Crystallographic Groups

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Introduction

These are notes on n-dimensional space groups, also known as crystallographic groups, or in two-dimensions, wallpaper groups. (Originally written up in 2011.)

Space groups provide an excellent introduction to many concepts of group theory, including group cohomology. They also play a fundamental role in crystallography and solid-state physics. Finally, Escher's drawings furnish lovely illustrations of all the wallpaper groups except one.

Note: the word "Fact" is used to signal that the following assertion, although true, may not be obvious; the proof may even be quite difficult.

Notation and Basic Concepts

E will denote n-dimensional Euclidean space throughout, and **V** will denote the n-dimensional vector space. **V** is basically **E** plus a distinguished point, the origin (always denoted O). Isom(**E**) is the group of isometries of **E**. Trans(**E**) is the subgroup of translations (a normal subgroup, as we'll soon see).

Elements of Isom(**E**) will be denoted by lower-case greek letters; τ usually denotes a translation.

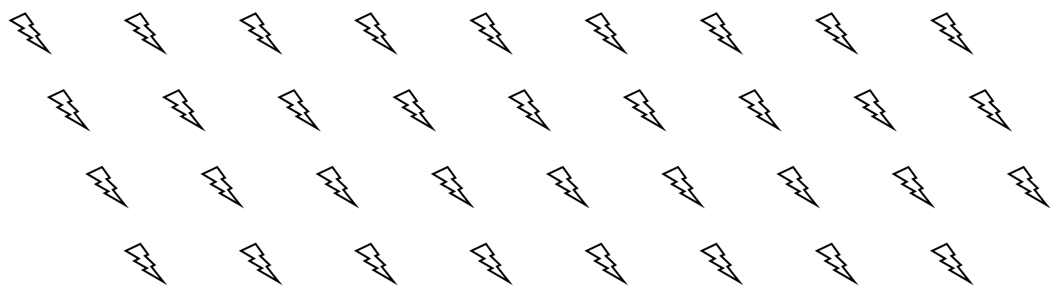
Points and vectors are denoted by lower-case latin letters. If p is a point and t is a vector, then $p+t$ stands for p translated by t.

There is an obvious canonical one-one correspondence between vectors and translations. If τ is the translation corresponding to t, then τp stands for the same point $p+t$. In general, τ_t is the translation corresponding to t. Because of the fundamental importance of this correspondence, we introduce a special notation for it: $t \Leftrightarrow \tau$ (or $\tau \Leftrightarrow t$) indicates that the vector t and the translation τ correspond.

A **space group** is a subgroup G of Isom(**E**) with the property that the translation subgroup $G \cap$Trans(**E**) is a finitely generated abelian group of rank n. Using the correspondence between translations and vectors, we can restate this: there are n vectors $t_1,\dots,t_n$ such that every translation in G corresponds to an integral linear combination of the t's. T will always stand for the translation subgroup of G.

Pick a point O in **E** to serve as the origin. Apply all elements of the translation subgroup T of G to it. We get the so-called **lattice** of G. The term is also applied to the corresponding set of vectors. The lattice of points is easy to picture. The lattice of vectors is a finitely generated abelian group, aka a **Z**-module. Likewise, of course, for the isomorphic group T.

Note that the point lattice depends on the choice of O, but the vector lattice does not. It is often useful, for pictorial reasons, to attach a little figure (called a motif) to each point in the lattice. Here's an example:



If we have chosen a set of basis vectors for **V**, say $v_1,\ldots,v_n$, it is also sometimes helpful to imagine "copies" of $v_1,\ldots,v_n$ attached to every lattice point.

Fact: a subgroup of Isom(**E**) is a space group iff (a) its point lattice is discrete (has no accumulation points), and (b) there is compact subset of **E** whose translates (via elements of the subgroup T) cover **E**. We won't need this fact, which was originally (for general n) a Hilbert problem.

O(n), Linear Maps, and the Point Group

Pick a point O in **E** to serve as the origin. That gives us a canonical one-one correspondence between **E** and **V**. Fact: every element ρ of Isom(**E**) can be written uniquely in the form

$$\rho x = Rx+t$$

where x does double-duty, standing for a point in **E** on the left, and the corresponding vector in **V** on the right; also R is a orthogonal linear map on **V**, and t is a vector in **V**. If we need to be more explicit about the distinction between points and vectors, we write this as:

$$\rho(O+x) = O + Rx+t$$

We will see shortly how R and t depend on the choice of O.

Notation: the group of all orthogonal linear maps is traditionally denoted O(n). Upper case latin letters will be used for elements of O(n). $[t{:}R]$ stands for the isometry $x \to Rx+t$, or $[t{:}R]_O$ if we want to make the choice of origin explicit.

We now do a simple computation for the group law in Isom(**E**):

$$\rho\sigma x = R(Sx+u)+t = RSx + Ru + t$$

so
$$[t{:}R]\,[u{:}S] = [t+Ru : RS]$$

We see immediately that the map sending $[t{:}R]$ to R is a homomorphism. The image, a subgroup of $O(n)$, is called the **point group** of G, and is denoted G_0. We see that the kernel is precisely the translation subgroup T, which is therefore a normal subgroup, as promised.

Finally, G_0 is isomorphic to G/T, by the first isomorphism theorem. We can regard the point group as a group of linear transformations, or more abstractly as a set of cosets of T.

The mapping $\rho = [t{:}R]$ to R is fundamental; we will see in the next section that it does not depend on the choice of origin. We denote this mapping by $\rho \Rightarrow R$.

In crystallography, the point group has a very natural physical interpretation. Basis vectors for T will be *very* microscopic — the typical interatomic distance in a crystal is less than a billionth of a meter. Thus many translations will not be visible to the naked eye[1].

Furthermore, every R in G_0 will look like an actual symmetry of the crystal to the naked eye[2]. For example, suppose we have a glide rotation $[t{:}R]$ where R is a 60° rotation. What if t is macroscopic, say length 1 cm? Well, then, compose $[t{:}R]$ with an element of T to get another glide rotation, say $[t-u{:}R]$, mapping to the same R. Since u can be any integral linear combination of basis vectors, we can get a glide rotation where the glide part is microscopic. To the naked eye, it looks like a pure 60° rotation.

Shifting to a New Origin

Suppose $[t{:}R]_O \in G$. We want to know what happens to t and R if we shift from O to a new origin, say O'. Let u be the vector pointing from the old origin to the new one; in other words, $O+u = O'$.

Result: R doesn't change, but t is replaced with $t + Ru-u$.

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[1] Since a real crystal is a finite hunk of rock, and not an infinite lattice, *none* of the translations is actually "visible to the naked eye" — the macroscopic one visibly move the rock.

[2] This statement also should be taken with few grains of salt. Literally: the point group for salt is the group of all symmetries of the cube. However, grains of salt won't usually be perfect cubes; the growth conditions might have favored one facet over another. Another example: 99.9% of snow crystals "in the wild" are misshapen clumps of ice, not displaying the familiar sixfold symmetry. The first photographer to compile a large collection selected just the pretty ones. So a more correct statement is, symmetries of the point group *can be* visible to the naked eye.

However, even if the so-called **crystal habit** does not manifest a point group symmetry, it can still be detected by studying the angles between facets. X-ray crystallography can reveal both point group and space group symmetries.

