Excursions in Computing Science: Book 8c. Symmetry: Simplifying Matrices. Part I Discrete symmetries and molecules.

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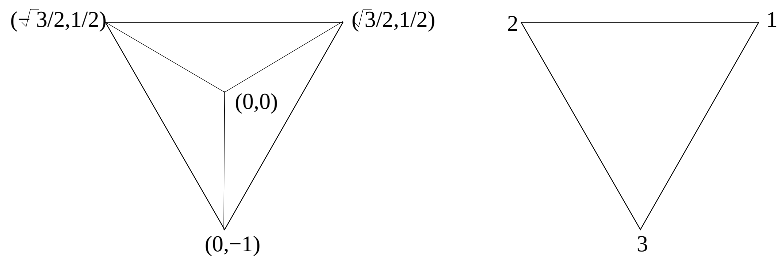
I. Prefatory Notes

1. Which operations preserve the triangle in part (a) of the figure?



a) by coordinates b) by abstract vertices

- The identity $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$,
- the rotations

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix} \text{ for } \frac{2\pi}{3} = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \text{ and}$$

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix} \text{ for } \frac{4\pi}{3} = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}, \text{ and}$$

- the reflections

$$x \leftrightarrow -x \quad : \quad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\text{and} \quad \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \text{ and}$$

$$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

2. How did we get the last two reflections?

One way is to generate them by combining $x \leftrightarrow -x$ with the two rotations.

What happens if we combine each of the six operations with every other one?

2nd \ first	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$
$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$
$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$
$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$
$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

The "2nd \ first" in this table is interpreted to mean that the operation from the top row is performed on the vector before the operation from the first column. That means, of course, that the "2nd" matrix is written before the "first" matrix. For example, in

$$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$ is the first operation to be applied to the coordinate vectors and $\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$ is the second.

Note that this multiplication table is self-contained: it is *closed*.

3. We can abstract all this to less clunky notation. In part (b) of the first figure the vectors giving the coordinates of each vertex have been replaced by the integer labels, 1, 2 and 3.

Rotating the triangle from this simpler point of view can be written

$$(123)$$

which means

$$1 \to 2, 2 \to 3, 3 \to 1$$

Similarly a reflection can be written

$$(12)$$

which means

$$1 \leftrightarrow 2$$

In this notation, each set of parentheses holds a *cycle* such as the two examples show. We can write

$$()$$

for the operation that leaves the triangle alone.

It should be clear how to write the other rotation and reflections in this cycle notation. Here is the table showing all the operations and their combinations. (Combining two operations could be called "multiplying" them, but a better term is "composing" them. So the table is a composition table.)

2nd \ first	()	(123)	(132)	(12)	(23)	(31)
()	()	(123)	(132)	(12)	(23)	(31)
(123)	(123)	(132)	()	(31)	(12)	(23)
(132)	(132)	()	(123)	(23)	(31)	(12)
(12)	(12)	(23)	(31)	()	(123)	(132)
(23)	(23)	(31)	(12)	(132)	()	(123)
(31)	(31)	(12)	(23)	(123)	(132)	()

Notice the pattern. For one thing, {(),(123),(132)} is also closed.

Let's rearrange to composition table to find other patterns.

2nd \ first	()	(12)	(23)	(123)	(31)	(132)
()	()	(12)	(23)	(123)	(31)	(132)
(12)	(12)	()	(123)	(23)	(132)	(31)
(23)	(23)	(132)	()	(31)	(123)	(12)
(132)	(132)	(23)	(31)	()	(12)	(123)
(31)	(31)	(123)	(132)	(12)	()	(23)
(123)	(123)	(31)	(12)	(132)	(23)	()

Note that the columns and rows are not in exactly the same order.

Now we see that {(),(12)} is closed, as are {(),(23)} and {(),(31)}.

4. These closed sets of operators have other properties:

- one operator, (), is the *identity*: $()g = g = g()$ for any operator g
- every operator g has an *inverse* g^{-1}: $gg^{-1} = () = g^{-1}g$
- composition is associative $(hg)k = hgk = h(gk)$

An algebraic structure which satisfies closure and these three axioms is called a *group*.

5. We have been looking at the effect of the group operators on the *space*, i.e., on the vectors

$$\left\{ \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} sqrt3/2 \\ 1/2 \end{pmatrix}, \begin{pmatrix} -sqrt3/2 \\ 1/2 \end{pmatrix} \right\}$$

What is their effect on *each other*?

Thinking about rotations and reflections (go back to the figure in Note 1), it is apparent that a reflected rotation is also a rotation, but in the opposite direction:

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} : \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \leftrightarrow \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

and the same for the other two reflections.

It is also apparent that a rotated reflection is one of the other reflections:

$$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} : \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

and backwards for the other rotation.

What matrix operations must we do to get these transformations?

In Week 7c we found out how to rotate a tensor T with the rotation matrix R

$$T' = RTR^{-1}$$

Tensor T was just a matrix itself and what we found out there applies to any transformation of any matrix.

Since the group elements are just abstractions of matrix operators, the effect of group element g on group element h must be

$$ghg^{-1}$$

Let's try reflecting a rotation.

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

as we wanted. (NB a reflection is its own inverse.)

Rotating a reflection:

$$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix} = \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

as we wanted. (NB the inverse of a rotation is its transpose.)

6. So something else we can do with a group is to study

$$ghg^{-1}.$$

for g and h elements of the group.

