Excursions in Computing Science: Book 8c. Symmetry: Simplifying Matrices. Part II Infinite symmetries and crystals.

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July 23, 2019

I. Prefatory Notes

19. Infinite groups. The integers form a group under +

$$\begin{array}{cccccc} & & \vdots & & & \\ & -2 & -1 & 0 & 1 & \\ .. & -1 & 0 & 1 & 2 & .. \\ & 0 & 1 & 2 & 3 & \\ & 1 & 2 & 3 & 4 & \\ & & \vdots & & & \end{array}$$

It is an infinite group.

It is commutative ("Abelian"): $m + n = n + m$.

So every element, m, is an invariant class by itself:

$$\forall n : n + m - n = m$$

(Let's put this into group terminology by writing

$$\begin{array}{rcl} t(n) & \text{for} & n \\ t(n)t(m) & \text{for} & n + m \\ \text{etc.} : & & \end{array}$$

$\forall n : t(n)t(m)t^{-1}(n) = t(m)$.)

So a representation, T, has an infinite number of elements

$$.., T(-1), T(0), T(1), T(2), ..$$

Since these matrices all commute with each other, they must all be simultaneously diagonal. or at least simultaneously diagonalizable.

The irreducible representations are thus 1×1 matrices, i.e., scalar numbers.

If $T(m)$ is a number and $T(m)T(n) = T(m + n)$ then $T(m) = a^m$ for some a.

Let's digress for a moment to the finite group of integers under addition modulo 3. Here $T(1 + 1 + 1) = T(1)^3 = T(0)$ and $T(0)$ must be 1, the identity 1×1 matrix. So $T(1)$ is a cube root of unity (see the Week 4 excursion "roots of unity") and to be different from 1 must be either $e^{2\pi i/3}$ or $e^{4\pi i/3}$. (Then $T(2)$ is the other one, namely $T(1)^2$.)

Back to regular arithmetic. Since we must distinguish each of the infinite number of irreducible representations from each other, we could use a parameter k. So it is handy to use $a = e^{-ik}$ for $0 \le k \le 2\pi$.

Here are some of these irreducible representations.

$$\begin{array}{rccccccccc} T_k(m) & k & m & -3 & -2 & -1 & 0 & 1 & 2 & 3 & \\ & 0 & .. & 1 & 1 & 1 & 1 & 1 & 1 & 1 & .. \\ & \pi/2 & .. & -i & -1 & i & 1 & -i & -1 & i & .. \\ & \pi & .. & -1 & 1 & -1 & 1 & -1 & 1 & -1 & .. \\ & 3\pi/2 & .. & i & -1 & -i & 1 & i & -1 & -i & .. \end{array}$$

Note that $T_{k+\ell}(m) = T_k(m)$ for any ℓ that is an integer multiple of 2π

$$e^{-i(k+\ell)m} = e^{-ikm}$$

Any subgroup of an Abelian (commutative) group is invariant. In particular, for the integers under addition we have the even integers, with odd integers forming the cofactor.

		:						
	-4	-2	0		-3	-1	1	
..	-2	0	2	..	-1	1	3	..
	0	2	4		1	3	5	
		:				:		
	-3	-1	1		-2	0	2	
	-1	1	3	..	0	2	4	..
	1	3	5		2	4	6	
		:				:		

The factor group is $I/2I = \{0, 1\}$ **mod** 2 where this has the group table

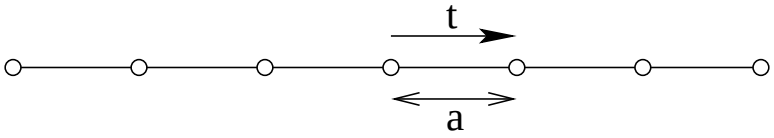
$+$		
	0	1
	1	0

(n **mod** 2 is the remainder of n divided by 2).

We can turn this around and write I as a *product group*

$$I = 2I \times \{0, 1\}\mathbf{mod}2$$

20. 1D crystals. Imagine an operator, t, which "translates" an infinite one-dimensional "crystal" by shifting it rightwards one atomic position. (a is the interatomic spacing in this crystal.)



Here is the group table. (e is the identity element, which does not shift the crystal at all.)

		:			
	$-2t$	$-t$	e	t	
..	$-t$	e	t	$2t$	..
	e	t	$2t$	$3t$	
	t	$2t$	$3t$	$4t$	
		:			

This is the same group as integers under addition. Operating with t is the same as adding a to the x-coordinate.

It has the same representations. For a physical system, the irreducible representations give, as for molecules, the possible modes of motion, whether this "motion" be the vibrations of the atoms in the crystal, the states the electrons may be in, the photons that may pass through the crystal, or anything else that might be interesting.

We have seen (Week 7a Note 2) what the form, e^{-ikm}, of the irreducible representations means physically. It means a *wave*.

The wave can be stationary or it can travel. The symmetry does not restrict us, except that the motion be a wave. So we can write it generally as a travelling wave.

$$e^{2\pi i(ft-\nu x)}$$

where f is the frequency and ν is the wavenumber. (We here use the crystallographer's convention that the 2π appears explicitly, rather than the physicist's implicit convention of Week 7a.)

Instead of measuring x in, say, nanometers, it might be convenient to measure in lattice spacings, a. If we call x measured in nanometers x_n and x measured in lattice spacings x_a then $x_a = x_n/a_n$

where the x-unit, a_n, is a measured in nanometers. Note that $a_n = a\times$ the 1-nanometer unit: coordinates are scaled by the reciprocal of a when the units are scaled by a.

Note also that the wavenumber, ν, in lattice units, scales oppositely to the distance, x. It is measured "per a" rather than "per nanometer", and so must be multiplied by a: $\nu_a = \nu_n \times a_n$. As a result, the products are the same: $\nu_a x_a = \nu_n x_n$.

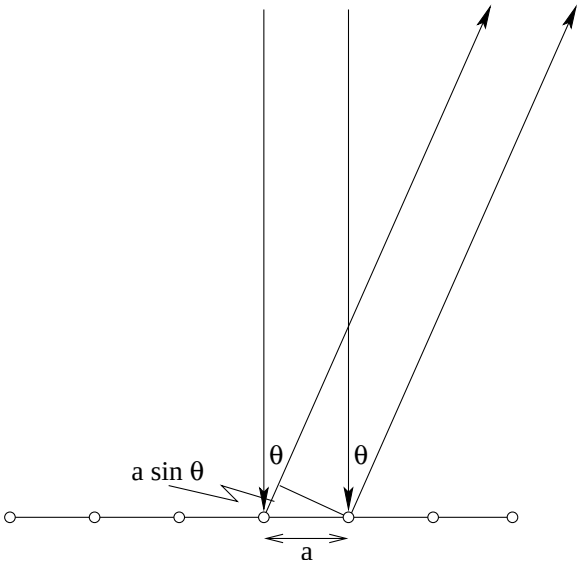
If we say we are measuring x in "lattice units" then we are measuring ν in "reciprocal lattice units". This distinction becomes more sophisticated in higher dimensions (next Note).

A one-dimensional crystal may seem implausible, but a *diffraction grating* is a very good realization.

Shine a laser pointer straight down on a CD disk placed horizontally near a wall and look for two distinct spots of light on the wall, apart from the pure reflection that should appear on the ceiling—or on your hand if you are really pointing straight down onto a horizontal CD.

Do not shine laser light anywhere near anybody's eyes or allow a reflected or a diffracted beam to get anywhere near an eye.

Let's see if we can explain these additional spots. The reasoning is that for the two-slit experiment in Week 5 Note 6. Each ridge of the diffraction grating (or "atom" in the "crystal" shown) acts as a new source of light. Rays will interfere destructively unless the path difference is an integer multiple of the wavelength. The path difference is $a \sin\theta$ where θ is the angle of the diffracted light from the perpendicular to the grating.



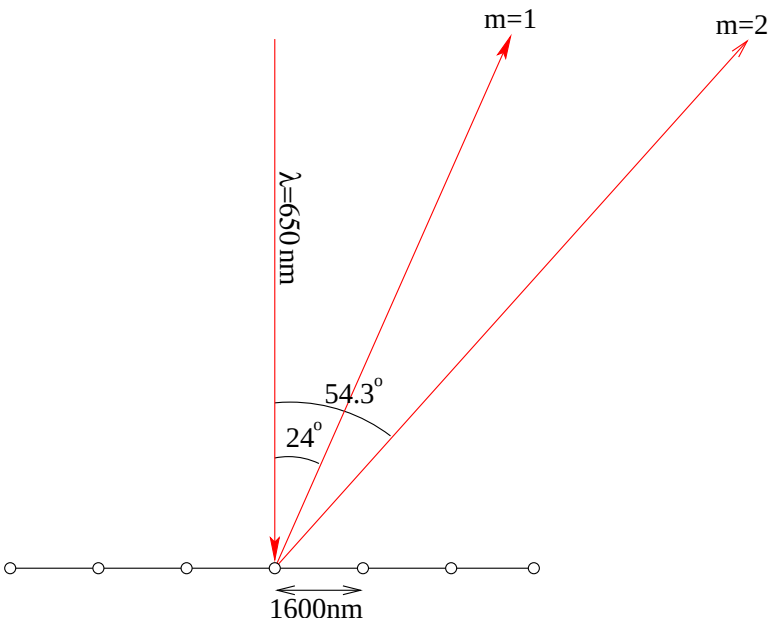
The diffraction grating has a much stronger effect than the two-slit experiment because there are many more than two ridges in the grating.

(Note that this figure differs from the corresponding figure in Week 5 Note 6, substantively in that this shows the incident rays parallel and the diffracted rays parallel, although they should be shown diverging from a point source and converging to a point detector, respectively. But the source and detector are a long way away.)

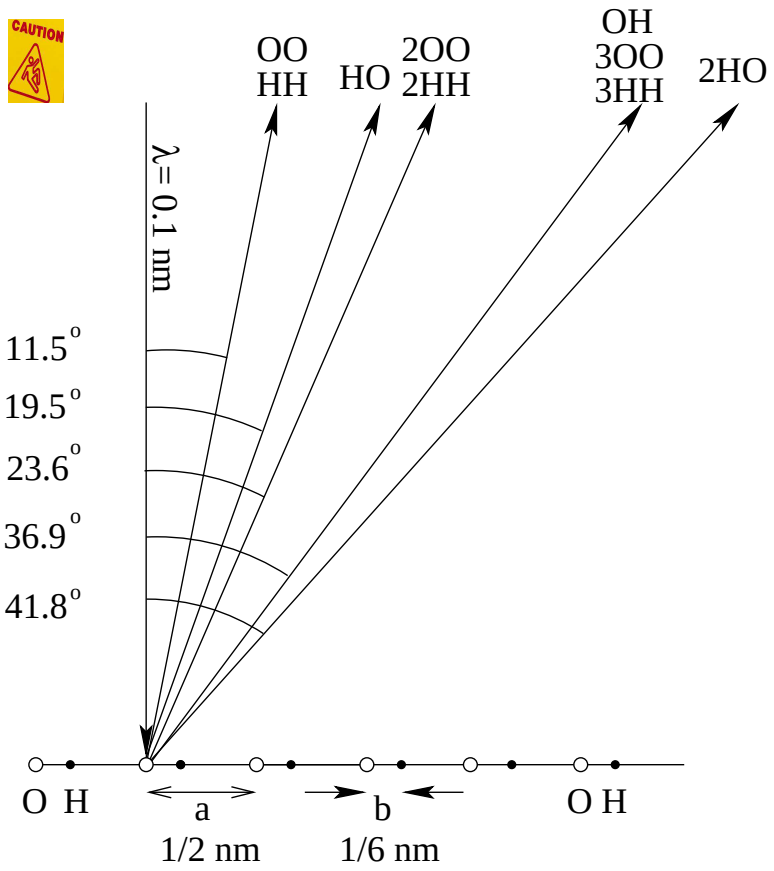
A CD has grooves about every 1.6 microns (micro-meters). A red laser pointer emits light at about 650 nanometers. So

$$\sin\theta = m\lambda/a = m650\text{nm}/1.6\mu\text{m} = 0.406m$$

and for $m = 1$ this gives $\theta = 24°$. For $m = 2$, $\theta = 54.3°$.