This is a simple computation: suppose a point p corresponds to vectors x and x' under the old and new origin (i.e., $p = O+x = O'+ x' = O + u + x'$ so $x = x'+u$). Let $\rho = [t{:}R]_O$. Then $\rho(O+x) = O+Rx+t = O+R(x'+u)+t = O+R\,x'+Ru+t = (O'-u)+R\,x'+Ru+t$, or

$$\rho(O'+ x') = O'+Rx' + t+Ru-u$$

so
$$\rho p = [t+Ru-u : R]_{O'}\, p$$

so
$$[t : R]_{\text{old}} \rightarrow [t+Ru-u : R]_{\text{new}}$$

Here is another, more visual way to look at it. Picture a vector attached to O, and the same vector (parallel and same length) attached to O'. By "attached", we mean that you should picture the vector emanating from the given point. The isometry ρ preserves parallelism and length of vectors. So ρ acts the same on the direction of the vector regardless of where it is attached. For example, if we are in the plane, and if ρ rotates the vector at O by 73°, then it will still change the direction of the vector by 73° when it is attached at O'. Or to take a 3D example, if ρ reflects the vector across some plane, it continues to do so even if we change the basepoint of the vector. Since R describes essentially how ρ affects the directions of vectors, it follows that R does not depend on the choice of origin.

We figure out the translation part of ρ by tracking what happens to a single point. The best choice of point is O'. O' moves from $O+u$ to $O+Ru$ to $O+Ru+t$, net change $Ru-u+t$.

Note: R does not depend on the choice of origin! So the homomorphism $\rho \Rightarrow R$ is also origin-independent, and the point group (regarded as a group of linear transformations) is also origin-independent.

2D and 3D examples and special cases

The choice of origin plays a subtle but crucial role in the theory of space groups; we will see that it is at the heart of the group cohomology of these groups. A few examples will strengthen our intuition.

First consider the planar case. Say we have a rotation by angle θ around O, followed by a translation by vector t. As we've just discovered, that's the same as rotation by angle θ around O', followed by translation by $t + Ru-u$, where as before, u is the vector from O to O', and R is the rotation. Special case: if $t + Ru-u = 0$, then we have a pure rotation about O'. Now, $Ru-u$ can be any vector we want by suitable choice of u. (Algebraically, $R-1$ is an invertible matrix.) So a rotation followed by a translation is always a rotation about some center. Conversely, a rotation about one center is the same as a rotation about some other center followed by a translation.

Next, say we have a reflection through a line l passing through O, followed by a translation by vector t. That's the same as a reflection through the line l' passing through O' and parallel to l, followed by translation by $t + Ru-u$, where now R is the reflection.

This time, $Ru-u$ is always perpendicular to l. (Algebraically, $R-1$ is no longer invertible, but has rank 1 instead.) So reflection followed by translation is a pure reflection when and only when the translation is perpendicular to the line of reflection. Conversely, a reflection through one line is the same as a reflection through a parallel line followed by a translation perpendicular to the line.

Suppose R is a reflection through a line l, and t is not perpendicular to l. We can decompose t into components perpendicular and parallel to l, say $t = t_\perp + t_\|$. Then R followed by $t_\perp$ is reflection through some line l' parallel to l. To get the full $[t{:}R]$ effect, we then have to follow with $t_\|$. In other words, a glide reflection can always be regarded as one where the translation is parallel to the line of reflection. On the other hand, if we have such a glide reflection, but we want the line of reflection to go through some given point O, we can always achieve this, but t may not be parallel to l anymore.

Turn to 3D. If R is rotation about an axis, then $R-1$ has rank 2, annihilating vectors along the axis. $Ru-u$ is always perpendicular to the axis. So we have glide rotations, and the translation component can be made parallel to the axis by choice of origin. If R is reflection through a plane, then $R-1$ has rank 1, and $Ru-u$ is always perpendicular to the plane. The translation component can be made parallel to the plane by choice of origin.

The Action of the Point Group on the Lattice

We noted that the homomorphism $\rho \Rightarrow R$ is origin-independent. This remarkable fact leads to one of the key algebraic structures, the action of G_0 on the vector lattice.

For starters, since T is a normal subgroup of G, we have the conjugation action of G on T: $\tau \to \rho\tau\rho^{-1}$, with $\tau\in T$ and $\rho\in G$. Useful notation: $\rho\tau\rho^{-1} = {}^{\rho}\tau$. (Note that ${}^{\rho}({}^{\sigma}\tau) = {}^{\rho\sigma}\tau$.)

G_0 acts on T via pullback followed by conjugation, thus: let $R\in G_0$, and let $\rho \Rightarrow R$. Now use ρ to conjugute τ, thus: $\tau \to {}^{\rho}\tau$. The result does not depend on the choice of ρ because T is abelian: if $\rho\sigma$ is some other pullback of r, with $\sigma\in T$, then ${}^{\rho\sigma}\tau = {}^{\rho}\tau$. More useful notation: ${}^{R}\tau$ denotes this result, i.e., the action of G_0 on T. Note that ${}^{R}({}^{S}\tau) = {}^{RS}\tau$.

It is not hard to describe the action of G_0 on T geometrically. The key thing to note is that a translation is completely determined by its action on a single point: if it sends p to q, then it corresponds to the vector from p to q.

Let R be in G_0, and let τ correspond to the vector t. Let R pull back to $\rho = [u{:}R] \in G$. We'll track the point O+u as $\rho\tau\rho^{-1}$ is applied to it; to reduce clutter, we'll leave out the initial "O+" throughout, implicitly identifying points and vectors. First ρ^{-1} sends u to the origin, and then the translation τ sends that to the point t, and then ρ sends that to Rt+u. In sum: $u \to O \to t \to Rt+u$. So $\rho\tau\rho^{-1}$ is translation by Rt. We can write this elegantly in a couple of ways:

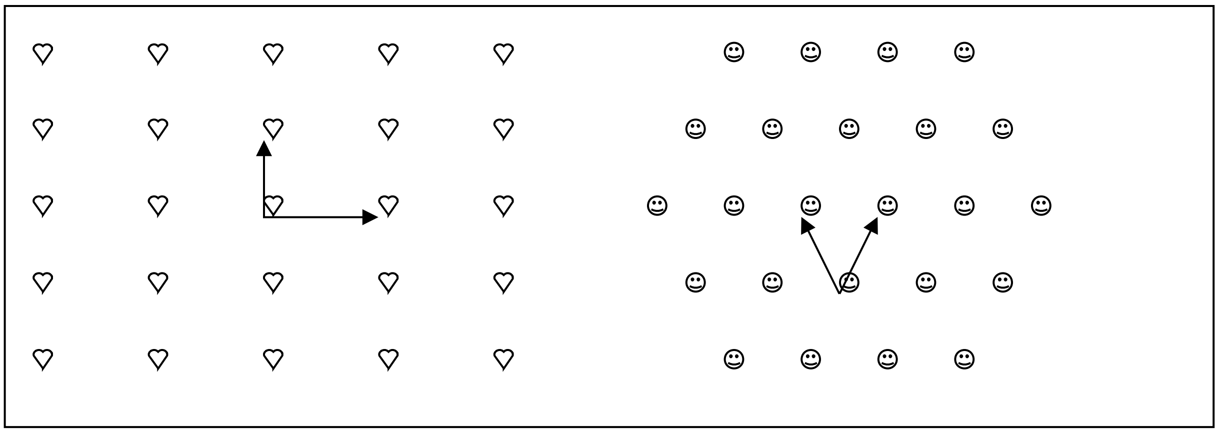
$$\text{If } t \Leftrightarrow \tau, \text{ then } Rt \Leftrightarrow {}^{R}\tau$$

$${}^{R}\tau_t = \tau_{Rt}$$

Examples of the Action in 2D

To picture the action, we look at what elements of G_0 do to the point lattice. We illustrate some subtleties by considering three planar examples, all with the same point group.