This operation can produce *invariant sets*: sets of elements h of the group that transform into themselves under all group elements g:

- the identity is invariant: $g()g^{-1} = ()$
- the two rotations form an invariant set (let r be (123) in which case $r^{-1} = r^2 = (132)$):
  - any reflection maps them into each other
  - rotations map them into themselves:

$$\begin{aligned} rrr^{-1} &= rrr^2 = r \\ r^2r(r^2)^{-1} &= r^2rr = r \\ rr^2r^{-1} &= rr^2r^2 = r^2 \\ r^2r^2(r^2)^{-1} &= r^2r^2r = r^2 \end{aligned}$$

- the three reflections form an invariant set (let f, f' and f'' be either (12) or (23) or (31)):
  - either rotation maps them into each other
  - reflections map them into each other:

$$f'f(f')^{-1} = f'ff' = f''$$

  Note that f'' must be a group element because the group is closed and, of those elements it must be a reflection because it is its own inverse $((f'ff')(f'ff') = ())$.

7. The rotation subgroup, $\{(), (123), (132)\}$, also forms an invariant set and is called an *invariant subgroup* (or *normal subgroup*).

Invariant subgroups are neat because they generate new groups from the original group.

To see this, we can abstract from the first composition table in Note 3. It has the pattern

$$\begin{array}{cc} E & A \\ A & E \end{array}$$

where E is the multiplication table for the subgroup $\{(), (123), (132)\}$ and A represents the products of the subgroup $\{(), (123), (132)\}$ and the "coset" $\{(12), (23), (31)\}$. Note that the elements do not appear in the same order in the two occurrences of A, but that they are exactly the same *set* of elements in both occurrences.

This new composition table

$$\begin{array}{cc} E & A \\ A & E \end{array}$$

also satisfies the group axioms.

E and A are the elements of a new group, the *factor group* (or *quotient group*) of

$$\begin{aligned} G &= \{(), (123), (132), (12), (23), (31)\} \text{ and} \\ H &= \{(), (123), (132)\} \end{aligned}$$

usually written G/H.

Note that the second composition table in Note 3 cannot be abstracted as a 3×3 composition table. It shows instead that the reflection subgroup, $\{(), (12)\}$ gets mixed into the other two reflection subgroups by the rotations.

There are two ways in which we can see, from a suitably arranged group composition table, whether a subgroup is invariant or not.

The first way considers $gHg^{-1} = H$ for any element g of the group G. This notation means that ghg^{-1}, for any element h of the subgroup H, is h', also an element of H.

The product Hg^{-1} can be viewed as a horizontal step in the composition table for G, rightwards from the sub-table for H.

The product $g(Hg^{-1})$ can be viewed as a vertical step downwards from Hg^{-1}.

So the composition sub-table for H keeps reappearing elsewhere in the composition table for G, as many times as there are elements of the factor group G/H.

In the example, E appears twice.

The second way of seeing the invariance of H uses $gH = Hg$, a rewriting of $gHg^{-1} = H$.

This is a kind of collective commutativity, and we can see in the first group composition table that the elements under the (12) column for the rows of H are the same set as the elements of the (12) row for the columns of H.

8. The title of this lecture mentions simplifying matrices but we seem to have wandered away from matrices into abstractions. This was *not* a digression, but let's get back to matrices.

The expression $gSg^{-1} = S$ for an invariant set S is significant if g and the elements of S are matrices.

In Week 7c the tensor T was a diagonal matrix of its eigenvalues (w and h in one example) under one set of coordinate axes, and non-diagonal when rotated using RTR^{-1} to some other set of coordinate axes: the eigenvalues in some sense stand for the "real" T, which just assumes different forms under rotations.

Here we are concerned less with "reality" but we can extract from that discussion that any matrix M is equivalent to RMR^{-1} under rotation R in the sense that both M and RMR^{-1} have the same eigenvalues.

This is also true for reflection, F: M and FMF^{-1} have the same eigenvalues.

Our group G consists of rotations and reflections. (This is true for any group representing geometric symmetry, except that *inversions* might also be included, which change the sign of all coordinates.)

So gsg^{-1} has the same eigenvalues as s.

So all elements of an invariant set S have the same eigenvalues, because each is mapped into some other by some element g of G, and if we work through all the elements of G we map every element of S into every other.

Any transformation which leaves eigenvalues $\lambda_1, \lambda_2, ...\lambda_n$ invariant also leave expressions such as the sum or product of all the eigenvalues invariant.

The product of eigenvalues is the *determinant* of the matrix: just apply the definition of determinant in Week 3 to a diagonal matrix.

The sum of eigenvalues is the *trace* of the matrix. In fact, the trace is easy to calculate for any matrix: just sum the diagonal.

We can see that this works for 2×2 matrices under rotations by summing the diagonal of

$$\begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} \lambda_1 & \\ & \lambda_2 \end{pmatrix} \begin{pmatrix} c & s \\ -s & c \end{pmatrix}$$

Because the trace is an easy invariant to calculate for any square matrix, and for other reasons which will become clear, we will study the traces of matrices in invariant sets.

Let's look at the traces of the matrices representing our triangle group, collected into classes of invariant sets.

()	(123)	(132)	(12)	(23)	(31)
$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$
2	-1	-1	0	0	0

Note how the traces (bottom row) reveal the invariant sets.

9. These 2×2 matrices are not the only representations of the triangle group.

They give the effect of the group on the 2-D space of coordinates of the triangle vertices.

But we could also look at the effect of the group on the 1-D space of the *direction of rotation*: $+1$ for counterclockwise and -1 for clockwise. Reflections change counterclockwise rotations to clockwise.

This representation will be 1×1 matrices, or just scalars.

()	(123)	(132)	(12)	(23)	(31)
1	1	1	-1	-1	-1

The traces are just the 1×1 matrices themselves.