Here is a one-dimensional "crystal" modelled after ice (Week_ii Note 9). It has two atoms per "unit cell", one oxygen and one hydrogen. a is 1/2 nm and b is a third of that.



Since this atomic spacing is far too fine for visible light, so let's think about shining X-rays on it at $\lambda = 0.1$nm. There will be diffraction from the OO and HH spacing, $a = 1/2nm$, from the HO

spacing, $b - a = 1/3nm$, and from the OH spacing, $b = 1/6nm$.

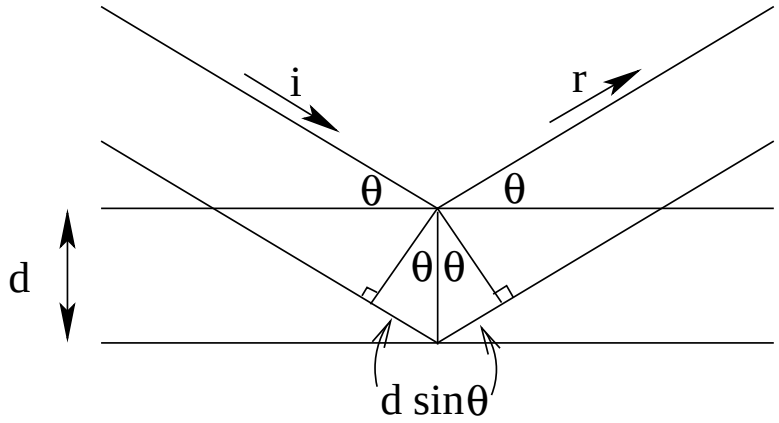
A fuller discussion of diffraction would discuss the intensities of each spot as well as their angles.

21. 2D crystals. Crystals are periodic lattices of atoms. If diffraction can tell us about the spacing of lines on a diffraction grating, maybe it can tell us something about how the atoms are arranged in a crystal.

We must work with shorter wavelengths than visible light because atom spacing in crystals is only a few nanometers. Hence we have X-ray crystallography, which has given us structures of crystals from table salt all the way up to crystallized proteins such as myoglobin.

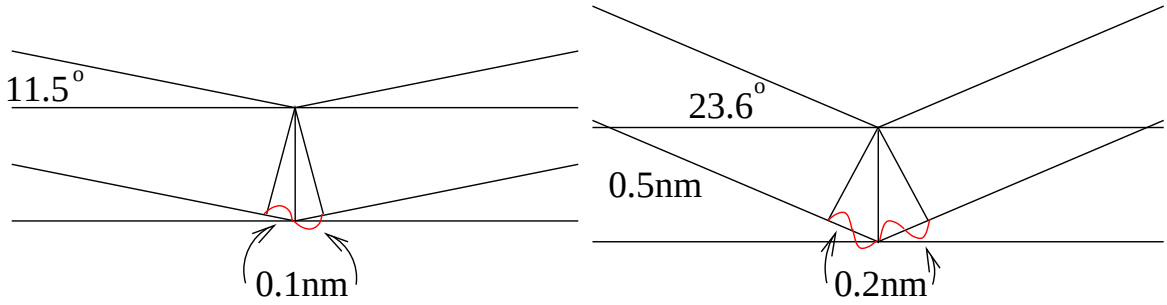
X-ray crystallography considers reflections (only) from the different planes of atoms that we can find in a crystal. The X-rays cannot be reflected at any angle, however, because reflections from different planes will interfere with each other.

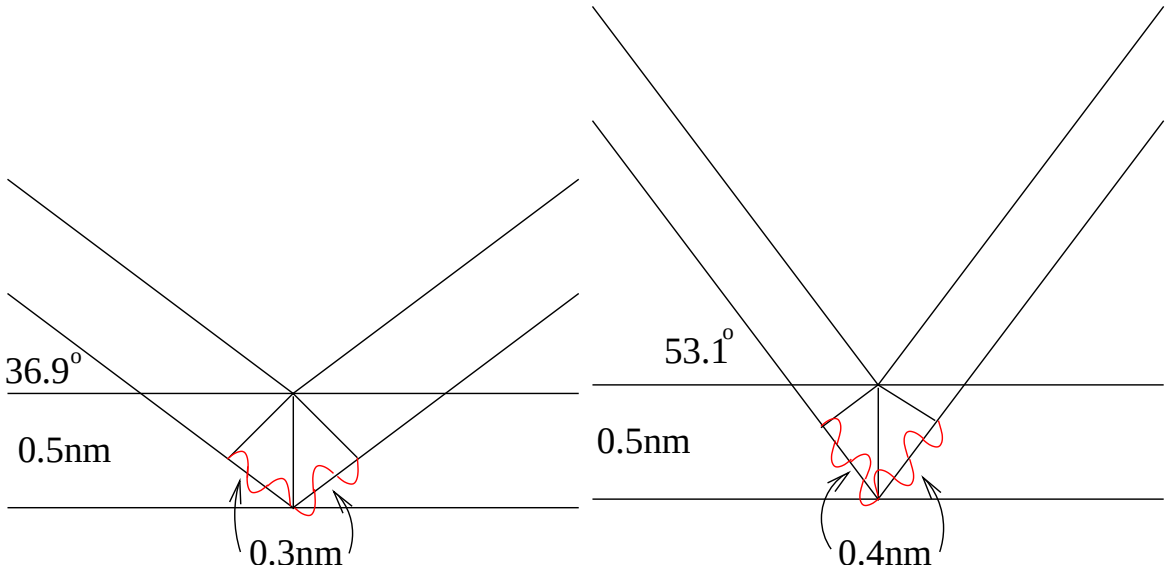
Here is Bragg's law governing which angles of reflection are allowed. Note that the math is very similar to the math for diffraction (previous Note) but that the incident and reflected angles are equal, and they are measured from the surface of the plane rather than from the perpendicular to the plane.



So the condition for constructive interference is $2d \sin\theta = n\lambda$ for any integer multiple, n, of the wavelength, λ.

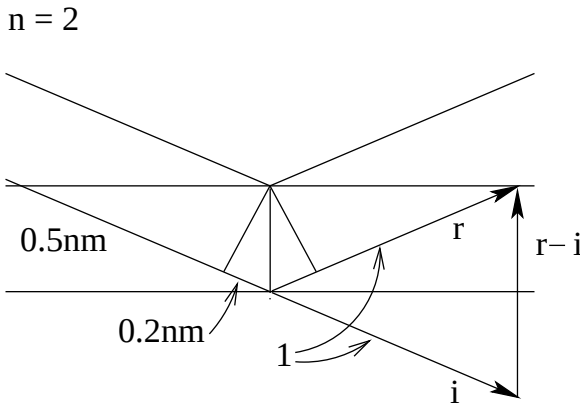
For plane separation $d = 0.5$ nm and wavelength $\lambda = 0.2$ nm, here are the possible reflections, $\theta = \sin^{-1} \frac{n\lambda}{2d}$.





Let's look at this in terms of vector differences.

Call the direction of the incoming ray $\vec{i}$ ($|\ \vec{i}\ | = 1$, unit vector) and the direction of the reflected (outgoing) ray $\vec{r}$ ($|\ \vec{r}\ | = 1$). The difference, $\vec{r} - \vec{i}$, is a vector perpendicular (normal) to the reflecting planes, and has length $2 \sin\theta = n\lambda/d$.



It is convenient to make this an integer multiple of $1/d$, as we'll see, so we divide everything by λ.

$$|\ \frac{\vec{r}}{\lambda} - \frac{\vec{i}}{\lambda}\ | = \frac{2\sin\theta}{\lambda} = \frac{n}{d}$$

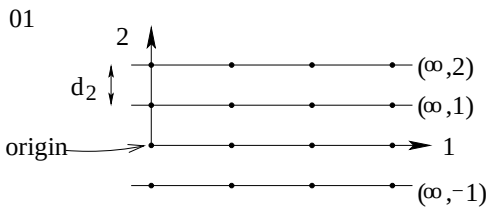
This is an improved way of looking at Bragg's law, called the Laue equations (equation*s*, plural, because two equations are given by the vector equation), because it relates the allowed reflections directly to the (normal to the) plane that causes them. In a crystal there are many planes, so this simple law can get confusing.

We'll work with two-dimensional "crystals" to keep things clear. "Planes" are now just lines.

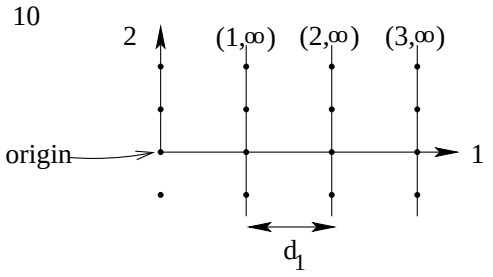
To keep things really simple, we'll start with *rectangular* 2D crystals.

We'll look at normals to planes with magnitude $1/d$, where adjacent planes are separated by d.

The basic planes are horizontal



and vertical



and I've shown the values at which each plane intersects with the 1 and 2 axes.

Since it is awkward to deal with ∞, we can get the same information from the reciprocal of the intersection values. Furthermore, we are not interested in each different plane but only in the whole class of parallel planes.

So we can consider only a plane next to the plane passing through the origin, and take the reciprocals of the intersections.

Thus, the class of horizontal planes, $(\infty, 0), (\infty, 1), (\infty, -1), (\infty, 2), ..,$ has reciprocal indices 01.

The class of vertical planes, $(0, \infty), (1, \infty), (-1, \infty), (2, \infty), ..,$ has reciprocal indices 10.

We call the vectors $\vec{b}_1 = \frac{1}{d_1}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\vec{b}_2 = \frac{1}{d_2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ the *reciprocal basis* vectors, or the basis of the *reciprocal lattice*. (d_1 and d_2 are the separations of the vertical and horizontal planes, respectively, as shown above.)

The reciprocal lattice is the reciprocal of the crystal lattice with bases $\vec{a}_1 = d_1\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\vec{a}_2 = d_2\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. Note, if we make a matrix, A, with columns $\vec{a_1}$ and $\vec{a_2}$, and a matrix, B, with rows $\vec{b_1}$ and $\vec{b_2}$, that

$$AB = \left(\begin{pmatrix} d_1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 \\ d_2 \end{pmatrix}\right)\begin{pmatrix} (1/d_1 & 0) \\ (0 & 1/d_2) \end{pmatrix} = I$$

i.e., they are inverses of each other.