Our point group is called D_1, and it is $\{1, R\}$, where R is a reflection about some line l. R must preserve the point lattice. Say x and y are basis vectors for the lattice. Consider the two possibilities shown below. On the left ("hearts"), the reflection line is the y-axis. The x and y vectors are horizontal and vertical, respectively. On the right, the reflection line is the vertical line in the direction $x+y$; the x and y vectors a both diagonal (with, say, x sloping northwest). So on the left, $Rx = -x$, $Ry = y$; on the right, $Rx = y$, $Ry = x$. The basis vectors are shown as arrows (although not labeled).



Although it is not obvious, these two wallpaper groups are not isomorphic. The one on the left is known as pm, the one on the right as cm (according to the International Tables for X-ray Crystallography).

Note that if, for example, we just changed the length of the x and y vectors on the left, we would get an isomorphic wallpaper group. We could replace x with, say, $6.358x$ and y with $2.91y$; there is an obvious isomorphism sending the old x and y to the new x and y. However, the angle between x and y must remain a right angle. (Also, if we changed x and y to have the same lengths, then new symmetries would appear.)

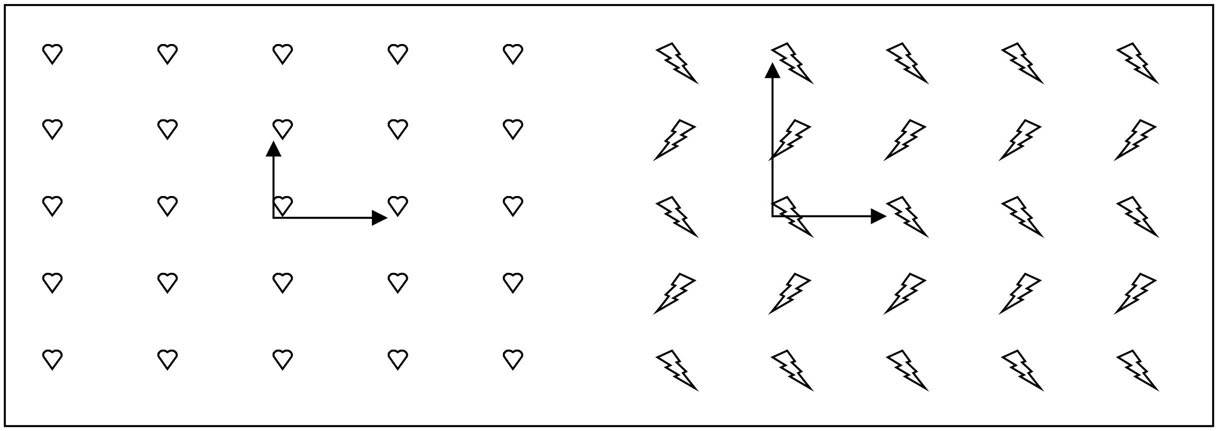
On the right, we could change the lengths of x and y, and also the angle between them. So long as the two lengths remain the same, we get an isomorphic group.

The lattice on the left contains a sublattice generated by $x+y$ and $-x+y$, which "looks the same" as the lattice on the right. In fact, the reflection R together with these two translations ($x+y$ and $-x+y$) generates a subgroup of pm that is isomorphic to cm.

On the other hand, the lattice on the right contains a sublattice generated by $x+y$ and $-x+y$, which "looks the same" as the lattice on the left. In fact, the reflection R together with these two translations ($x+y$ and $-x+y$) generates a subgroup of cm that is isomorphic to pm.

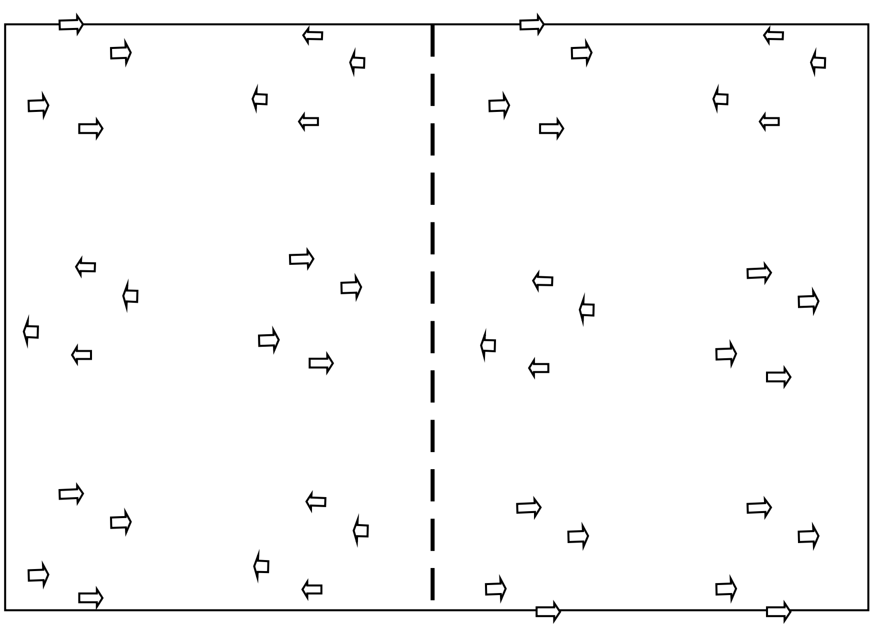
Notice that both pm and cm contain subgroups isomorphic to D_1. In fact, the stabilizer of the origin (i.e., the set of all elements of G leaving the origin fixed) is $\{1, R\}$ in both cases.

Our next pair of examples is pm again ("hearts" on the left), and a group known as pg on the right ("lightning"). This time x is horizontal and y is vertical in both pictures; also, R



acts the same way on both lattices, namely $Rx = -x$, $Ry = y$. However, R is not a symmetry of pg. Instead, R pulls back to a glide reflection ρ. We let $\rho = [\frac{1}{2}y{:}R]$.

Notice that ρ^2 is a pure translation, namely y.



One last example: the group p4g, shown above. This has a different point group, known as D_4; this is the group of symmetries of the square, and is generated by a 90° rotation, say R, and a reflection, call it F (for "flip"). F pulls back to a reflection about the dashed line. The group p4g confronts us with a new aspect of the origin choice issue. It is clear where the centers of rotation are, and the line of reflection does not pass through them. If we make the origin a center of rotation for R, we are forced to pull F back to $[\frac{1}{2}x{:}F]$ or something similar. Note, however, that there *are* glide reflections whose reflection lines passes through centers of rotation.

Determining the Translations

Suppose we have isomorphic space groups G and G'. Do translations necessarily correspond to translations? In other words, is there a purely group-theoretic way to determine the translations?

Answer: yes. We have a canonical homomorphism $G \to G_0$. Fact: the point group is always finite. Let m be the order of G_0. Then $R^m = 1$ for all $R \in G_0$. So ρ^m maps to 1 for any $\rho \in G$, so ρ^m is a translation. So ρ^m commutes with all translations. So a necessary condition for σ to be a translation is that it commutes with all the ρ^m.

This is also sufficient, or in other words, if σ commutes with all the ρ^m, then σ is a translation. Proof: among the ρ^m, we have all the τ^m, or in other words all the translations by mt for all the t in the lattice. If σ commutes with all these, that means the conjugation action of σ on these translations is trivial. Say $\sigma \Rightarrow S$. Since $\tau^m \Leftrightarrow mt$, we have ${}^S(\tau^m) \Leftrightarrow S(mt)$. So S leaves all the mt fixed, so S=1, and σ is a translation.