We can also see this as a representation of the 2-element factor group $G/\{(),(123),(132)\}$

{(),(123),(132)}	{(12),(23),(31)}
1	-1

Simplest of all is the *trivial representation*, which we can think of as the effect of the group on the 1-D space of the *radius of the triangle vertices*: always 1.

()	(123)	(132)	(12)	(23)	(31)
1	1	1	1	1	1

But there are less trivial representations. Let's consider the matrices that give the effect of the group as *permutations of three objects*.

()	(123)	(132)	(12)	(23)	(31)
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$
3	0	0	1	1	1

The traces tell us something about this. Let's put them all down as one table, and give names to the representations at the same time.

rep.	()	(123)	(132)	(12)	(23)	(31)
triv	1	1	1	1	1	1
direc	1	1	1	−1	−1	−1
2D	2	−1	−1	0	0	0
perm	3	0	0	1	1	1

Look closely: **triv**, **direc** and **2D** are mutually orthogonal. These are the *irreducible representations* of this group.

("Orthogonal" is a generalized word meaning "perpendicular". In this case, the six-dimensional vector, (1,1,1,1,1,1) is orthogonal to $(2, -1, -1, 0, 0, 0)$ because the sum of the products of each term is 0:

$$1 \times 2 + 1 \times -1 + 1 \times -1 + 1 \times 0 + 1 \times 0 + 1 \times 0 = 0$$

Which of the others is (3,0,0,1,1,1) orthogonal to?)

Note also that the trace of () is the dimensionality of the representation and that the sum of the *squares* of the dimensions of the irreducible representations = 6, the size of the group.

Look closely again: **perm** = **triv** + **2D**.

10. Finally, we've come to simplifying matrices.

The simplest matrices are diagonal. (Well, the **perm** matrices look pretty simple, just 0s and 1s, but that's not the way we are going.)

It is too much to hope that we can diagonalize all the matrices of a representation simultaneously.

But we can *block-diagonalize* them all simultaneously. *This decomposes the space they operate in to a sum of spaces of smaller dimensions.*

Since **perm** = **triv** + **2D** we should be able to decompose the 3-D space operated in by the **perm** matrices into a 1-D space (**triv**) and a 2-D space (**2D**).

We can: try SgS^{-1} on each **perm** matrix g where

$$S = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{2} & \sqrt{2} & \sqrt{2} \\ \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \end{pmatrix}$$

We get

()	(123)	(132)	(12)	(23)	(31)
$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & -1/2 & -\sqrt{3}/2 \\ & \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & -1/2 & \sqrt{3}/2 \\ & -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & 1/2 & \sqrt{3}/2 \\ & \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1 & & \\ & 1/2 & -\sqrt{3}/2 \\ & -\sqrt{3}/2 & -1/2 \end{pmatrix}$
3	0	0	1	1	1

To get S we must find out that (1,1,1) is the one-dimensional subspace and {(1,−1,0), (1,1,−2)} spans the two-dimensional subspace that the space of **perm** decomposes into.

To find these vectors, we must find projections from the 3-D space onto its 1-D and 2-D decompositions.

The traces of **triv** and **2D** representations together with the 3×3 matrix representing **perm** gives these projections. ($P_{()}$ is the **perm** matrix giving group element (), and so on.)

$$\begin{aligned}
P_{\mathbf{triv}} &= \frac{1}{6}(1 \times P_{()} + 1 \times P_{(123)} + 1 \times P_{132)} + 1 \times P_{(12)} + 1 \times P_{(23)} + 1 \times P_{(31)}) \\
&= \frac{1}{6}\begin{pmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \\ 2 & 2 & 2 \end{pmatrix} \\
&= \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}(1\ 1\ 1)\frac{1}{\sqrt{3}} \\
P_{\mathbf{2D}} &= \frac{2}{6}(2 \times P_{()} - 1 \times P_{(123)} - 1 \times P_{(132)}) \\
&= \frac{1}{3}\left(\begin{pmatrix} 2 & & \\ & 2 & \\ & & 2 \end{pmatrix} - \begin{pmatrix} & & 1 \\ 1 & & \\ & 1 & \end{pmatrix} - \begin{pmatrix} & 1 & \\ & & 1 \\ 1 & & \end{pmatrix}\right) \\
&= \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \\
&= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}(1\ \ {-1}\ 0)\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}(1\ 1\ \ {-2})\frac{1}{\sqrt{6}}
\end{aligned}$$

and note that the **direc** representation does not participate:

$$\begin{aligned}
P_{\mathbf{direc}} &= \frac{1}{6}(1 \times P_{()} + 1 \times P_{(123)} + 1 \times P_{132)} - 1 \times P_{(12)} - 1 \times P_{(23)} - 1 \times P_{(321)}) \\
&= 0
\end{aligned}$$

Note that the ratios $\frac{1}{6}$ and $\frac{2}{6}$ are the sizes of the component representations divided by the size of the group.

These three vectors, normalized, give the rows of the block-diagonalizing matrix S (and the columns of its inverse S^{-1}).

11. Every group has a *regular representation* consisting of $\mid G \mid \times \mid G \mid$ matrices, where $\mid G \mid$ is the number of elements in the group G—the size of G.

Each vector operated on by the regular representation is all zeros except for a single 1. The $\mid G \mid$ vectors might just as well be labelled by the $\mid G \mid$ group elements.