Going back to X-ray reflection, note that for the horizontal planes

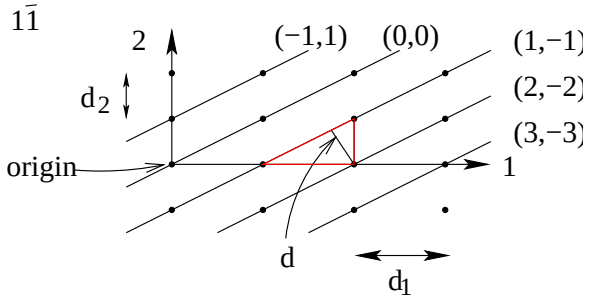
$$\frac{\vec{r} - \vec{i}}{\lambda} = nb_2$$

and for the vertical planes

$$\frac{\vec{r} - \vec{i}}{\lambda} = nb_1$$

So it seems that if we can find the reciprocal lattice we can find the allowed reflections.

Let's look at some other planes in our rectangular crystal.



The reciprocal indices are 1 and -1, abbreviated $1\bar{1}$.

The distance between adjacent planes, d, can be found by calculating the area, Δ, of the red triangle in two different ways.

$$d_1 d_2 = 2\Delta = d\sqrt{d_1^2 + d_2^2}$$

so $d = \frac{d_1 d_2}{\sqrt{d_1^2+d_2^2}}$ and $\frac{1}{d} = \frac{\sqrt{d_1^2+d_2^2}}{d_1 d_2}$.

The unit vector normal to the planes is

$$\frac{1}{\sqrt{d_1^2 + d_2^2}} \begin{pmatrix} d_2 \\ -d_1 \end{pmatrix}$$

because the "plane" in this 2D example is just the vector (d_1, d_2). (Recall that

$$(d_1, d_2) \begin{pmatrix} d_2 \\ -d_1 \end{pmatrix} = 0$$

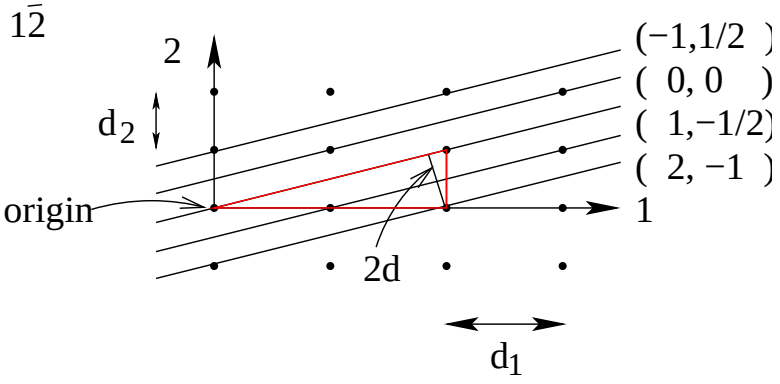
is a multiple of the cosine of the angle between the vectors, which, being zero, means the angle is a right angle.)

Dividing this by d (reciprocal vectors have magnitudes that are the reciprocal of the separation)

$$\frac{\sqrt{d_1^2 + d_2^2}}{d_1 d_2} \frac{1}{\sqrt{d_1^2 + d_2^2}} \begin{pmatrix} d_2 \\ -d_1 \end{pmatrix} = \begin{pmatrix} 1/d_1 \\ -1/d_2 \end{pmatrix} = \vec{b_1} - \vec{b_2}$$

Since $\frac{\vec{r}-\vec{i}}{\lambda} = \frac{n}{d}$ (unit normal to the reflecting planes) we see that reflection off the $1\bar{1}$ planes is just a vector in the reciprocal lattice with integer coefficients.

Let's try one more set of planes



The reciprocal indices are 1 and -2 or $1\bar{2}$ and the twice-too-big red triangle has area Δ

$$2d_1d_2 = 2\Delta = 2d\sqrt{(2d_1)^2 + d_2^2}$$

So $1/d$ times the unit normal is

$$\frac{1}{d_1d_2}\begin{pmatrix} d_2 \\ -2d_1 \end{pmatrix} = \begin{pmatrix} 1/d_1 \\ -2/d_2 \end{pmatrix} = \vec{b_1} - 2\vec{b_2}$$

It should be clear now that in general 1/d times the unit normal to plane hk is $hb_1 + kb_2$ and reflections from these planes satisfy

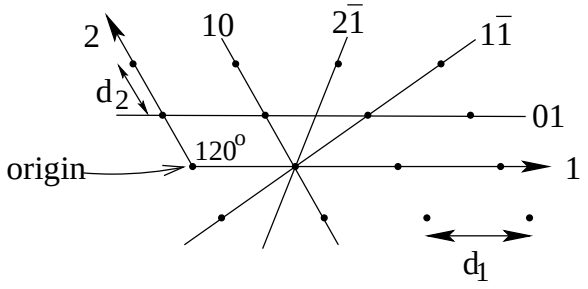
$$\frac{\vec{r} - \vec{i}}{\lambda} = n(hb_1 + kb_2)$$

That is, reciprocal lattice vectors with integer coefficients correspond to X-ray reflection spots.

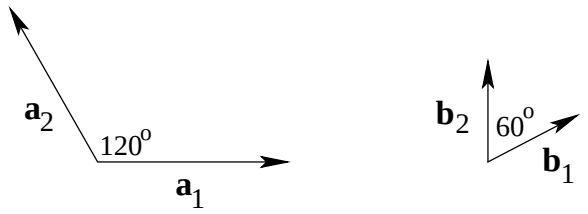
The object of X-ray crystallography is to work backwards from the spots to the crystal structure. This is relatively easy if, as for table salt, we can guess the structure and calculate the spots to check with the measurement. It is very difficult if, as for vitamin B12 or myoglobin (which each generated a Nobel prize), such guessing is impossible.

We won't pursue X-ray crystallography further here, except to show that non-rectangular lattices can be handled by the same mathematics.

First, the indexing convention for planes is just the same.



Second, the rule for finding the reciprocal lattice is the same.



$$\begin{aligned}
(\vec{b_1}\vec{b_2})^T &= (\vec{a_1}\vec{a_2})^{-1} \\
&= \left(\begin{pmatrix} d_1 \\ 0 \end{pmatrix}\begin{pmatrix} -d_2/2 \\ d_2\sqrt{3}/2 \end{pmatrix}\right)^{-1} \\
&= \frac{2}{d_1d_2\sqrt{3}}\begin{pmatrix} d_2\sqrt{3}/2 & d_2/2 \\ 0 & d_1 \end{pmatrix} \\
&= \begin{pmatrix} (1/d_1 & 1/d_1/\sqrt{3}) \\ (0 & 2/d_2/\sqrt{3} \end{pmatrix}
\end{aligned}$$

so $b_1 = \frac{1}{d_1}\begin{pmatrix} 1 \\ 1/\sqrt{3} \end{pmatrix}$ and $b_2 = \frac{1}{d_2}\begin{pmatrix} 0 \\ 2/\sqrt{3} \end{pmatrix}$.

Finally, since vectors in the recirocal lattice are $1/d$ long and perpendicular to planes, they give reflection spots for plane hk in exactly the same way

$$\frac{\vec{r} - \vec{i}}{\lambda} = n(hb_1 + kb_2)$$

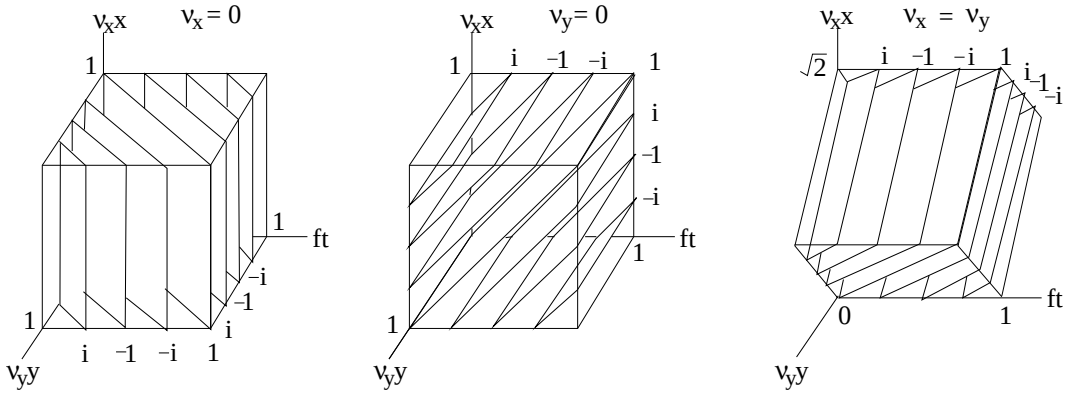
All these generalize readily to real crystals in three dimensions, using three indices for the planes, $hk\ell$.

These indices are called Miller indices.

22. 2D waves. A wave travels in one direction, i.e., one dimension, even in the context of two or more dimensions. By analogy with one-dimensional waves (Note 20, Week 7a Note 2), the form will be $e^{2\pi i(ft - g(x,y))}$, for some function, $g()$, of the two coordinates x and y. This function must also involve the wavenumbers, ν_x and ν_y. The wave velocity has a direction and hence x- and y-components. For an observer attached to the crystal, it would make sense that these components should be f/ν_x and f/ν_y, respectively.

This will happen if $g(x, y) = \nu_x x + \nu_y y$: try changing x by Δ_x and t by Δ_t without changing y, and calculate Δ_x/Δ_t for the timespace change that keeps the phase the same. (This is the argument used for one dimension in the "visualizing waves" excursion of Week 7a.) Do the same for Δ_y/Δ_t keeping x unchanged.

Here is a picture of the planes of constant phase for three different wave directions.



But this is just the dot product of the vector $\vec{\nu}$ and the vector (x, y), which we can call $\vec{w}$, meaning the wave direction:

$$e^{2\pi i(ft - \vec{\nu}.\vec{w})}$$

From this Book's excursion, "dot product", this is also easily calculated from the reciprocal coordinates of $\vec{\nu}$ and the lattice coordinates of $\vec{w}$:

$$e^{2\pi i(ft - (\nu_x w_x + \nu_y w_y))} = e^{2\pi i(ft - (\nu^1 w_1 + \nu^2 w_2))}$$

We get exactly the same thing from the group representations.

The translation operations under which the crystal is invariant are now t_1, in the direction of lattice axis 1, and t_2, in the direction of lattice axis 2. Clearly these commute: t_1 followed by t_2 gives the same final position as t_2 followed by t_1.

So the translation group, $T^{(t_1,t_2)}$, is the product of two one-dimensional groups,

$$T^{(t_1,t_2)} = T^{(t_1)} \times T^{(t_2)}$$

and the irreducible representations are also products, of the one-dimensional irreducible representations we found in Note 19.

$$\begin{aligned} T_{k_1,k_2}(m_1,m_2) &= T_{k_1}(m_1) \times T_{k_2}(m_2) \\ &= e^{-ik_1m_1} \times e^{-ik_2m_2} \\ &= e^{-i(k_1m_1+k_2m_2)} \\ &= e^{-i\vec{k}.\vec{m}} \end{aligned}$$

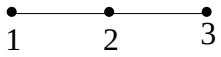
and I have written these roots of unity in the notation used in Note 19, but they could equally well be written as above

$$e^{2\pi i(ft-\vec{\nu}.\vec{w})}$$

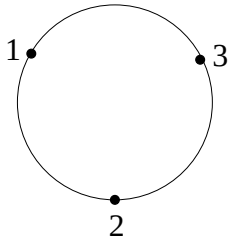
because the $e^{2\pi ift}$ component is just a phase change independent of position that does not involve the space, and the 2π is just to allow us to use wavenumber, ν, instead of angular wavenumber, k.