Let G and G' be isomorphic space groups. We don't know *a priori* that their point groups have the same order. However, we can pick a common multiple of the two orders. The previous argument immediately generalizes to show that if m is any multiple of the order of G_0, then σ is a translation iff it commutes with all the ρ^m. So translations map to translations.

Isomorphic Space Groups

Let G and G' be isomorphic space groups, as above. So the translation subgroups T and T' correspond, and the point groups G_0 and G_0' are also isomorphic, as they are isomorphic to G/T and G'/T' respectively. Also the conjugation actions of G and G' on T and T' correspond: if $\rho \leftrightarrow \rho'$ and $\tau \leftrightarrow \tau'$ then ${}^\rho\tau \leftrightarrow {}^{\rho'}\tau'$.

All this is general "diagram chasing", but it leads to something important. The plan of attack is to use the group isomorphism on translations, plus the canonical correspondence between translations and vectors, to set up a vector space isomorphism between **V** for G and[3] **V**$'$ for G'. Consider this done, and call the isomorphism U.

Next, we will use the action of G_0 on T, and the group isomorphism on translations, to carry R in G_0 over to R' in G_0'. Finally we will invoke the basic fact about this action: if $\tau \Leftrightarrow t$, then ${}^R\tau \Leftrightarrow Rt$, and likewise with primed entities. So if ${}^R\tau \leftrightarrow {}^{R'}\tau'$, then also $Rt \leftrightarrow R't'$, and by the way U is defined, U carries $Rt \leftrightarrow R't'$.

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[3] Actually, with our setup, all the n-dimensional space groups act on the same Euclidean space **E**, so it's the same **V** for G for G'. So it's really a vector space automorphism. As it happens, that fact makes no difference.

We now define R' and check that ${}^{R}\tau \leftrightarrow {}^{R'}\tau'$. Start with R in G_0. Pull it back to $\rho \Rightarrow R$. We defined ${}^{R}\tau$ to be ${}^{\rho}\tau$, and we noted that ${}^{\rho}\tau$ did not depend on which pullback of R we chose. Note that all the possible pullbacks form a coset of T in G.

Under the isomorphism between G and G', this coset of T maps to a coset of T', and all members ρ' of the coset give the same result for ${}^{\rho'}\tau'$. Furthermore, the entire coset maps to the same linear map (call it R') under the homomorphism $G' \to G_0'$. As we already noted, if $\rho \leftrightarrow \rho'$ and $\tau \leftrightarrow \tau'$ then ${}^{\rho}\tau \leftrightarrow {}^{\rho'}\tau'$. So we must also have ${}^{R}\tau \leftrightarrow {}^{R'}\tau'$.

As promised, we now invoke the basic fact about the action: if $\tau \Leftrightarrow t$, then ${}^{R}\tau \Leftrightarrow Rt$. Likewise, if $\tau' \Leftrightarrow t'$, then ${}^{R'}\tau' \Leftrightarrow R't'$. Since ${}^{R}\tau \leftrightarrow {}^{R'}\tau'$, we must have $Rt \leftrightarrow R't'$. By the way U is defined, we must have $Ut = t'$ and $U(Rt) = R't'$. In other words, $URt = R'Ut$. This holds for all t in the vector lattice, and by linearity, for all of $\mathbf{V}$. So $UR = R'U$, so $URU^{-1} = R'$.

We turn this into a computational test by choosing basis vectors for the vector lattices of G and G'. Recall that the lattices are $\mathbf{Z}$-modules, so by "basis vectors" we mean generators over $\mathbf{Z}$. It is clear that the matrix for U must have integer entries, but this also true for U^{-1}. So U is an element of $\mathrm{GL}_n(\mathbf{Z})$. Note that this is a necessary condition for G to be isomorphic to G'. The example of pm and pg shows that it is not sufficient, since the point groups and the actions are the same in that case.

This test will show that pm and cm are not isomorphic. The trick is to reduce the matrices modulo 2; this will prove that the matrices for the two reflections (in pm and cm) are not conjugate in $\mathrm{GL}_2(\mathbf{Z})$.

Space Group Equivalence

Most of the material in these notes came out of the (successful) efforts to classify the symmetry groups of crystals. It is time to take stock and ask, what do we mean when we say that there are 17 essentially different wallpaper patterns? What is the right notion of equivalence for space groups?

One simple (and OK) answer is isomorphism: there are 17 non-isomorphic wallpaper groups. However, group isomorphism is rather abstract and not immediately geometric. For example, consider the point groups $C_2 = \{1, R\}$ and $D_1 = \{1, F\}$, where R is a 180° rotation and F is a reflection. As groups, these are obviously isomorphic, but the geometry is very different.

Another possible definition: conjugacy classes in the group $\mathrm{Isom}(\mathbf{E})$. However, this is *not* the right approach. We can see this with the group pm on page 6. Consider pm, generated by translations x and y and and a reflection. If we conjugate this with an isometry $[u{:}U]$, we get translations Ux and Uy. These necessarily have the same lengths as the original x and y. So if we have two copies of pm, one with translations x and y and the other with (say) translations $6.358x$ and y with $2.91y$, they would belong to different conjugacy classes in $\mathrm{Isom}(\mathbf{E})$.

As we noted on page 6, there *is* a vector space isomorphism U sending x to $6.358x$ and y to $2.91y$. So these two copies of pm are conjugate by an element of $GL_2(\mathbf{R})$.

More generally, we can consider conjugacy in the group Aff(**E**) of **affine motions**, that is, mappings that can be expressed in the form $x \to Ux+u$, where U is invertible. This turns out to be the right notion of equivalence for space groups. For example, two copies of cm, differing only in the angle between the basis vectors, will be conjugate in Aff(**E**).

Perhaps you are wondering, how do we insure that the basis vectors x and y have the same length in each copy of cm? Or for pm, how do we guarantee that the basis vectors remain perpendicular?

This is enforced by the point group. Let U be a linear mapping of the plane that changes the angle between the basis vectors x and y. Let R be the reflection about the y-axis, so $Rx = -x$, $Ry = y$. If we conjugate by U, we get R', x', and y' satisfying the same equations, but it is not hard to see that this R' is not an isometry.

So *if* we have two wallpaper groups, and *if* they are conjugate by an element of Aff(**E**), and *if* one of them is a copy of pm, *then* the other one will also be a copy of pm: it will contain a reflection about one of the basis vectors, and its lattice will be rectangular. (As an exercise, verify this assertion. Also as an exercise, do a similar analysis for cm.)

Given an affine motion ψ and an isometry ρ, $\psi\rho\psi^{-1}$ will not usually be an isometry. Only in special circumstances will this obtain. So the idea is, we first collect all subgroups of Isom(**E**) satisfying the space group condition, and then we use conjugacy in the larger group Aff(**E**) to define equivalence.

Remarkable fact: two space groups are isomorphic iff they are conjugate in Aff(**E**)! Of course, we have already proved part of this (the existence of a U making the point groups conjugate) in the previous section.

Crystal Classes

Our ultimate goal is classifying space groups up to isomorphism, or equivalently, up to conjugacy in Aff(**E**). We could regard this purely as an algebraic problem, but we would like also to understand the geometric significance of the various steps.

So far, we've identified three key algebraic invariants: the translation subgroup T, the point group G_0, and the action of G_0 on T. T can be pictured as a lattice of points (or vectors by preference), and elements of G_0 are orthogonal linear mappings that map T onto itself ("preserve the lattice").