E.g., for the triangle group

$\mid () >$	$\mid (123) >$	$\mid (132) >$	$\mid (12) >$	$\mid (23) >$	$\mid (31) >$
1	0	0	0	0	0
0	1	0	0	0	0
0	0	1	0	0	0
0	0	0	1	0	0
0	0	0	0	1	0
0	0	0	0	0	1

Then the matrix representing a group element g_1 maps the vector labelled for g_2 into the vector labelled for $g_1 g_2$

$$R(g_1) \mid g_2 >=\mid g_1 g_2 >$$

Thus

$$\begin{aligned}
R(\,()\,) &= \begin{pmatrix} 1 &&&&& \\ & 1 &&&& \\ && 1 &&& \\ &&& 1 && \\ &&&& 1 & \\ &&&&& 1 \end{pmatrix} R(\,(12)\,) = \begin{pmatrix} &&& 1 && \\ &&&& 1 & \\ &&&&& 1 \\ 1 &&&&& \\ & 1 &&&& \\ && 1 &&& \end{pmatrix} \\
R(\,(123)\,) &= \begin{pmatrix} && 1 &&& \\ 1 &&&&& \\ & 1 &&&& \\ &&&& 1 & \\ &&&&& 1 \\ &&& 1 && \end{pmatrix} R(\,(23)\,) = \begin{pmatrix} &&&& 1 & \\ &&&&& 1 \\ &&& 1 && \\ && 1 &&& \\ 1 &&&&& \\ & 1 &&&& \end{pmatrix} \\
R(\,(132)\,) &= \begin{pmatrix} & 1 &&&& \\ && 1 &&& \\ 1 &&&&& \\ &&&&& 1 \\ &&& 1 && \\ &&&& 1 & \end{pmatrix} R(\,(31)\,) = \begin{pmatrix} &&&&& 1 \\ &&& 1 && \\ &&&& 1 & \\ & 1 &&&& \\ && 1 &&& \\ 1 &&&&& \end{pmatrix}
\end{aligned}$$

The traces of this regular representation are

()	(123)	(132)	(12)	(23)	(31)
6	0	0	0	0	0

amd we can see that **reg** = **triv** + **direc** + 2×**2D**.

As in Note 10, here are the projection operators that decompose the space

$$\begin{aligned}
P_{\mathbf{triv}} &= \frac{1}{6}(1 \times R_{()} + 1 \times R_{(123)} + 1 \times R_{132)} + 1 \times R_{(12)} + 1 \times R_{(23)} + 1 \times R_{(31)}) \\
&= \frac{1}{6} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \\
P_{\mathbf{direc}} &= \frac{1}{6}(1 \times R_{()} + 1 \times R_{(123)} + 1 \times R_{132)} - 1 \times R_{(12)} - 1 \times R_{(23)} - 1 \times R_{(321)})
\end{aligned}$$

$$
= \frac{1}{6}\begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix}
$$

$$
\begin{aligned}
P_{\mathbf{2D}} &= \frac{2}{6}(2 \times R_{()} - 1 \times R_{(123)} - 1 \times P_{(132)}) \\
&= \frac{1}{3}\begin{pmatrix} 2 & -1 & -1 & & & \\ -1 & 2 & -1 & & & \\ -1 & -1 & 2 & & & \\ & & & 2 & -1 & -1 \\ & & & -1 & 2 & -1 \\ & & & -1 & -1 & 2 \end{pmatrix}
\end{aligned}
$$

From these we have two one-dimensional and one four-dimensional subspaces, whose (possible) basis vectors are

triv	**direc**	2×**2D**			
$\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{pmatrix}$	$\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \\ -2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ -2 \end{pmatrix}$

These vectors giving the subspaces, if normalized, also give the block-diagonalizing transformation

$$
S = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ \sqrt{3} & \sqrt{3} & 0 & 0 & 0 & 0 \\ 1 & 1 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & \sqrt{3} & 0 \\ 0 & 0 & 0 & 1 & 1 & -2 \end{pmatrix}
$$

Note that the column vectors have been transposed into row vectors. S^{-1} transposes them back again.

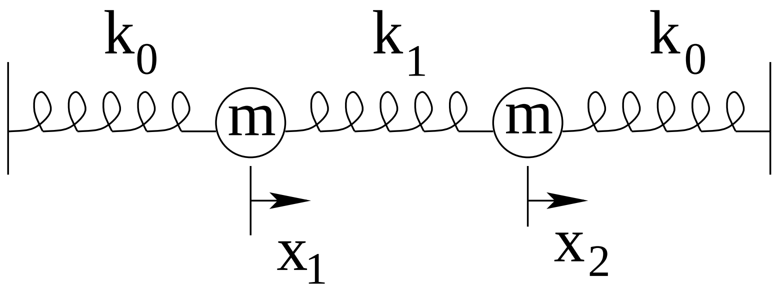
12. Molecules. Using symmetry to simplify matrices also simplifies scientific problems described by matrices.

For instance, finding the configurations of electrons on molecules so as to predict their chemical properties is a hard quantum-mechanical problem.

But much of it can be done by symmetry alone. We'll do the calculations, but to keep the physics to a minimum we'll find out instead how a molecule can vibrate. This is also useful in determining, for instance, what energies a greenhouse gas molecule of CO_2, methane or water vapour can absorb in the upper atmosphere.

We'll consider an imaginary molecule shaped like the triangle we've been studying in previous Notes.

But first let's look at the physics of a simpler, one-dimensional, system: two "atoms" connected by forces modelled as springs to each other and to fixed walls.