Since we cannot make this concrete for infinite crystals, let's look at a couple of finite examples. First, a one-dimensional "crystal" of three atoms, 1, 2 and 3.

Periodic boundary conditions. Since waves in a finite crystal, especally a three-atom one, will be dominated by the effects of the boundaries where the crystal stops, we use a standard trick: we pretend that the crystal forms a ring so that atom 3 appears before atom 1 and atom 1 after atom 3.



1−D "crystal"



periodic boundary

··1 2 3 1 2 3 **1 2 3** 1 2 3 1 2 3··

"infinite"

Now the translations are simply (123) and its inverse, (132).

The translation group, its irreducible representations, and *perm*, which gives the projections, are

	()	(123)	(132)
triv	1	1	1
left	1	$e^{2\pi i/3}$	$e^{-2\pi i/3}$
right	1	$e^{-2\pi i/3}$	$e^{2\pi i/3}$
	3	0	0
perm	$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} & & 1 \\ 1 & & \\ & 1 & \end{pmatrix}$	$\begin{pmatrix} & 1 & \\ & & 1 \\ 1 & & \end{pmatrix}$

Since **perm** = **triv** + **left** + **right**, the modes are given by the projections

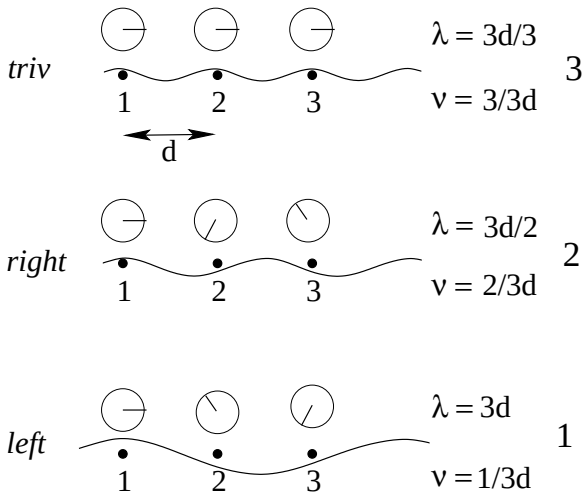
$$P_{\mathbf{triv}} = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}(1,\ 1,\ 1)\frac{1}{\sqrt{3}}$$

$$P_{\mathbf{left}} = \frac{1}{3}\begin{pmatrix} 1 & e^- & e^+ \\ e^+ & 1 & e^- \\ e^- & e^+ & 1 \end{pmatrix} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ e^+ \\ e^- \end{pmatrix}(1,\ e^-,\ e^+)\frac{1}{\sqrt{3}}$$

$$P_{right} = \frac{1}{3}\begin{pmatrix} 1 & e^+ & e^- \\ e^- & 1 & e^+ \\ e^+ & e^- & 1 \end{pmatrix} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ e^- \\ e^+ \end{pmatrix}(1,\ e^+,\ e^-)\frac{1}{\sqrt{3}}$$

where we have abbreviated $e^{2\pi i/3}$ by e^{+} and $e^{-2\pi i/3}$ by e^{-}, and where we (always!) apply the 2-number (complex) conjugate when we transpose a vector or a matrix.

The resulting modes can be drawn as little clocks showing the phase at each atom or as cosines to convey more graphically the idea of waves.



Also shown for each wave are the wavelength, λ, in terms of $3d$, the width of the crystal (atoms spaced d apart), and the wavenumber, ν, in terms of "per $3d$". Since the wavenumber is proportional to the frequency and is just an integer in units of $1/3d$, we emphasize ν here and now on.

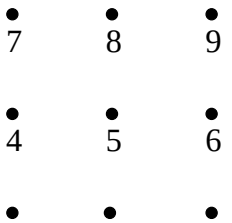
Notice that the clock "goes around" (counterclockwise) twice as fast when ν is 2 as when ν is 1, and three times as fast when ν is 3. Or that there are three whole waves across the crystal when ν is 3, two when ν is 2 and one when ν is 1.

Note that, if this math is describing atomic vibrations, the "wave" for ν is 3 need not be a wave at all: all atoms are moving in the same direction, and there may be no restoring force to make them vibrate. On the other hand, the math may be describing electron positions, and the (2-number) wave makes sense.

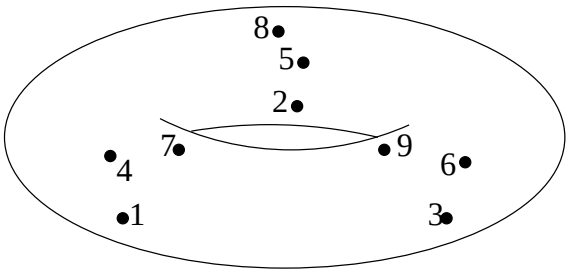
Note also that waves of larger ν are not distinguishable from what we have already shown. For instance, halving the wavelength where ν is 3 still has all atoms moving in the same direction: the extra peaks halfway between each atom fall on no atoms and so describe no motion.

The smallest ν is 1: the full crystal must hold at least one wave. This is a result of the periodic boundary condition.

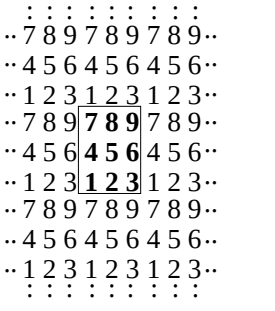
With this one-dimensional preamble, we can go on to two dimensions. This time consider a 3×3 "crystal", again with periodic boundary conditions. The double cycle of the boundaries is harder to imagine in 2-D: think of one direction curled up to make a cylinder, then the cylinder curled around in the other direction to make a doughnut.



2−D "crystal"

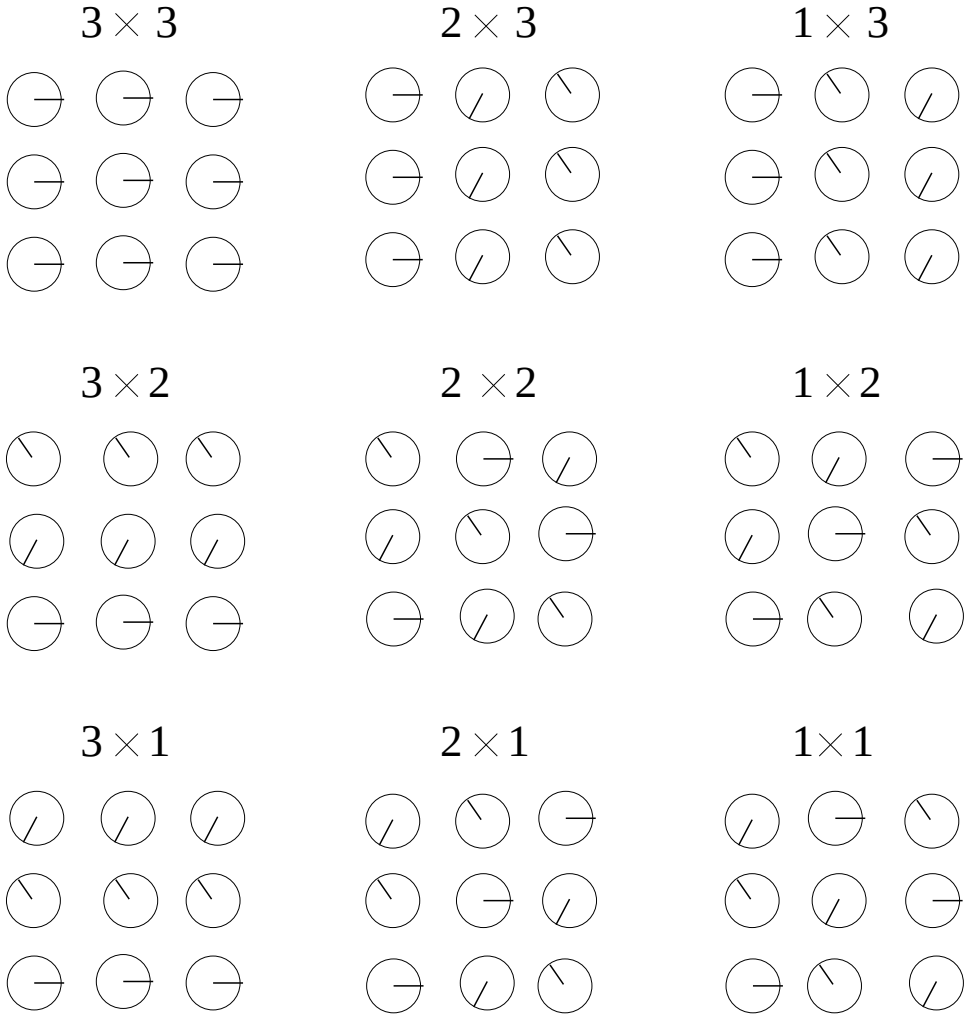


periodic boundaries



"infinite"

Since the one-dimensional crystal has three modes, which we called 3, 2 and 1 (with 3 corresponding to the **triv** representation), let's do this one backwards, starting with guessing the modes. It seems likely that there will be nine modes, which we can call 3×3 (corresponding to *triv*), $3\times 2, 3\times 1, 2\times 3$ and so on down to 1×1.



Here are plausible mode vectors, using 1 to stand for 1, \ to stand for $e^{2\pi i/3}$ (the drawings above and below show why) and / to stand for $e^{-2\pi i/3}$.

We can further suppose that the x- and y-motions are the same, except for lying respectively in the x- and y-directions. So the drawing above and the vectors below need not be redone for the other direction.

atom	3×3	3×2	3×1	1×3	2×3	1×2	2×1	1×1	2×2
1	1	1	1	1	1	1	1	1	1
2	1	1	1	\	/	\	/	\	/
3	1	1	1	/	\	/	\	/	\
4	1	/	\	1	1	/	\	\	/
5	1	/	\	\	/	1	1	/	\
6	1	/	\	/	\	\	/	1	1
7	1	\	/	1	1	\	/	/	\
8	1	\	/	\	/	/	\	1	1
9	1	\	/	/	\	1	1	\	/

The nine translation group elements have the form (123)(456)(789) etc. and are shown below in columns of three cycles. The **perm** representation is nine 9×9 matrices and we have room to show only their traces. We see below that **perm** is just the sum of all the irreducible representations. These are named for the waves they generate, so **perm** = '3 × 3' + '3 × 2' + '3 × 1' + '1 × 3' + '2 × 3' + '2 × 1' + '1 × 2' + '1 × 1' + '2 × 2'.

In addition, the representation for the x and y coordinates at each atom consists entirely of 2×2 identity matrices, so their traces are all 2 and their representation **xy** = 2×**triv**.