We have a notion of equivalence for these (G_0,T) pairs, namely conjugacy by vector space isomorphism U taking T to T'. When the space groups are isomorphic, the associated (G_0,T) pairs are equivalent in this manner.

By an **arithmetic crystal class**, we mean a class of such (G_0,T) pairs under the equivalence relation just described. So T is a lattice and G_0 is a group of orthogonal linear mapping preserving T.

What does an arithmetic crystal class "look like"? Let's take pm as our first example. The lattices are all rectangular, but the rectangles can have different heights and widths. Even if the height happens to equal the width (a square lattice), this is accidental and is not manifested in the point group $G_0 = D_1$. $D_1 = \{1, R\}$, where R flips the lattice about one of the axes. The orientation of the rectangles is unimportant, even though we usually draw them with horizontal and vertical sides.

Clearly there are other orthogonal mappings that preserve the lattice but do not belong to D_1. For example, there is a 180° rotation, and a reflection about the other axis. In the picture on page 6, we killed those other symmetries by attaching a motif to each lattice point.

Fact: there are 13 arithmetic crystal classes in 2D, and 73 arithmetic crystal classes in 3D. To bring some order to the list, it is traditional to focus on **maximal** point groups; in other words, given a lattice, to look at *all* the point group symmetries that preserve it. All crystal classes with a given maximal point group are said to belong to the same **crystal system**.

It turns out that there are four crystal systems in 2D, and seven crystal systems in 3D.

In 2D, the crystal systems are labeled by the groups C_2, D_2, D_4, and D_6; D_k in general is the group of $2k$ symmetries of the regular k-gon. The associated lattices look like this:

Point Group	**Lattice**
C_2	parallelograms
D_2	rectangular or rhombic
D_4	square
D_6	hexagonal

To give a sense of how the classification of space groups works out, we now describe all the wallpaper groups in the D_2 system. Of course, it would take quite a bit of geometric reasoning to justify our assertions.

D_2 is the group of symmetries of the regular 2-gon, which is an unoriented line segement, or what amounts to the same thing, a rectangle. D_2 has four elements, 1, F, R, and RF, where F is a reflection ("flip") about an axis, R is a 180° rotation, and $RF = FR$ is a flip about the perpendicular axis.

There are two non-conjugate actions of D_2 on T: either F can negate one basis vector and leave the other fixed, or F can interchange the basis vectors,. Choosing basis vectors gives us matrix representations for F, namely $\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$ and $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. These are not conjugate in $GL_2(\mathbf{Z})$ by a modulo 2 argument. (Reduce modulo 2. Then the first matrix becomes the identity matrix, which is conjugate only to itself.)

If F leaves one basis vector fixed and negates the other, then the basis vectors must be perpendicular, so we have rectangular lattice. If F interchanges the basis vectors, then they must have equal length, so we have a rhombic lattice.

Start with the rectangular lattices. D_2 has three proper non-trivial subgroups, $\{1,R\}$, $\{1,F\}$, and $\{1,RF\}$. Abstractly these are all $\mathbf{Z}_2$. Geometrically these are C_2, D_1, and D_1. Here C_2 is the cyclic rotation group of order 2, and D_1 is the symmetry group of the 1-gon (a line segment with a "top" and a "bottom", so it can't be rotated by 180°).

So arithmetic crystal classes with rectangular lattices could have point group 1, C_2, D_1, or D_2. But if the point group is C_2, then the class really belongs to another crystal system. Its lattice is, so to speak, "accidentally rectangular"; the point group treats it as if it were parallelogramic.

Suppose the point group is D_1. We have now narrowed our scope down to a single crystal class. The $\{1,F\}$, and $\{1,RF\}$ cases are conjugate in $GL_2(\mathbf{Z})$. Let's pick the $\{1,F\}$ case. The R and RF symmetries have been killed. (See the "hearts" illustration of pm, for example.) What wallpaper groups belong to this class?

Well, it all depends on the pullback of F. It turns out that either F can pull back to a reflection, and then we get pm. Or else F must pull back to a non-trivial glide reflection, in which case we get pg (see page 7).

Next we consider the D_2 point group, still with a rectangular lattice. Either F and RF both pull back to reflections (yielding a wallpaper group called pmm), or F does but RF demands a glide reflection (the wallpaper group called pmg), or RF does but F demands a glide reflection (isomorphic to the last case), or F and RF both demand glide reflections (yielding the group called pgg).

That exhausts the rectangular cases. Turn to the rhombic lattice. Again we need to consider the D_1 subgroup. It turns out the F can always be pulled back to a reflection. We get a single wallpaper group, called cm (and illustrated on page 6).

For the D_2 case, it turns out that both F and RF can always be pulled back to reflections, so we get only one wallpaper group, called cmm.

Summing up, we have four arithmetic crystal classes in this system: rectangular D_1 and D_2, and rhombic D_1 and D_2. We have seven wallpaper groups in these four classes: pm and pg (in rectangular D_1), pmm, pmg, and pgg (in rectangular D_2), cm (in rhombic D_1), and cmm (in rhombic D_2).

In the four 2D crystal systems, there are five kinds of lattices, as shown in the table. It turns out that there are 14 lattices types in 3D; these are known as the **Bravais lattices**.

For example, the cubic crystal system has point group O_h, the group of all symmetries of the cube. It turns out that there are three Bravais lattices in the cubic system, known as simple cubic, body centered cubic (bcc), and face centered cubic (fcc). There are a total of 15 arithmetic crystal classes in the cubic system, and 36 space groups.

Cohomology

The examples of the previous section highlight the importance of pullbacks. To take the easiest example, pm and pg have isomorphic point groups, acting the same way on the vector lattices, with the space groups still not being isomorphic. In pm, the reflection pulls back to a pure reflection; in pg, it pulls back to a glide reflection.

The algebraists have put this in a more general context. We have a short exact sequence

$$1 \to T \to G \to G_0 \to 1$$

where T is abelian. Any time we have such a sequence, $G_0 \cong G/T$, and G_0 acts on T via pullback plus conjugation. One says that ***G* is an extension of *T* by G_0**. The goal of group cohomology is to classify all such extensions.

In the case of a group like pm (or for that matter, in the group Isom(**E**)), G contains a group isomorphic to G_0; in fact, there is what is called a **splitting homomorphism**, a map η: $G_0 \to G$, which, when composed with the map π: $G \to G_0$, gives the identity on G_0 ($\pi \circ \eta = \mathrm{id}_{G0}$). This means we can basically regard G_0 as a subgroup of G. It turns out in this case that G is canonically isomorphic to the **semi-direct product** of T and G_0: the set $T \times G_0$ given a group structure by the multiplication law $(a, R)(b, S) = (a+Rb, RS)$, where we have written the group operation in T additively, in G_0 multiplicatively, and used Rb to indicate R acting on b. (Compare the formula for composition of isometries: $[t{:}R]\,[u{:}S] = [t+Ru : RS]$).

To classify extensions $1 \to T \to G \to G_0 \to 1$, we need to consider all possible ways of pulling back $R \in G_0$ to $\rho \in G$. In the geometric context of space groups, we can be more concrete: we need to consider all possible $[t{:}R] \in G$. Note that t will not necessarily be a translation in G. If it is, we can follow $[t{:}R]$ with $[-t,0]$ and conclude that $[0{:}R]$ is also in G; in other words, the point group element R can be regarded as an element of G. If we can do this for *all* elements of the point group, with a single choice of origin, then crystallographers say that the space group is **symmorphic**.