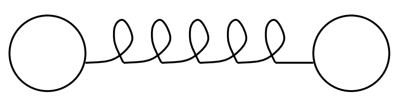
This is classical (pre-quantum, pre-timespace) physics needing Newton's law $F = ma$, Young's law for springs $F = -kx$ and differential equations. But we'll skip right to the matrix equation we get when we assume $x_1 = a_1 e^{i\omega t}, x_2 = a_2 e^{i\omega t}$ and $\lambda = m\omega^2$ for the displacements x_1 and x_2 of the two atoms, each of the same mass m. We must solve for the two (non-quantum) amplitudes, a_1 and a_2, of the vibrations in terms of the spring constants, k_0 and k_1:

$$\lambda \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} -k_0 - k_1 & k_1 \\ k_1 & -k_0 - k_1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

This is an eigenvalue/eigenvector problem, which we solve by viewing it as $\lambda a = Ka$ or $(K - \lambda I)a = 0$ and noting that solutions apart from $a = 0$ requires $\det(K - \lambda I) = 0$.

$$\begin{aligned} \text{I.e., } 0 &= \begin{vmatrix} -(k_0 + k_1 + \lambda) & k_1 \\ k_1 & -(k_0 + k_1 + \lambda) \end{vmatrix} \\ &= (k_0 + k_1 + \lambda)^2 - k_1^2 \\ &= \lambda^2 + 2(k_0 + k_1)\lambda + k_0^2 + 2k_0 k_1 \\ \text{So } \lambda &= -(k_0 + k_1) \pm k_1 \\ &= \begin{cases} -k_0 \\ -k_0 + 2k_1 \end{cases} \end{aligned}$$

Why did we need those fixed walls? Let's just have a free molecule: $k_0 = 0$.



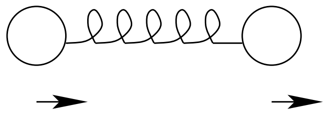
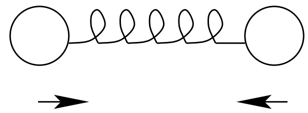
$$\text{So } m\omega^2 = \begin{cases} 0 \\ 2k_1 \end{cases}$$

ω is the (angular frequency of vibration, so $\omega = 0$ must mean the molecule is just flying around rigidly.

The next step is to find the eigenvectors.

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} : \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} m\omega^2 - k_1 & k_1 \\ k_1 & m\omega^2 - k_1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

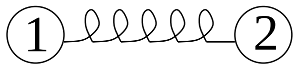
$$\begin{aligned} \text{So } a_2 &= (1 - m\omega^2/k_1)a_1 \\ &= \left(1 - \left\{ \begin{matrix} 0 \\ 2 \end{matrix} \right\}\right) a_1 \\ &= \left\{ \begin{matrix} 1 \\ -1 \end{matrix} \right\} a_1 \end{aligned}$$

Whew!

What if we tried doing it by *symmetry*?

Z_2	()	(12)
()	()	(12)
(12)	(12)	()



This group, called Z_2 has the trivial representation, {1,1}, and one other irreducible representation, {1,−1}, both needing only scalars, not matrices.

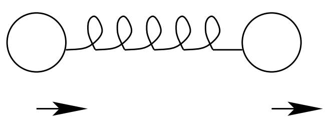
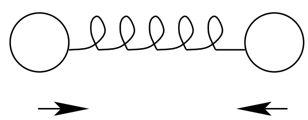
Its **perm** representation is also its **reg** representation

$$\begin{array}{cc} () & (12) \\ \hline \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} & \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \end{array}$$

and these project into **triv** and the other representation, which we can call **1D**, by

$$\begin{aligned} P_{\mathbf{triv}} &= \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} + \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} (1\ 1) \\ P_{\mathbf{1D}} &= \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} - \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} (1\ \ -1) \end{aligned}$$

which immediately give the two modes of motion

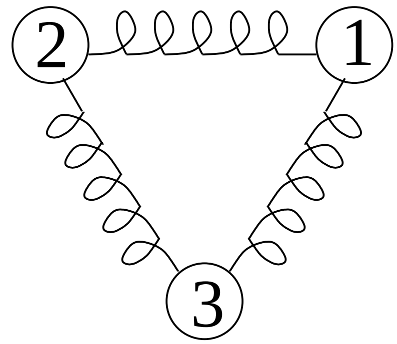
$$\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad\qquad \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

(symmetric under (12)) (antisymmetric under (12))

We got a lot by symmetry alone without needing any physics: we did not get the frequencies (energies) but we did get the two modes of motion.

Since this approach avoids the physics, the problem we've solved with it could be the original, classical-physics problem of the motions of balls on a spring, but it could equally well tell us the distribution of electrons in a diatomic molecule, or any other scientific problem involving Z_2 symmetry.

13. Let's see what we can learn about the modes of motion of a three-atom molecule in two dimensions, using our triangle symmetry.



This system must be described as a combination of the three-element permutation of the three atoms (the **perm** representation) and the 2-D motions of each atom $(x_1, y_1), (x_2, y_2), (x_3, y_3)$ (the **2D** representation).

The nature of this combination is a *tensor product* (Week 6): the 3-D **perm** representation combines with the 2-D **2D** representation to give a 6-D representation (which is not **reg**). Here it is

$$() \quad \rightarrow \quad \left(\begin{array}{cc|cc|cc} 1 & & & & & \\ & 1 & & & & \\ \hline & & 1 & & & \\ & & & 1 & & \\ \hline & & & & 1 & \\ & & & & & 1 \end{array}\right)$$

$$(123) \quad \rightarrow \quad \left(\begin{array}{cc|cc|cc} & & & & -1/2 & -\sqrt{3}/2 \\ & & & & \sqrt{3}/2 & -1/2 \\ \hline -1/2 & -\sqrt{3}/2 & & & & \\ \sqrt{3}/2 & -1/2 & & & & \\ \hline & & -1/2 & -\sqrt{3}/2 & & \\ & & \sqrt{3}/2 & -1/2 & & \end{array}\right)$$

$$(12) \quad \rightarrow \quad \left(\begin{array}{cc|cc|cc} & & -1 & & & \\ & & & 1 & & \\ \hline -1 & & & & & \\ & 1 & & & & \\ \hline & & & & -1 & \\ & & & & & 1 \end{array}\right)$$

and so on.