The combination, **perm**×**xy**, gives the representation for all motions. We see below that **permxy** = **perm**×**xy** is twice the sum of all the irreducible representations, **permxy** = 2×**perm**. This factor 2 means that x and y may be treated independently and identically, as we supposed above.

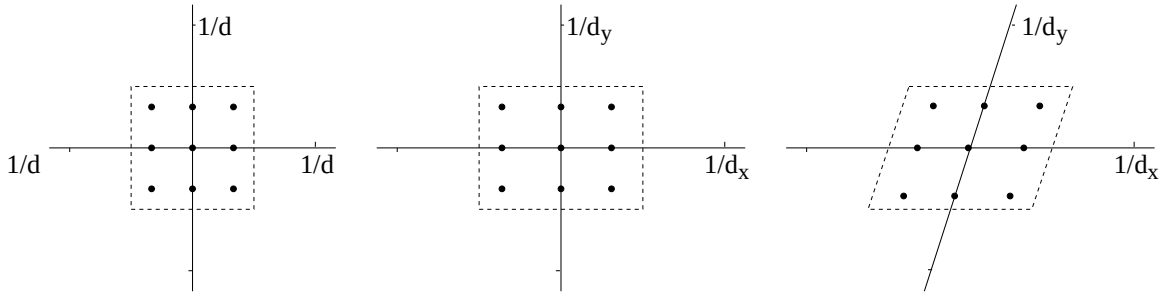
	()	(123) (456) (789)	(132) (465) (798)	(147) (258) (369)	(174) (285) (396)	(159) (267) (348)	(195) (276) (384)	(168) (249) (357)	(186) (294) (375)
'3 × 3'	1	1	1	1	1	1	1	1	1
'3 × 2'	1	1	1	/	\	/	\	/	\
'2 × 1'	1	1	1	\	/	\	/	\	/
'1 × 3'	1	\	/	1	1	\	/	/	\
'2 × 3'	1	/	\	1	1	/	\	\	/
'1 × 2'	1	\	/	/	\	1	1	\	/
'2 × 1'	1	/	\	\	/	1	1	/	\
'1 × 1'	1	\	/	\	/	/	\	1	1
'2 × 2'	1	/	\	/	\	\	/	1	1

23. Brillouin zone. We saw that $\nu = 6/3d$, say, is indistinguishable in a 3-crystal (1-D) from $\nu = 3/3d$, because both lead to the same displacement of the three atoms. By the same reasoning, adding any multiple of the reciprocal lattice, $1/d$, to any of the allowed wavenumbers gives motion indistinguishable from the original wavenumber.

In particular, we could replace $\nu = 3/3d$ by $\nu = 0/3d = 3/3d - 1/d$, and so relabel "3" everywhere above by "0". We could also replace $\nu = 2/3d$ by $\nu = -1/3d$, so that "2" becomes "−1".

The *Brillouin zone* of a crystal is defined to be all the allowed wavenumbers, normalized to lie between $-1/d$ and $1/d$.

This notion generalises to higher dimensions. Here are Brillouin zones for three 3-by-3 lattices, one square ($d_x = d_y$), one rectangular (in this case $d_x < d_y$) and one rhombic (in this case also $d_x < d_y$).



It is not hard to see that a 4-by-4 crystal would have 16 allowed wavenumbers within the same $-[1/2d_x, 1/2d_y] \times [-1/2d_x, 1/2d_y]$ region, a 4-by-3 would have 12, and so on. So a realistically large crystal of, say 10^{10}-by-10^{10} atoms would have 10^{20} allowed wavenumbers within the same region.

There are also reciprocal lattices and Brillouin zones in three dimensions. A realistically-sized crystal might be 10^7-by-10^7-by-10^7.

Adding any reciprocal lattice vector to any allowed wavenumber just maps it to the corresponding

point in an image of the Brillouin zone about some other point in the reciprocal lattice. It has no effect whatsoever on the motions about each atom, whether displacements of the atom itself, actions on the electrons of the atom, reflection of photons, or any other physical interpretation of the mathematics.

The Brillouin zone is the simplification extracted by group theory from translational symmetry. We do not need to worry about wavenumbers outside of it.

24. Non-translational crystal symmetries. Crystals usually have symmetries beyond the translational. The non-translational symmetries form *point groups*, and the combined groups are *space groups*.

The one-dimensional crystal of Note 22 has reflection symmetry as well as translation. Combining these groups gives the full triangle group we saw in Note 1. (All six elements of the group can be generated from (123) for translation and (12) for reflection about 3—or, equally, about the halfway point between 1 and 2.)

We saw the irreducible representations of the triangle group in Note 9 and their interpretation for a triangular molecule in Note 13. For the one-dimensional, 3-atom crystal of Note 22, the motions are given by **perm** (see Note 9) and the projection vectors are $1/\sqrt{3}(1,1,1)$, $1/\sqrt{2}(1,-1,0)$ and $1/\sqrt{6}(1,1,-2)$. The first is a wave of wavelength d (or ∞: see Note 23) and amplitude $1/\sqrt{3}$. The second and third are both waves of wavelength $3d$ and amplitude $\sqrt{2/3}$, the first with a maximum at atom 1 and the second with a maximum halfway between atoms 1 and 2.

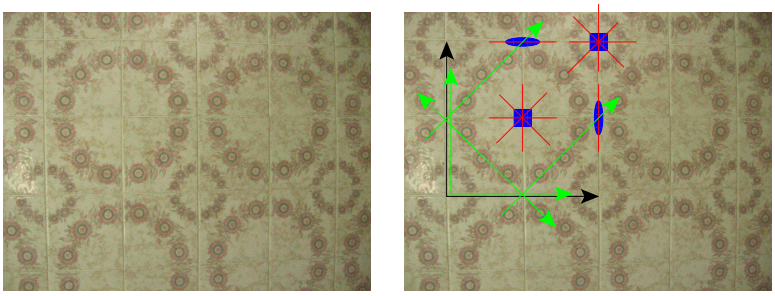
This one-dimensional point group, {(), (12)}, can be reduced to {()} by "breaking" the reflection symmetry, The only way to do that in this case is by inserting a second atom associated with each atom already in the lattice. The second atom can be different from the first or it can be the same and inserted asymmetrically into the lattice, i.e., closer to the associated lattice atom than to its neighbour. An example, where the second atom is both different and asymmetrically placed, is the one-dimensional "ice" of Note 20. Then we are back to purely translational symmetry and the space group is just the translation group.

In two dimensions we can have square symmetry, with rotations and reflections as well as translations, or hexagonal symmetry, or any of a number of broken sub-symmetries. The figure showing Brillouin zones in Note 23 above shows how rotational symmetry can be lost by changing the square lattice to a rectangular lattice, and how reflection symmetry can be lost by skewing one of the axes of the lattice.

One way we can break square symmetry is, again, by associating a second atom with each lattice atom, either of different type or asymmetrically placed. This introduces the idea of a "unit cell", an internal structure of more than one atom, or point, which must be translated as a whole to give the translational symmetry. In wallpaper and other examples of translational symmetry, the unit cell consists of many points, the entire repeated pattern.

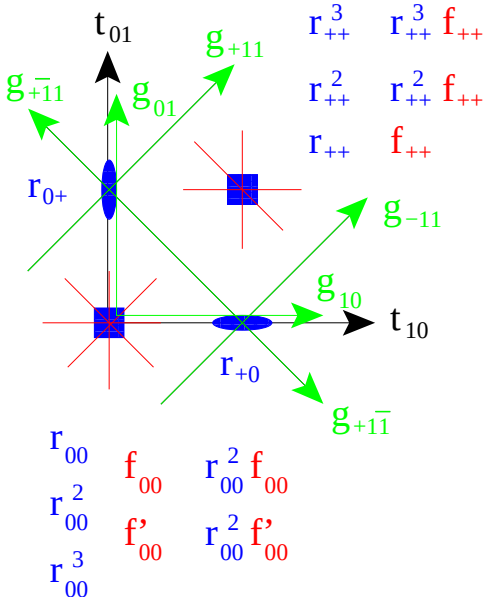
An important way to break symmetry in a crystal is to pass a wave through it. A wave belonging to the trivial representation has wavenumber 0 and the crystal propagating it has the full symmetry of the undisturbed crystal. Any other wave will reduce the symmetry of the crystal by favouring the direction it is travelling in. This is not very richly illustrated by the small crystals we have looked at explicitly, but becomes significant in crystals of realistic sizes. The physics of crystals is strongly influenced by symmetries broken by wave propagation.

25. Wallpaper groups. The simplest 2D pattern is highly symmetrical, just a square tiling. Let's see if we can extract all the symmetry operators. Here is an example with a pattern but which has the full symmetry.



This shows all the basic rotations (blue square for fourfold, ellipse for twofold) and reflections (red lines). All other operations can be found from these using translational symmetry, including the "glide reflections" (green lines). These follow a translation by a reflection. We will go on to find which of the operations shown can also be derived.

Meanwhile, we need names for them all.



The rotations and reflections about the origin are handled by matrices.

$$r_{00} : \begin{pmatrix} & -1 \\ 1 & \end{pmatrix} \times, \quad f_{00} : \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \times$$

The translations can be expressed by adding a vector.

$$t_{10} : + \begin{pmatrix} d \\ 0 \end{pmatrix}, \quad t_{01} : + \begin{pmatrix} 0 \\ d \end{pmatrix}$$

where d is the lattice spacing, the same in both directions for squares.

It is going to be a little hard to mix these two forms, namely matrix multiplication and vector addition. Here's a trick.

$$r_{00} = \begin{pmatrix} & -1 & \\ 1 & & \\ & & 1 \end{pmatrix}, \quad f_{00} = \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$$

$$t_{10} = \begin{pmatrix} 1 & & d \\ & 1 & \\ & & 1 \end{pmatrix}, \quad t_{01} = \begin{pmatrix} 1 & & \\ & 1 & d \\ & & 1 \end{pmatrix}$$

These 3×3 matrics are to be applied to the augmented vector

$$\begin{pmatrix} x \\ y \\ 1 \end{pmatrix}$$

As well as rotation and reflection at the origin, we will need rotation and reflection at $(d/2, 0), (0, d/2)$ and $(d/2, d/2)$ as shown above.

A rotation about a point P can be calculated by 1) translating to the origin, 2) rotating about the origin, and 3) translating back to P. For example, the rotation about (1/2,1/2)d ("+" is supposed to be "1" cut in half)

$$\begin{aligned}
r_{++} &= Y_{1/2}X_{1/2}r_{00}X_{-1/2}Y_{-1/2} \\
&= \begin{pmatrix} 1 & & \\ & 1 & d/2 \\ & & 1 \end{pmatrix}\begin{pmatrix} 1 & & d/2 \\ & 1 & \\ & & 1 \end{pmatrix}\begin{pmatrix} & -1 & \\ 1 & & \\ & & 1 \end{pmatrix}\begin{pmatrix} 1 & & -d/2 \\ & 1 & \\ & & 1 \end{pmatrix}\begin{pmatrix} 1 & & \\ & 1 & -d/2 \\ & & 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & & d/2 \\ & 1 & d/2 \\ & & 1 \end{pmatrix}\begin{pmatrix} & -1 & \\ 1 & & \\ & & 1 \end{pmatrix}\begin{pmatrix} 1 & & -d/2 \\ & 1 & -d/2 \\ & & 1 \end{pmatrix} \\
&= \begin{pmatrix} & -1 & d \\ 1 & & \\ & & 1 \end{pmatrix}
\end{aligned}$$

The same process works for reflection in axes that do not include the origin.