Obviously a symmorphic space group is the semi-direct product of the translation group and the point group. I suspect that conversely, if the space group is the semi-direct product of the translation group and point group (with the usual conjugation action), then the space group is symmorphic[4]. Fact: of the 219 3D space groups, only 73 are symmorphic. In 2D, 13 of the 17 wallpaper groups are symmorphic.

Suppose $\rho = [r{:}R]$ and $\sigma = [s{:}R]$ are both in G; then $\rho^{-1}\sigma$ is a pure translation τ (it maps to the identity element of G_0), and from $\sigma = \rho\tau$ we conclude that $s = r+t$ for some translation t in the lattice. So the pullback is determined uniquely modulo elements of T.

Let's now look at a piece of the classification theorem for wallpaper groups: the proof that there are just three extensions of a 2D lattice by D_1, namely pm, pg, and cm. Going through this case will motivate the cohomological machinery.

So let $D_1 = \{1,F\}$, where F is a reflection about a line; we will picture the line as vertical. We let x and y be basis vectors for the translation lattice T. Some geometric reasoning shows that we can choose basis vectors so that one of two cases holds: either F negates x and leaves y fixed, or F interchanges x and y. I won't go through this part of the argument.

Let F pull back to $[f{:}F]$. We know that f is determined up to translations in T, i.e., $\{f + t : t\in T\}$ is the set of all possible choices for f. (If you're being persnickety, we're now using T both for the set of translations in G, and for the set of corresponding vectors.)

Since $F^2 = 1$, it follows that $[f{:}F]^2$ is in T. But $[f{:}F]\,[f{:}F] = [f + Ff : 1]$, so $f + Ff$ is in T. At this point we need to use our information about how F acts on the basis vectors. Let f have coordinates (a,b) in the x,y basis.

In the rectangular case, where $Fx = -x$ and $Fy = y$, we have $f + Ff = (a,b)+(-a,b) = (0,2b)$. So $2b\in\mathbf{Z}$. Since f is determined only modulo T, we can assume that $0\le b<1$. So either $b = 0$, or $b = ½$.

Now, a is completely arbitrary. However, note that (a,b) gives the decomposition of f into the component perpendicular to the reflection line (namely $(a,0)$), and the component parallel to the reflection line (namely $(0,b)$). We observed much earlier that by shifting our choice of origin, we can always make the perpendicular component of any glide reflection vanish.

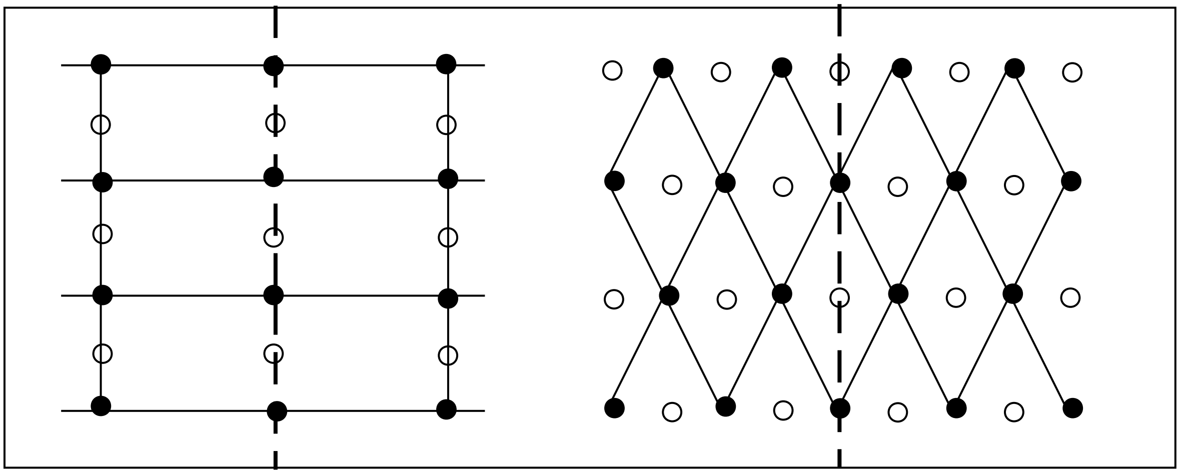
Summing up the rectangular case, either $[f{:}F]$ is a pure reflection (and $f = 0$), or $[f{:}F]$ is a glide reflection by one-half the y basis vector (and $f = ½y$). These are the cases pm and pg.

Turn to the rhombic case, where $Fx = y$ and $Fy = x$. Then $f + Ff = (a,b)+(b,a) = (a+b,b+a)$. So $a+b\in\mathbf{Z}$. We can add any vector $(k,l)\in\mathbf{Z}\times\mathbf{Z}$, since f is only determined modulo T. So we can assume $a+b = 0$, and $f = (a, -a)$. But then f is perpendicular to the reflection line, and by changing the origin, we can make $f = 0$. So we have a pure reflection. This is the cm case.

[4] Hiller's article states that a semi-direct product space group is called symmorphic by crystallographers.

The diagram below illustrates the essential difference between the rectangular and rhombic cases. The light lines indicate the lattice. The heavy dashed line is a reflection line for F. The dots indicate possible values for f. The origin has already been shifted so that it lies on the reflection line; assume it's the bottom solid dot.

The rectangular case $b \equiv 0 \pmod{\mathbf{Z}}$ and rhombic case $a+b \equiv 0 \pmod{\mathbf{Z}}$ have solid dots; the cases $b \equiv \frac{1}{2}$ and $a+b \equiv \frac{1}{2}$ have hollow dots.



Because f is determined only modulo T, we can use any dot of the same "color" (solid or hollow) as our glide. In the solid dot cases, F pulls back to a pure reflection. In the cm hollow dot case, one possible pullback uses the glide from the origin to the hollow dot horizontally to the right. But this is just a pure reflection about the vertical line midway between the two dots. However, in the pm hollow dot case, there is no choice of glide perpendicular to the reflection line, and so the glide cannot be eliminated.

Time to generalize. As we've seen, we need to consider possible pullbacks of R for R in the point group. For every $R \in G_0$, chose $[a_R : R] \in G$. So $a_R \in \mathbf{V}$, the set of all translations of Euclidean space, but not necessarily in T. Let α_R be the image of a_R under the natural mapping $\mathbf{V} \to \mathbf{V}/T$. Thus α_R is determined uniquely.

Our previous discussion hinged around the implications of the equation $F^2=1$ for a_F (and, implicitly, α_F). More generally, let's see what we can say about α_{RS} for R and S in the point group. Since $[a_R:R]\ [a_S:S]$ is a possible pullback for RS, we must have $a_R + Ra_S \equiv a_{RS} \pmod{T}$, or $\alpha_R + R\alpha_S = \alpha_{RS}$. (Note that $R\alpha_S$ is well-defined because the point group leaves T invariant.) A function $\alpha: G_0 \to \mathbf{V}/T$ satisfying these conditions:

$$\alpha_R + R\alpha_S = \alpha_{RS}, \quad \alpha_1 = 0$$

is called a **1-cocycle** of G_0.

One can check that any 1-cocycle gives a way to construct a space group out of the translation lattice and the point group.

Shifting the origin also played a crucial role. We noted much earlier that changing the origin from O to $O' = O+u$ has this effect on the translation part:

$$[t : R]_{\text{old}} \to [t{+}Ru{-}u : R]_{\text{new}}$$

This suggests that if we set $\alpha_R' = \alpha_R + R\upsilon - \upsilon$ for some fixed $\upsilon \in \mathbf{V}/T$, then we should regard α' and α as equivalent in some sense. A function of the form $\beta_R = R\upsilon - \upsilon$ is called a **1-coboundary**. It turns out the set of all 1-cocyles forms an abelian group under pointwise addition, and the set of all 1-coboundaries is a subgroup. The group of 1-cocyles mod 1-coboundaries is the **1-dimensional cohomology group $H^1(G_0,\mathrm{V}/T)$, with coefficients in V/*T***.