Each matrix has three copies of the **2D** matrix: one copy in place of each 1 in the **perm** matrix.

We can see directly that the traces are 6, 0 and 0 for the respective invariant sets—just like **reg**.

We can see this more formally by the rule that the *trace of a tensor product is the product of the traces of its components.*

rep.	()	(123)	(132)	(12)	(23)	(31)
perm	3	0	0	1	1	1
2D	2	−1	−1	0	0	0
molec	6	0	0	0	0	0

Like **reg**, **molec** = **triv** + **direc** + 2×(**2D**).

The projection operators have the same formula as **reg** (Note 11) but of course are different matrices because the **molec** representation matrices differ from **reg**'s.

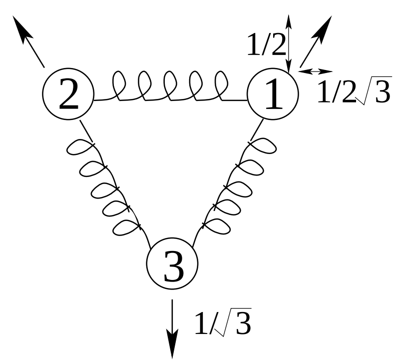
$$P_{\mathbf{triv}} = \begin{pmatrix} 1/2 \\ \sqrt{3}/6 \\ -1/2 \\ \sqrt{3}/6 \\ 0 \\ -1/\sqrt{3} \end{pmatrix} (1/2, \sqrt{3}/6, -1/2, \sqrt{3}/6, 0, -1/\sqrt{3})$$

$$P_{\mathbf{direc}} = \begin{pmatrix} -\sqrt{3}/6 \\ 1/2 \\ -\sqrt{3}/6 \\ -1/2 \\ 1/\sqrt{3} \\ 0 \end{pmatrix} (-\sqrt{3}/6, 1/2, -\sqrt{3}/6, -1/2, 1/\sqrt{3}, 0)$$

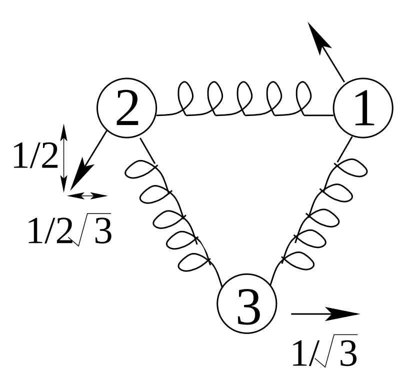
$$P_{2\times\mathbf{2D}} = \left(\begin{array}{cc|cc|cc} 2/3 & 0 & 1/6 & -\sqrt{3}/6 & 1/6 & \sqrt{3}/6 \\ 0 & 2/3 & \sqrt{3}/6 & 1/6 & -\sqrt{3}/6 & 1/6 \\ \hline 1/6 & \sqrt{3}/6 & 2/3 & 0 & 1/6 & -\sqrt{3}/6 \\ -\sqrt{3}/6 & 1/6 & 0 & 2/3 & \sqrt{3}/6 & 1/6 \\ \hline 1/6 & -\sqrt{3}/6 & 1/6 & \sqrt{3}/6 & 2/3 & 0 \\ \sqrt{3}/6 & 1/6 & -\sqrt{3}/6 & 1/6 & 0 & 2/3 \end{array}\right)$$

To interpret these projections as modes of motion we can apply the first two as (x, y)-coordinates to the triangle.

Triv gives a "breathing" mode. Note that $x_1 + x_2 + x_3 = 0 = y_1 + y_2 + y_3$ and that each vector has length $1/\sqrt{3}$.

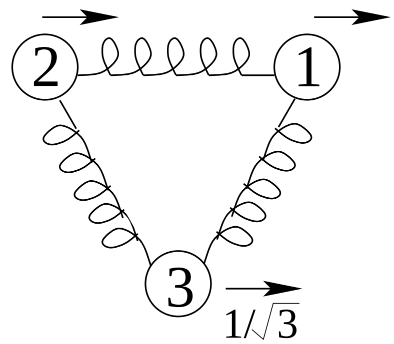


Direc gives a rotation mode—so the frequency will be zero.

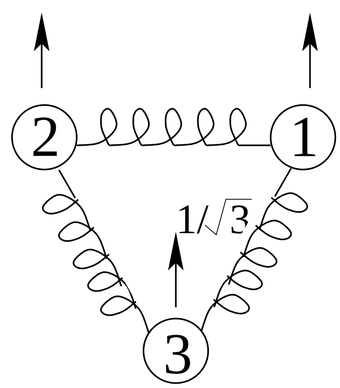


To analyze the four dimensions of $2\times\mathbf{2D}$ (note that the trace of $P_{2\times\mathbf{2D}} = 4$) we can think about what motions are missing.

