since the gauge-invariant values completely determine the phase function.[28] 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 Z_1. A more convenient basis would include an invariant like $\mathbf{k}_h[g] - \mathbf{k}_g[h]$, and each basis element can be thought of as corresponding to a hole in a topological space.

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[22] That is, just that part of the classification that concerns families of gauge-equivalent phase functions.[6]

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