With these two ideas, we can write down all the matrices.

First, the point group rotations.

$$r_{00} = \begin{pmatrix} & -1 & \\ 1 & & \\ & & 1 \end{pmatrix}, \quad r_{00}^2 = \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}, \quad r_{00}^3 = \begin{pmatrix} & 1 & \\ -1 & & \\ & & 1 \end{pmatrix}$$

Second, the point group reflections.

$$\begin{aligned}
f_{00} &= \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}, \quad f'_{00} = \begin{pmatrix} & 1 & \\ 1 & & \\ & & 1 \end{pmatrix} = r_{00}f_{00} \\
r_{00}^2 f_{00} &= \begin{pmatrix} -1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \quad r_{00}f'_{00} = \begin{pmatrix} & -1 & \\ -1 & & \\ & & 1 \end{pmatrix} = r_{00}^3 f_{00}
\end{aligned}$$

We are going to see that the rest can be derived from these plus the translations. So, third, the translations.

$$t_{10} = \begin{pmatrix} 1 & & d \\ & 1 & \\ & & 1 \end{pmatrix}, \quad t_{11} = \begin{pmatrix} 1 & & \\ & 1 & d \\ & & 1 \end{pmatrix}$$

Fourth, the two-fold rotations about the halfway points along the axes.

$$r_{+0} = \begin{pmatrix} -1 & & d \\ & -1 & \\ & & 1 \end{pmatrix}, \quad r_{0+} = \begin{pmatrix} -1 & & \\ & -1 & d \\ & & 1 \end{pmatrix}$$

Fifth, the rotation about the face centre.

$$r_{++} = \begin{pmatrix} & -1 & d \\ 1 & & \\ & & 1 \end{pmatrix}, \quad r_{++}^2 = \begin{pmatrix} -1 & & d \\ & -1 & d \\ & & 1 \end{pmatrix}, \quad r_{++}^3 = \begin{pmatrix} & 1 & \\ -1 & & d \\ & & 1 \end{pmatrix}$$

Sixth, the reflection at the face centre.

$$f_{++} = \begin{pmatrix} 1 & & \\ & -1 & d \\ & & 1 \end{pmatrix}, \quad r_{++}^2 f_{++} = \begin{pmatrix} -1 & & d \\ & 1 & \\ & & 1 \end{pmatrix}, \quad r_{++}^3 f_{++} = \begin{pmatrix} & -1 & d \\ -1 & & d \\ & & 1 \end{pmatrix}$$

Seventh, the glide reflections along the translation axes.

$$g_{10} = \begin{pmatrix} 1 & & d \\ & -1 & \\ & & 1 \end{pmatrix}, \quad g_{01} = \begin{pmatrix} -1 & & \\ & 1 & d \\ & & 1 \end{pmatrix}$$

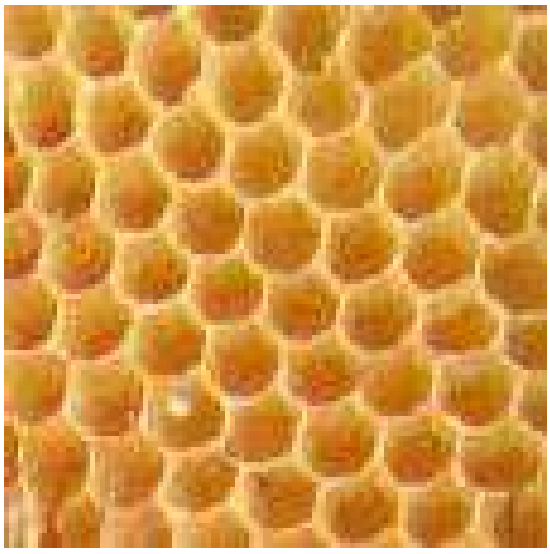
Eighth, the glide reflections along the diagonals.

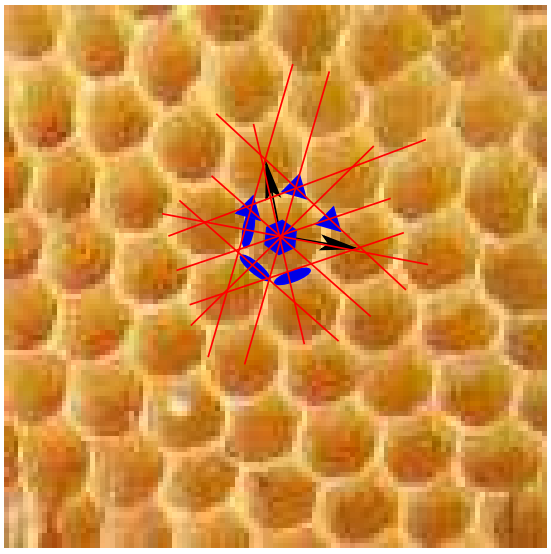
$$g_{-11} = \begin{pmatrix} & 1 & d \\ 1 & & \\ & & 1 \end{pmatrix}, \quad g_{+11} = \begin{pmatrix} & 1 & \\ 1 & & d \\ & & 1 \end{pmatrix}$$

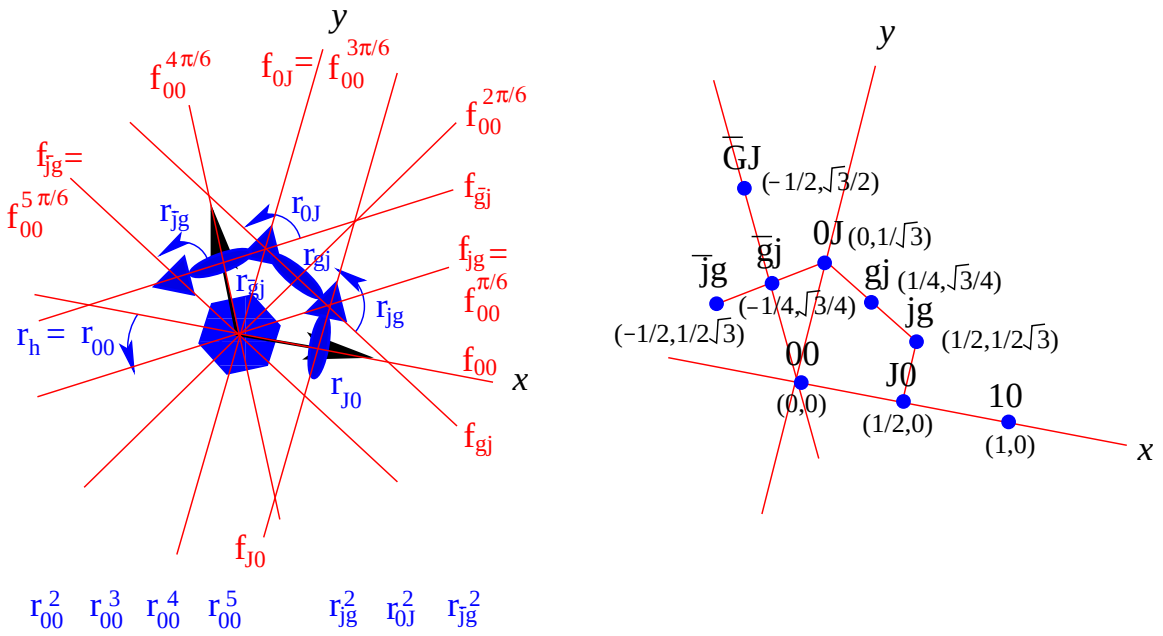
$$g_{-1\overline{1}} = \begin{pmatrix} & -1 & d \\ -1 & & \\ & & 1 \end{pmatrix}, \quad g_{+\overline{1}1} = \begin{pmatrix} & -1 & \\ -1 & & d \\ & & 1 \end{pmatrix}$$

There are four basic operations in all this. The point group of eight elements is generated by r_{00} and f_{00}. The infinite translation group is generated by t_{10} and t_{01}. Combining these gives the infinite space group.

The best illustration of honeycomb symmetry is a honeycomb.







The group elements are generated by the basic rotation and reflection of the point group. (The subscript labels refer to the point the operation is centered on, and we use r_h for "hexagon" instead of r_{00} so as not to confuse it with the basic square rotation above.)

$$r_h = \begin{pmatrix} 1/2 & -\sqrt{3}/2 & \\ \sqrt{3}/2 & 1/2 & \\ & & 1 \end{pmatrix} \qquad f_{00} = \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$$

and by two translations

$$t_{10} = \begin{pmatrix} 1 & & 1 \\ & 1 & \\ & & 1 \end{pmatrix} \qquad t_{\overline{G}J} = \begin{pmatrix} 1 & & -1/2 \\ & 1 & \sqrt{3}/2 \\ & & 1 \end{pmatrix}$$

(We used the subscript J in Week 6 to mean $1/2$, since J resembles an upside-down 2. The subscripts jg and gj are visually intermediate between $J0$ and $0J$, to give the counterclockwise sequence JO, jg, gj, $0J$ in the figure. This sequence continues with $\overline{g}j$ and $\overline{j}g$ to give all the centres of, alternately, 3-fold and 2-fold rotations, and all the reflections. $\overline{G}J$ is the lattice point twice as far from 00 as $\overline{g}j$, and GJ, $G\overline{J}$, $\overline{GJ}$ similarly are lattice points although not shown. 10 is of course the other lattice point.

The only confusion I foresee in the gj and jg notation might come in a discussion between an anglophone and a francophone.)

The point group consists of twelve elements, r_h and its powers 2, .., 5, and f_{00} and its transforms, which can be written variously (if you inspect the figure and check the matrix products) as $f_{00} = f_{J0}$, $f_{00}^{\pi/6} = f_{jg} = r_h f_{00}$, $f_{00}^{2\pi/6} = r_h^2 f_{00}$, $f_{00}^{3\pi/6} = f_{0J} = r_h^3 f_{00}$, $f_{00}^{4\pi/6} = r_h^4 f_{00}$, and $f_{00}^{5\pi/6} = f_{\overline{j}g} = r_h^5 f_{00}$.

(From Note 8 of Week 7c you can derive the matrix form of a reflection of a general point (x, y) about a general line of direction (c, s) as

$$(e_1, e_2) \begin{pmatrix} c^2 - s^2 & 2cs \\ 2cs & s^2 - c^2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

to check the above matrix products.)

The remaining honeycomb symmetry relations identified in the figure are

$$r_{jg} = t_{jg}\, r_h^2\, t_{jg}^{-1} = t_{10}\, r_h^2$$

and its successor r_{jg}^2,

$$r_{0J} = t_{0J}\, r_h^2\, t_{0J}^{-1} = t_{GJ}\, r_h^2 = r_h\, r_{jg}\, r_h^{-1}$$

and its successor r_{0J}^2,

$$r_{\overline{jg}} = t_{\overline{jg}}\, r_h^2\, t_{\overline{jg}}^{-1} = t_{\overline{G}J}\, r_h^2 = r_h^2\, r_{jg}\, r_h^{-1}$$

and its successor $r_{\overline{jg}}^2$,
and the 2-fold rotations.