Translation is one: two components could be $(1/\sqrt{3}, 0, 1/\sqrt{3}, 0, 1/\sqrt{3}, 0)$



and $(0, 1/\sqrt{3}, 0, 1/\sqrt{3}, 0, 1/\sqrt{3})$



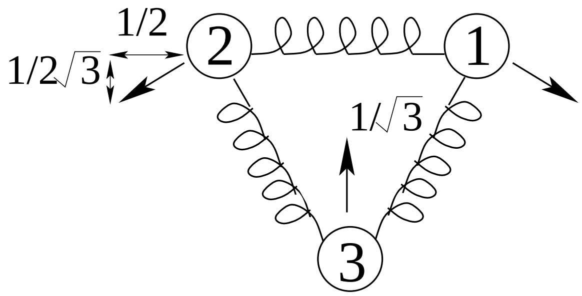
Subtracting these two translation modes

$$\begin{pmatrix} 1/\sqrt{3} \\ 0 \\ 1/\sqrt{3} \\ 0 \\ 1/\sqrt{3} \\ 0 \end{pmatrix} (1/\sqrt{3}, 0, 1/\sqrt{3}, 0, 1/\sqrt{3}, 0) + \begin{pmatrix} 0 \\ 1/\sqrt{3} \\ 0 \\ 1/\sqrt{3} \\ 0 \\ 1/\sqrt{3} \end{pmatrix} (0, 1/\sqrt{3}, 0, 1/\sqrt{3}, 0, 1/\sqrt{3})$$

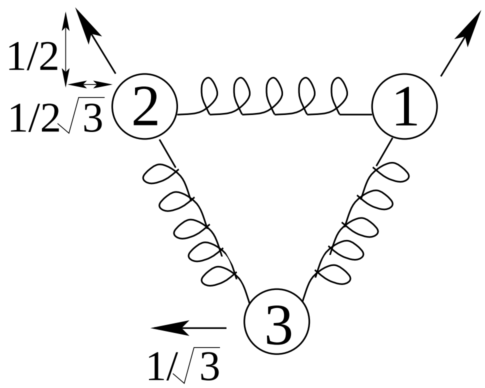
from $P_{2\times\mathbf{2D}}$ gives

$$\begin{aligned}
M &= \left(\begin{array}{cc|cc|cc} 1/3 & 0 & -1/6 & -\sqrt{3}/6 & -1/6 & \sqrt{3}/6 \\ 0 & 1/3 & \sqrt{3}/6 & -1/6 & -\sqrt{3}/6 & -1/6 \\ \hline -1/6 & \sqrt{3}/6 & 1/3 & 0 & -1/6 & -\sqrt{3}/6 \\ -\sqrt{3}/6 & -1/6 & 0 & 1/3 & \sqrt{3}/6 & -1/6 \\ \hline -1/6 & -\sqrt{3}/6 & -1/6 & \sqrt{3}/6 & 1/3 & 0 \\ \sqrt{3}/6 & -1/6 & -\sqrt{3}/6 & -1/6 & 0 & 1/3 \end{array}\right) \\
&= \begin{pmatrix} 1/2 \\ -\sqrt{3}/6 \\ -1/2 \\ -\sqrt{3}/6 \\ 0 \\ 1/\sqrt{3} \end{pmatrix} (1/2, -\sqrt{3}/6, -1/2, -\sqrt{3}/6, 0, 1/\sqrt{3}) + \begin{pmatrix} \sqrt{3}/6 \\ 1/2 \\ \sqrt{3}/6 \\ -1/2 \\ -1/\sqrt{3} \\ 0 \end{pmatrix} (\sqrt{3}/6, 1/2, \sqrt{3}/6, -1/2, -1/\sqrt{3}, 0) \\
&= a'a + b'b
\end{aligned}$$

corresponding to two vibration modes, mode M1



and mode M2



How did we get this breakdown? First we got a' by normalizing the last column of the matrix M. Think of this as disturbing the system by pulling down on atom 3, or, mathematically, by operating with M on $v = (0, 0, 0, 0, 0, 1)'$.

Second, we rotated the whole system by $2\pi/3$ to get a linearly independent vector $c = (0, 1/\sqrt{3}, 1/2, -\sqrt{3}/6, -1/2, -\sqrt{3}/6)'$.

Third, we find the component of c orthogonal to a and normalize that to give b.

In summary, three of the six modes of motion of the triangular molecule involves relative displacements of the atoms. Thus they stretch and squeeze the springs and so are *vibrations* (having *frequencies* which symmetry alone cannot calculate).

The other three modes, the rotation and the two translations, are not resisted by the springs, and so have vibrational frequencies of zero.

We can guess that the frequencies for the last two vibrations, due to matrix M, will be the same. When we use the six projection vectors to block-diagonalize all six 6×6 group element matrices, we get two 1×1 and two 2×2 blocks: the two vibration modes for M are independent of everything else. (As are the two translation modes, the breathing mode and the rotation mode.)

$$\begin{pmatrix} () & & \\ & () & \\ & & () \end{pmatrix}, \begin{pmatrix} () & & \\ & (123) & \\ & & (132) \end{pmatrix},$$

$$\begin{pmatrix} () & & \\ & (132) & \\ & & (123) \end{pmatrix}, \begin{pmatrix} (12)^\sim & & \\ & (12) & \\ & & (12)^\sim \end{pmatrix},$$

$$\begin{pmatrix} (12)^\sim & & \\ & (23) & \\ & & (23)^\sim \end{pmatrix}, \begin{pmatrix} (12)^\sim & & \\ & (31) & \\ & & (31)^\sim \end{pmatrix}$$

where (), (123), etc. are the 2×2 matrices in Note 1 and where $\sim$ transposes a matrix about its secondary diagonal, e.g.,

$$\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}^{\sim} = \begin{pmatrix} -1 & \\ & 1 \end{pmatrix}$$

This shows that the frequencies for both modes in each two-dimensional subspace are the same. Since modes M_1 and M_2 are mixed with each other, but not with any other modes, under all the symmetry operations, their properties (and in particular their frequencies) must be indistinguishable.

This is also true, of course, for the two translation modes.

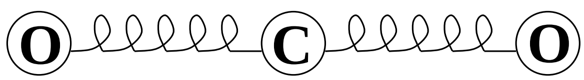
14. Greenhouse gases. Simpler, but also more realistic, molecules are the greenhouse gases, CO_2, H_2O (vapour), methane and ozone.