It will not surprise you to learn that k-dimensional cohomology groups for all integer k can be defined, with various coefficient groups. I won't go into this, but will briefly describe the **2-dimensional cohomology group, $H^2(G_0,T)$, with coefficients in *T***. Fact: $H^1(G_0,\mathrm{V}/T)$ and $H^2(G_0,T)$ are isomorphic.

In the case of a semi-direct product extension, we have a homomorphism η: $G_0 \to G$, which, when composed with π: $G \to G_0$, gives the identity on G_0. In the case of a general extension, we can still look at functions η: $G_0 \to G$ for which $\pi \circ \eta = \mathrm{id}_{G0}$ (these are called **sections**). We won't necessarily have $\eta(R)\eta(S) = \eta(RS)$; in fact, $\eta(R)\eta(S)\,\eta(RS)^{-1}$ in some sense measures the failure of η to be a homomorphism. Define

$$c(R, S) = \eta(R)\eta(S)\,\eta(RS)^{-1}$$

Since $c(R, S)$ maps to the identity under the π mapping, $c(R, S)$ must be in T.

The associative law in G translates into a condition on $c(R, S)$; I won't spell out the details. The set of all c:$G_0 \times G_0 \to T$ satisfying this condition turns out to be a group under pointwise addition, called the **group of 2-cocycles**.

Now $c(R, S)$ depended on the choice of section η. Choosing a different section η' leads to a different c', but one can show that the difference $c'-c$ is always of a certain form. The set of all b: $G_0 \times G_0 \to T$ of this form is a subgroup of the group of 2-cocycles, called the group of **2-coboundaries**; of course, 2-cocycles mod 2-coboundaries gives us the 2-dimensional cohomology group, $H^2(G_0,T)$, with coefficients in T.

These definitions work for any extension of an abelian group by another group acting on it. In our special case, where $\eta(R) = [a_R{:}R]$ for some $a_R \in \mathbf{V}$, we can say more.

We have $c(R, S) = [a_R{:}R]\,[a_S{:}S]\,[a_{RS}{:}RS]^{-1} = [a_R + Ra_S{:}RS][-(RS)^{-1}a_{RS} : (RS)^{-1}] =$
$[a_R + Ra_S - a_{RS} : 1]$. Now π sends $c(R, S)$ to 1, so we must have $a_R + Ra_S - a_{RS} \in T$. Reducing modulo T gives us the 1-cocycle condition. We already see a connection between the two cohomology groups $H^1(G_0,\mathbf{V}/T)$ and $H^2(G_0,T)$. Working through the details yields the isomorphism mentioned above.

The 17 Wallpaper Groups

We have now sketched all the machinery needed for the classification of space groups. Morandi's notes give full details for the 2D case, proving that there are 17 wallpaper groups[5]. Here's an outline of the argument. 2D is assumed throughout.

The first two chapters cover the basic geometry (translations, rotations, shift of origin). Chapter 3 on the point group shows that the only possible point groups are C_1, C_2, C_3, C_4, C_6, and D_1, D_2, D_3, D_4, D_6. (Supposedly this fact was known to Leonardo da Vinci.) This is known as the **crystallographic restriction** (in 2D).

Morandi shows that isomorphic wallpaper groups have isomorphic point groups with conjugate actions on the lattice (conjugate in $GL_2(\mathbf{Z})$), as we noted earlier. (He also states incorrectly on p.23 that the converse is true.)

He then determines all possible actions of these point groups on the lattices, leading to five types of lattices and 13 arithmetic classes. The arithmetic classes are labeled by embellishing the subscript on the point group. For example, $D_{1,p}$ is D_1 acting on a rectangular lattice, and $D_{1,c}$ is the rhombic case.

The arguments involve chosing a lattice basis in a smart way. For example, if the point group contains a rotation R of order 3, 4, or 6, and t is a lattice vector of minimal length, then $\{t, Rt\}$ is a basis. (Typo on p.26: D_3 has three reflections and D_6 has six.)

The 17 wallpaper groups and 13 arithmetic classes are given in the following table:

Arithmetic Class	**Lattice**	**Wallpaper Groups**
C_1	Parallelogramic	p1
C_2	Parallelogramic	p2
C_3	Hexagonal	p3
C_4	Square	p4
C_6	Hexagonal	p6
$D_{1,p}$	Rectangular	pm, pg
$D_{1,c}$	Rhombic	cm
$D_{2,p}$	Rectangular	pmm, pmg, pgg
$D_{2,c}$	Rhombic	cmm
D_4	Square	p4m, p4g
$D_{3,s}$	Hexagonal; reflection exists leaving one basis vector fixed	p31m
$D_{3,l}$	Hexagonal; no such reflection	p3m1
D_6	Hexagonal	p6m

The arithmetic classes are shown to be distinct by using the "conjugate in $GL_2(\mathbf{Z})$" criterion.

[5] Unfortunately Morandi's notes contain a few minor errors, which I will note.

Chapter 4 develops group cohomology in some detail. The machinery is then applied to calculate the 2-dimensional cohomology groups for all the possible point groups. It turns out that these are all trivial except for three cases: $D_{1,p}$ has cohomology $\mathbf{Z}_2$, $D_{2,p}$ has cohomology $\mathbf{Z}_2 \oplus \mathbf{Z}_2$, and D_4 has cohomology $\mathbf{Z}_2$.

Chapter 5 then gives the proof of the classification theorem, first using the cohomology results, then repeating the argument without explicit use of cohomology[6]. We know there are 13 symmorphic wallpaper groups; the only other possible groups then come from the three cases $D_{1,p}$, $D_{2,p}$, and D_4.

First a general result: for any of the point groups, whether a C_k or a D_k, it is always possible to chose the origin so that the rotations pull back to pure rotations. This is easy: pick a generator R for the (sub)group C_k and pull it back to ρ. We know that ρ is a rotation about *some* center. Then ρ^i can be used as the pullback for R^i. Whenever the point group has a non-trivial rotation, Morandi chooses the origin in this manner.

The fun, then, revolves around the pullbacks of reflections in the point group. Just as we saw with D_1, if F pulls back to $[f{:}F]$, then $f + Ff$ is in T. $D_{1,p}$ yields the groups pm and pg, pretty much as we outlined above. $D_{1,c}$ yields the group cm, also as shown above.

$D_{2,p}$ initially yields four groups, pmm, pmg, pgm, and pgg, since there are two reflections to deal with (the 180° rotation is their product). Each reflection has, modulo T, two possible pullbacks. However, pmg and pgm are isomorphic, being conjugate under an element of $GL_2(\mathbf{Z})$ that swaps the basis vectors[7].

$D_{3,s}$, $D_{3,l}$, and D_6 all give only symmorphic groups. We get to use a new cocycle condition for these. Let R be a rotation and let F be a reflection. First note that by our choice of origin, $\alpha_R = 0$. Next, $\alpha_{RF} = \alpha_R + R\alpha_F = R\alpha_F$. Finally, RF is a reflection, so $(RF)^2 = 1$, so $RFR = F$. So $\alpha_F = \alpha_{RFR} = \alpha_{RF} + RF\alpha_R = \alpha_{RF} = R\alpha_F$. So $R\alpha_F - \alpha_F = 0$. In other words, $Ra_F - a_F \in T$.