The remaining reflections are

$$\begin{aligned} f_{J0} &= t_{J0}\, f_{00}\, t_{J0}^{-1} = t_{10}\, f_{00} \\ f_{gj} &= t_{gj}\, f_{\overline{jg}}\, t_{J0}^{-1} = t_{GJ}\, f_{\overline{jg}} \\ f_{\overline{g}j} &= t_{\overline{g}j}\, f_{jg}\, t_{\overline{g}j}^{-1} = t_{\overline{G}J}\, f_{jg} \end{aligned}$$

Since $t_{GJ} = t_{10} + t_{\overline{G}J}$ all these can be generated using only the two basic translations.

All the infinite other symmetry operations can be found by simple translation of the operations shown.

26. Continuous groups.
27. Spherical symmetry.
28. Commutator algebra.
29. Representations of the spherical group.
30. Spherical harmonics.
31. Atomic physics.
32. SU(2) formal and informal,
33. SU(3).
34. Isospin and quarks
35. Symmetry and Conservation: Complementary Quantities
36. Symmetry and Conservation: Energy
37. Principle of Stationary Action
38. Symmetry and Conservation: Noether's Theorem
39. The Hamiltonian and Schrödinger's Equation
40. Summary (These notes show the trees. Try to see the forest!)

Part I Discrete symmetries and molecules.

Notes 1–11. Symmetries of an equilateral triangle abstracted to groups. Invariant sets and subgroups. Traces and further matrix representations. Decomposing into irreducible representations and block-diagonalizing matrices.

Notes 12–17. Finding fundamental vibration modes of molecules from their symmetries: greenhouse gases CO_2 and H_2O.

Notes 16–18. Symmetries of the platonic solids: tetrahedron, octahedron/cube, dodecahedron/icosahedron.

Part II Infinite symmetries and crystals.

Notes 19–25. Translation symmetries and crystals in one and two dimensions: crystallography and waves.

Part III Continuous symmetries and the atom.

Notes 26–29. Rotational symmetry in two and three dimensions. Commutator algebra and representations of the spherical group.

Notes 30, 31. Spherical harmonics and atomic physics.

Part IV Abstract symmetries and lots of physics

Notes 32–34. From SU(2) (the atom) to SU(3) (the quarks). Isospin and hypercharge.

Notes 35–39. Symmetry and conservation laws. Complementary quantities, energy, Lagrangian, principle of stationary action, Noether's theorem, Hamiltonian, Schrödinger's equation and the quantum harmonic oscillator.

II. The Excursions

You've seen lots of ideas. Now *do* something with them!

1. a) Show that integers form a group under addition by checking each of the group axioms.
   b) What property of the addition table shown in Note 19 tells us addition is commutative?
   c) Do the integers form a group under multiplication? What about the rationals?

2. a) Show that multiples of 3, $\{..,-6,-3,\ 0,\ 3,\ 6,\ ..\}$, form an invariant subgroup $3I$ of the integers under $+$.
   b) Show that $I = 3I \times \{0,1,2\}$ **mod** 3.

3. Translations in one dimension might seem a boring symmetry, but they are the basis for western poetry and music. The keys to making this symmetry interesting are the idea of a "unit cell" and the notion of "broken symmetry".
   A unit cell is the unit of repetition in translational symmetry. In poetry it is the "foot" and in music the "bar". Feet have a certain number of syllables and bars have a certain number of beats.
   For example, two-syllable feet come in four varieties, depending on where the stress is put. If we symbolise the unstressed syllable as lower-case `a` and the stressed syllable as upper-case `A`, then an *iamb* is `aA` ("To be or not to be"), a *trochee* is `Aa`, a *spondee* is `AA` and a *pyrrhic* is `aa`.
   Of course, these last two definitions do not make sense from the simple point of view of translational symmetry, because if the rhythm is `AAAA`.. or `aaaa`.., how can we tell that the unit cell (the foot) has two syllables? So we might modify the definition, against poetic convention, to say that the spondee is the stressed one-syllable foot, `A`, and the pyrrhic is the unstressed one-syllable foot, `a`.
   That approach would give two basic forms for the one-syllable unit cell (foot) and two for the two-syllable unit cell (foot), since two of the four theoretically possible are reducible to single syllables.
   Three-syllable feet then have six (out of eight) possibilities: `aaA` *anapest*, `aAa` *amphibrach*, `Aaa` *dactyl*, `aAA` *bacchic*, `AaA` *cretic*, and `AAa` *antibacchic*; the remaining two being reducible to one-syllable feet.
   a) Collect examples of verse with two- and three-syllable feet. For example, iambs are the favourite of Shakespeare; anapests are the basis of a common and often vulgar form of verse; amphibrachs were extensively used by a famous writer of children's books; an extended poem about the British dispersion of the Acadians is dactyllic.

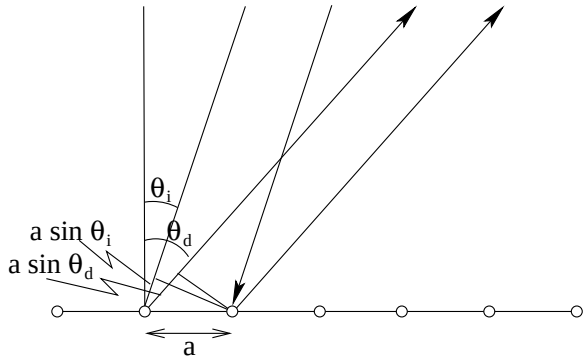
b) Analyse this verse. From it, deduce the pronunciation of the last syllable of the place name. See if you can find out how to pronounce the first syllable.
Note that the poet has broken the symmetry to emphasize the colloquialisms in the second and fifth lines. How? Where else?
Find or invent limericks about other places with obscure pronunciations, such as Dun Laoghaire.

```
A Canadian stayed in Milngavie.
Raised his glass: "Here's mud in your avie!
It was easier when
We lived in Bearsden
To say 'Let's drink the pub dravie!'"
```

c) How many four-syllable feet can there be, on the above reasoning? Look up their names.
d) The names of these rhythms are unusual words. Look them up.
e) Poetry has multiple levels of symmetry. The level up from rhythm is rhyme. Verse is constructed out of lines of a certain number of feet—the meter (anapestic trimeter and anapestic dimeter in the above limerick)—which rhyme with each other in various patterns. For instance, the limerick rhyme pattern is AABBA. What does this higher structure do to the unit cell?
f) The unit cell in music is the "bar", which has a certain number of beats and an internal rhythmic structure. For instance, "waltz time" is dactylic. Rock'n'Roll usually uses "4/4" time, four "quarter-notes" to the bar, with a rhythm which is not quite two trochees: the second stressed beat is less stressed than the first. Collect as many different musical beats as you can. (Try Dave Brubeck's album "Take Five". Try classical Indian ragas.) What happens to the rhythms of poetry when set to music in songs? (What is the dfference between "Twinkle, twinkle, little star" and "Baa, baa, black sheep"?)

4. a) Explain why the spots diffracted from the CD in Note 20 appear as short circular arcs.
b) Why is there no CD diffracted beam corresponding to $m = 3$ in Note 20?
c) Why are there no spots corresponding to the spacings between every second atom/ridge or every third atom/ridge, or so on?
d) If you have a green laser pointer, the wavelength is about 530 nm. Recalculate the CD diffraction angles of Note 20. Will there be an $m = 3$ beam?
e) Try the laser experiment with a DVD. Measure the angle and calculate what the spacing on the DVD must be. Given that a DVD holds about six times more data than a CD, and that both store data on a two-dimensional surface, discuss whether your calculated spacing makes sense. If you have one of the original 12" analogue optical disks, try that one, too. What do you observe about the fineness of the spacing and the diffraction angle?
f) Confirm the angles of diffraction for one-dimensional "ice" in Note 20. What might be wrong with this prediction? Will all of the spots appear? Any?

5. a) Show that the angle of diffraction, θ_d, from a grating for light originally incident at angle θ_i satisfies $$a(\sin\theta_d + \sin\theta_i) = m\lambda$$



b) In Week 5 Note 6 (two-slit diagram), what implicit assumption did we make about the light source?
c) Redraw this figure for light incident from the other side of the perpendicular, i.e., negative θ_i. Does the formula still hold?
d) In this figure and all the diffraction figures in Note 20, what is missing? (Did you look at the other wall when you shone the laser on the CD?)

6. Why does white light, reflected off an optical disc, break into the rainbow of its coloured components?

7. Show that the diffraction condition, $d\sin\theta = m\lambda$, and the Bragg reflection law, $2d\sin\theta = n\lambda$, (remembering that θ has quite different, indeed, complementary, meanings in the two formulae) give the same result for light *within* a one-dimensional "crystal", i.e., travelling in the same dimension as the "atoms" are lined up.

8. Confirm that the $1/d$ perpendicular to plane $2\bar{1}$ is $2\vec{b_1} - \vec{b_2}$ in the 120° non-rectangular lattice in Note 21.

9. What is the spacing of the ridges on the scales of the Morpho peleides butterfly that gives rise, by Bragg diffraction, to its blue colour?

10. Show that all possible reflection spots are reciprocal lattice points lying on the *Ewald sphere* (*Ewald circle* in two dimensions), which passes through the end of the $\vec{i}/\lambda$ vector and whose centre is at the beginning of the $\vec{i}/\lambda$ vector.
(Note that we must change the angle of the beam to pick up different multipliers, n. This is usually done by rotating the crystal in the beam.)

11. Try extending the math of Note 21 to three dimensions. Try it on a table salt crystal with the chlorine atoms missing. Try it with both sodium and chlorine atoms.

12. Look up Auguste Bravais 1811–63, Paul Peter Ewald 1888-1985, Sir William Lawrence Bragg 1890–1971, Dorothy Mary Crowfoot Hodgkin 1910–94, Max Ferdinand Perutz 1914–2002 and John Cowdery Kendrew 1917–1997. What did they do for crystallography? Which of them won Nobel prizes?

13. **Dot product.** Show that the dot product between two vectors, $\vec{u} = (u_x, u_y)$ and $\vec{v} = (v_x, v_y)$, which is $u_x v_x + u_y v_y$, becomes $u^1 v_1 + u^2 v_2$ when the vectors are expressed in terms of a crystal lattice, $\vec{v} = v_1\vec{a_1} + v_2\vec{a_2}$, and its reciprocal lattice, $\vec{u} = u^1\vec{b_1} + v^2\vec{b_2}$. Hint: using $\vec{u_j} = \vec{u}.\vec{b_j}d_j$ and $\vec{v^j} = \vec{a_j}.\vec{v}/d_j$, $j = 1, 2$ (why?) combine the $\vec{a_j}$s and the $\vec{b_i}$s in $u^1 v_1 + u^2 v_2$ so that they form a matrix which you can show from the definition of the $\vec{b_j}$ in terms of the $\vec{a_j}$s to be the identity matrix.
(The subscripted coordinates, v_j, are called *covariant* and the superscripted coordinates, u^j, are called *contravariant*. When dealing with coordinate systems whose bases are not orthonormal (i.e., perpendicular to each other and of unit length) using co- and contravariant coordinates from the basis and its reciprocal make dot products just as easy as in orthonormal bases. There is even a convention, the "Einstein summation convention", that a combination of superscript and subscript implies a sum: $u^j v_j \stackrel{\text{def}}{=} \sum_j u^j v_j$. The matrix $(\vec{a_1}\vec{a_2}) \times (\vec{a_1}\vec{a_2})^T$ is called the *metric tensor*. What are the equivalents of covariant and contravariant coordinates and the metric tensor in one dimension?
Look up the Excursion "Nonorthogonal axes and tensor notation" in Week 7c.)