Choosing a suitable basis (with the basis vectors at 120° to each other), and working through some simple algebra[8], we conclude in the D_6 case that α_F is (0,0). In the D_3 cases, α_F can also be (−1/3, 1/3), or (−2/3, 2/3); pictorially, these appear as dots in the centroids of the equilateral triangles of the lattice.

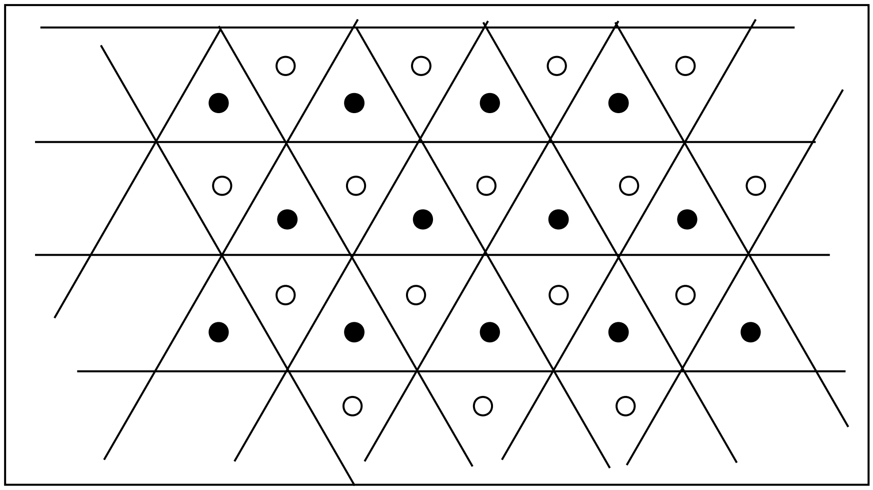
For $D_{3,l}$, you can show that if α_F is (−1/3, 1/3) or (−2/3, 2/3), then the other cocycle condition $\alpha_F + F\alpha_F = 0$ is violated. For $D_{3,s}$, there is always a choice of glide (one of the centroid dots) perpendicular to the reflection line. So by shifting the origin, our glide

[6] Typos on p.53: Morandi writes g instead of t_g in three places, twice near the top and once near the bottom.

[7] Be careful with Morandi's generators g_2 and g_3 on p.50. Conjugation by U does not swap them, although he correctly states that it does establish an isomorphism between pmg and pmg′ (as he calls pgm).

[8] Typos on p.55: $\equiv -2u \pmod{T}$ instead of $\equiv 2u \pmod{T}$; $f(u) \equiv -u$ (same line); in displayed equation, should have $(\alpha t_1 + \beta t_2)$ and $(\alpha - \beta)$.

reflection becomes a pure reflection. In fact, you can check the origin gets shifted to another centroid dot, and also that all the centroid dots are centers of 120° rotations. So in all the D_3 cases, the wallpaper group is symmorphic.

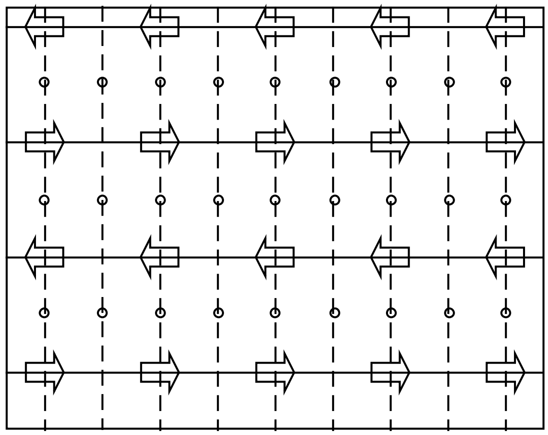


For D_4, we use the same cocycle condition $R\alpha_F - \alpha_F = 0$ that we used in D_3 and D_6. (The proof did not depend on the order of the rotation.) It turns out that this forces α_F to be either (0,0) or (½, ½). These yield the groups p4m and p4g.

It remains to be prove various non-isomorphisms. Groups in different arithmetic classes are automatically non-isomorphic, as was shown earlier. So we have only a few pairs to check.

Let's begin with pm vs. pg. It is easy to see that pg has no elements of order 2 (and in fact no non-identity elements of finite order), while pm does of course.

Next, pmm, pmg, and pgg. First, pmm has two reflections whose product is a 180° rotation, thus two elements of order 2 whose product is of order 2. The elements of pmg



fall into four sets as shown in the figure: the translations; the 180° rotations (hollow dots); the horizontal glide reflections (solid lines); the vertical glide reflections (dashed lines). We choose as the origin a center of rotation. You can see that the only elements of order two are the 180° rotations, and those horizontal glide reflections that happen to be pure reflections. You can also verify that in no case do we two elements of order 2 whose product is of order 2. Note that none of the pure reflection lines passes through a center of rotation, which is why the product of a pure reflection and a rotation does not give another pure reflection[9]. For pgg, the only elements of order 2 are the 180° rotations, and the product of two such has infinite order (or is the identity). To show that pmg and pgg are not isomorphic, note that an isomorphism would have to send a reflection in pmg to a rotation in pgg (order 2 goes to order 2). But we know the isomorphism can be realized by conjugation in $GL_2(\mathbf{Z})$, which preserves determinants.

The last pair to check is p4m and p4g. Now p4m contains a subgroup isomorphic to D_4, thus it contains an element ρ of order 4, and an element φ of order 2 other than ρ^2. Moreover, $\rho\varphi$ is of order 2, being a reflection. If you go back and look at the picture for p4g (p.7), you will note that p4g also has an element ρ of order 4 (a rotation), and an element φ of order 2 other than ρ^2. However, $\rho\varphi$ is a non-trivial glide reflection and thus has infinite order. In fact, one can check that this is true for any such ρ and φ in p4g.

Epilog: Fourier Space

From the early days of X-ray crystallography, Fourier analysis has been the order of the day in crystallography. Let $\rho(x)$ be the electron density (or some other physical property) in a crystal at location x. Then $\rho(x) = \rho(x+t)$ for all t in the vector lattice. Applying the Fourier inversion formula in 3D, it then transpires that $\rho(x)$ can be expressed in the form $\rho(x) = \Sigma_r\, \rho_g \exp(2\pi i\; r{\cdot}x)$, where the ρ_g are the Fourier coefficients, and the sum Σ_r ranges over a set of vectors in another lattice, known as the **reciprocal lattice**. (A

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[9] Error on p.51 of Morandi: $\{(rf,nt_2){:}n\in\mathbf{Z}\}$ is not right for the pure reflections, since his origin is a center of rotation. It should be $\{(rf, (n+½)t_2\}$. Similar issue for pgg.

mathematician would say that the r's really live in the dual space of 1-forms on $\mathbf{R}^3$, and the dot product is not really needed.) Fact: the reciprocal lattice has the same point symmetry group as the original lattice (called, in this context, the **real space lattice** or **direct space lattice)**.

In 1984, the first **quasicrystals** were discovered; these are substances that have a kind of long-range order, but lack three-fold translational symmetry. They can have point group symmetries forbidden by the crystallographic restriction; for example, the first quasicrystal discovered had fivefold rotational symmetry.

The theory of space groups can be translated into Fourier space, and this turns out to be a powerful tool for studying quasicrystals. The Fourier space approach to crystal symmetries had already appeared in 1962, before the advent of quasicrystals, but that discovery gave it new life, with a new wave of papers starting around 1996.

Finally, starting around 2002, the physicists realized the value of group cohomology for this field.