14. Confirm that the one-dimensional representations, '3×3', '3×2', .., '1×1', of the 3-by-3 atom translation group in Note 22 are orthogonal to each other and are therefore all the irreducible representations, that they sum to the **perm** representation, and that the mode vectors given in Note 22 are also given by the projections of **perm** into its one-dimensional decompositions. (Remember to use the 2-number (complex) conjugate when you transpose vectors to take the dot product: this swaps \ and /.)

15. Draw, as cosine curves, some of the waves that result from the 3-by-3 translational symmetry.

16. For a 2-by-2-atom "crystal" with periodic boundary conditions what are
a) the translation group,
b) its irreducible representations,
c) the motion representation, **perm**, and its decompositions, and, hence,
d) the modes of vibration? Compare your results with the 3-by-3 "crystal" of Note 22.
Extend this translation group by adding the point group, assuming square symmetry around each atom, and answer the above four questions. Discuss the changes from the first case where the only symmetry was translational. Which two symmetry operators can generate the whole group? Note that putting in rotation about an atom automatically generates rotation about centres halfway between atoms.

17. What does a wavenumber of 0 mean in the one-dimensional crystal of Note 22?
Confirm in two dimensions that adding any reciprocal lattice vector to any wavenumber vector within the Brillouin zone gives exactly the same atomic displacements and so gives nothing new.

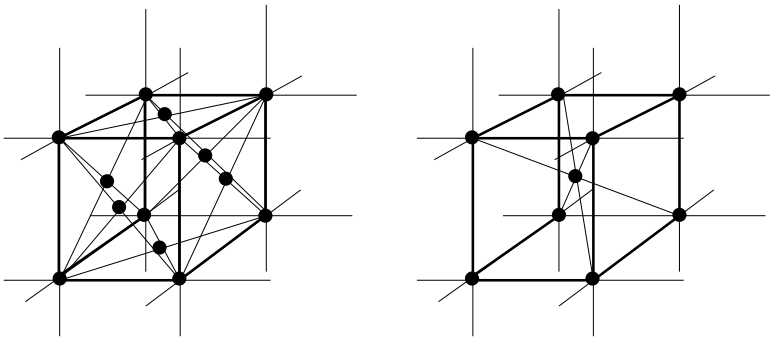
18. Draw the Brillouin zone for a hexagonal two-dimensional lattice.

19. Look up Léon Brillouin, 1889–1969. What is Brillouin scattering?

20. Show that the projection vectors given in Note 24 for the one-dimensional three-atom crystal with both translation and reflection symmetry give waves of the wavelengths claimed.

21. Show that n-fold rotational symmetries are allowed in a two-dimensional crystal only if $n =$ 1, 2, 3, 4 or 6:
a) Show that $n \leq 6$ by considering the length of $\vec{r} - \vec{r'}$ where $\vec{r}$ is a minimum-length translation vector and $\vec{r'}$ is its rotated image: $\mid \vec{r} - \vec{r'} \mid = 2 \mid \vec{r} \mid \sin(2\pi/2n)$ must be no less than $\mid \vec{r} \mid$ because we said $\vec{r}$ is a shortest translation vector, but $\vec{r} - \vec{r'}$ must also be a translation vector.
b) Show that $n = 5$ is excluded because the length of the *sum* of two opposite rotations, $\vec{r'}$ and $\vec{r''}$, of $\vec{r}$ must also be no less than the length of $\vec{r}$, or else exactly zero: write out this length divided by $\mid \vec{r} \mid$ for $n =$ 1, 2, 3, 4, 5 and 6, the only values allowed by (a) above.
c) Look up "Penrose tiles" and figure out how fivefold rotational symmetry is worked into patterns that completely cover ("tile") the plane. Can you find examples of such tiling from before they were proposed by Roger Penrose [e.g., 1974]?

22. The 3D cubic symmetries require different unit cells for "face-centred" and "body-centred" lattices.



Face−centered cubic Body−centred cubic

a) Find the unit cells.
b) What pattern do both of these reduce to in 2D? Why do we not need a 2-point unit cell in 2D? What are the basic translations?
c) What pattern do they reduce to in 1D? Why do we not need a 2-point unit cell in 1D? What are the basic translations?

23. **Wallpaper groups.** David E. Joyce at Clark University has posted examples of all seventeen two-dimensional space groups [Joy97].
a) Make a photographic collection of as many different wallpapers as you can find and try to collect examples of all seventeen groups. (E.g., look up William Morris, 1834–96.)
b) Draw your own examples of the seventeen groups, using as few lines as possible to distinguish each symmetry group from the others.
c) Go on to three dimensions and look up the 32 crystallographic point groups.

24. What are the symmetries in time and in space of Norman McLaren's "Pas de deux" (1967, National Film Board of Canada)?

25. What is the 3D interpretation of the 3×3 matrices applied to the augmented vector $(x, y, 1)^T$ in Note 25?

26. Confirm that $(a+x, b+y, 1)^T$ transforms correctly under $t_{ab}\, r\, t_{ab}^{-1}$ where

$$t_{ab} = \begin{pmatrix} 1 & & a \\ & 1 & b \\ & & 1 \end{pmatrix} \quad \text{and} \quad r = \begin{pmatrix} c & -s & \\ s & c & \\ & & 1 \end{pmatrix}$$

27. Show that the translation matrices X and Y commute with each other but not with rotations or reflections in Note 25.

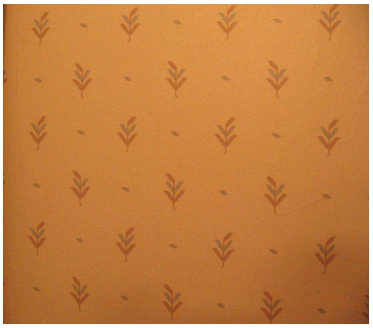
28. Verify and explore the symmetry operations given in Note 25 for the square tile example, especially the glide reflection operations to be sure you understand them.

29. Work out the matrices for the glide reflections missing from the square tile example in Note 25. Hint: which translation operators are also missing?

30. For the square tiling in Note 25
a) Show that $r_{+0} = t_{10} r_{00}^2$, $r_{++} = t_{10} r_{00}$, $r_{++}^2 f_{++} = t_{10} r_{00}^2 f_{00}$, $g_{10} = t_{10} f_{00}$, $g_{-11} = t_{10} r_{00} f_{00}$ and $g_{+1\overline{1}} = t_{10} r_{00}^3 f_{00}$.
b) Which combinations of $t_{10} \times$ {the point group} are missing from (a)?
c) Find combinations of the four generators of the space group that give the other operations listed in Note 25.
d) Find the combinations giving the operators for the square tiling not listed in Note 25.

31. Which subgroup of the `p4m` wallpaper group of Note 25 define the symmetries of the following (mostly square) wallpaper groups?





Which of Joyce's [Joy97] wallpaper groups are they?

32. Look up glide reflections in [Joy97]. Note that the "glide reflections" in the square example of Note 25 are derived from the fundamental reflection and translations. They are not fundamental themselves. These are not usually counted as glide reflections.
Explore glide reflections in group `p4g`.

33. Here are some typical wallpapers. Find their point and space groups.



34. Quilt designs can be more adventurous than wallpapers. Porter [Por06] illustrates half a dozen wallpaper groups. Have a look.

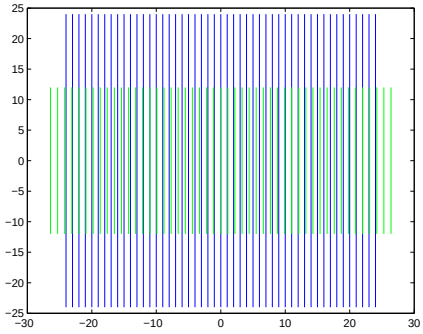
35. What are the representations of the wallpaper groups discussed in the notes or that you have found independently?

36. a) If the honeycomb of Note 25 had each hexagon turned into a perspective cube by adding three lines, which subgroup of the honeycomb group gives its symmetry?
b) Which wallpaper groups [Joy97] are the honeycomb group and the cubic honeycomb group?

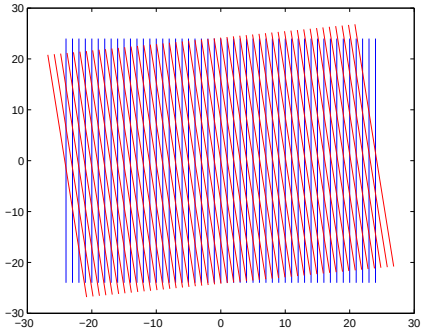
37. Find symmetries in the following.



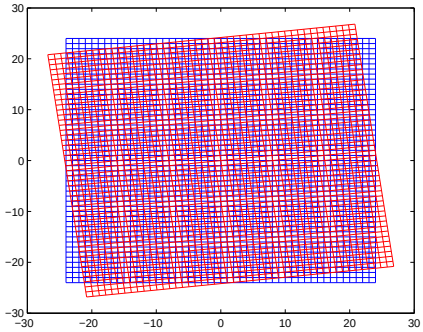
38. **Periodic interactions.** Write a MATLAB program to draw the three figures below in this excursion. Write a loop to animate the drawings for a range of different distortions of the green and red periodicities.
a) The green lattice of vertical lines is stretched 10% over the blue base lattice. This is the simplest form of "moiré pattern".



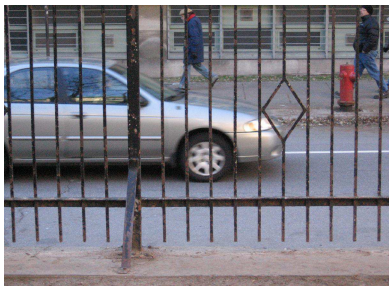
What is the relationship among the three periods? Note that all three are in the same one dimension. Hint: work with frequencies.
Look up "beats" between two musical tones. Write a program to plot the sum of the sine waves.
Look up the "Vernier" method to increase precision of measurements and figure out how to increase precision ten times.
b) The red lattice of vertical lines is tilted about seven degrees (about 1/8 radian) from the base blue lattice. Both have the same spacings.



(The moiré pattern here shows clearly the irregularities in `gplot`, the MATLAB function I used to draw the figures.)
Now the two periods in (more-or-less) the x-direction produce "beats" in the y-direction. What is the relationship among these periods?
Here, for instance, is the same rotation for a square grid.



c) Watch the wagon wheels next time you look at a Wild West movie. Do they turn the right way? Supposing movies are filmed at 24 frames/sec., calculate the apparent rotational velocity of the wheels for various translational velocities of the wagon.
Alternatively, watch hubcaps through a spoked fence and do the same calculation.



39. Any part of the Preliminary Notes that needs working through.

References

[Joy97] David E. Joyce. The 17 plane symmetry groups. URL www.clarku.edu/∼djoyce/wallpaper/seventeen.html (accessed 2008/12), 1997.

[Por06] Christine Porter. *Tesselation Quilts*. David & Charles, Newton Abbott, UK, 2006.