The constituents of carbon dioxide are carbon, C^6, and oxygen, O^8. Oxygen has eight electrons, arranged 2+6 (see Week 6 excursions): two in the inner shell, and six in the outer shell responsible for chemistry.

Carbon has 6 = 2+4 electrons, and CO_2 is constructed by each oxygen atom "borrowing" two electrons from the carbon atom, so that each atom now has a complete outer shell:

oxygen	2+8
carbon	2

Because of the symmetry of this borrowing, it makes sense that CO_2 is a linear molecule: the atoms form a straight line. Here it is, with the electron bonding modelled as springs.



We'll look at the symmetry of this molecule assuming the central, carbon, atom is pinned to a fixed position.

The result should closely resemble the two-atom molecule of Note 12, except we considered that in one dimension, but we'll look at CO_2 in two.

The symmetry group consists of the identity element and the operation of swapping the two oxygens: CO_2 {(),(12)}.

Its irreducible representations are both one-dimensional

	()	(12)
triv	1	1
swap	1	−1

The permutation representation and the representation giving the effect of the group on the (x, y) coordinates of a 2-D space containing the molecule are both two-dimensional

	()	(12)
perm	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$
(x,y)	$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & \\ & 1 \end{pmatrix}$

Therefore the representation that combines the swapping of the oxygens with the 2-D vibrations of each of them is the four-dimensional tensor product

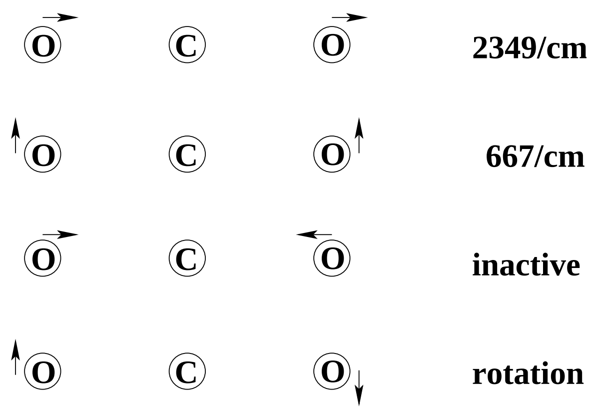
$$
\begin{array}{c|cc}
 & () & (12) \\
\hline
\mathbf{CO_2} & \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} & \begin{pmatrix} & & -1 & \\ & & & 1 \\ -1 & & & \\ & 1 & & \end{pmatrix} \\
\text{trace} & 4 & 0
\end{array}
$$

From the traces we can see that

$$\mathbf{CO_2} = 2 \times \mathbf{triv} + 2 \times \mathbf{swap}$$

is the irreducible decomposition of this representation.

This gives the following modes of motion (recalling that we've pinned down the carbon atom).



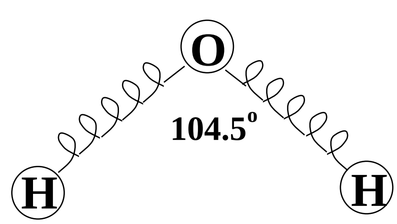
(Why is there no mode corresponding to translation of the molecule?)

The quantities shown, 2349/cm and 667/cm give the wavelengths of the infrared (IR) electromagnetic radiation that have been measured for two of the modes. This IR light is absorbed by the molecule by causing it to vibrate in the corresponding mode.

Electromagnetic radiation can only be absorbed or emitted by a molecule (or any other system) if the mode of vibration changes the "electric dipole moment". Since the oxygen atoms have borrowed electrons from the carbon, the first two modes cause a change in the relative positions of the negative (O) and positive (C) charges, and this changes the dipole moment. The "inactive" and "rotation" modes do not.

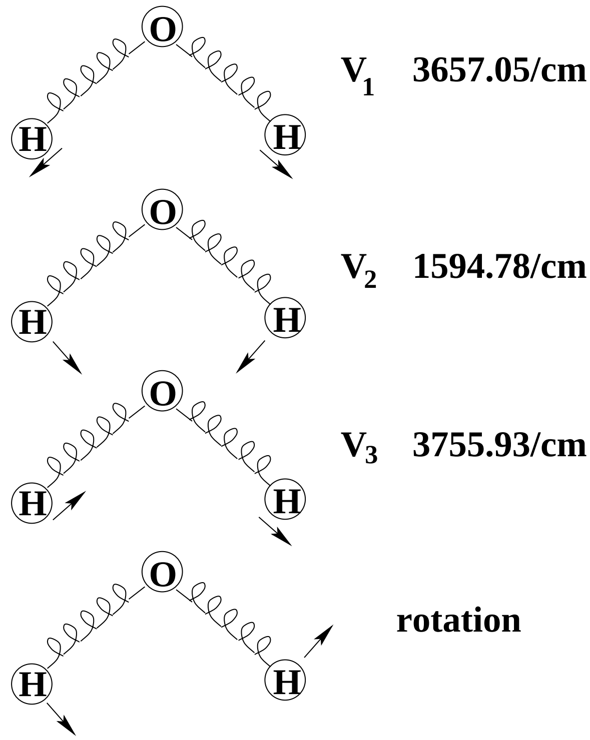
15. The water vapour molecule, H_2O, is not linear in structure because the four pairs of electrons that constitute the filled outer shell of the oxygen atom are arranged tetrahedrally for symmetry, distributing them equally (they all repel each other electrically, so stay as far apart as possible).

The oxygen atom could be thought of as being at the centre of a tetrahedron of hydrogen atoms (which it is in an ice crystal), except that here there are only two hydrogen atoms, and that the vapour molecule is planar (which it must be, consisting of only three atoms).



This triangle is not equilateral, and there are only two bonds, so Note 13 does not apply. (The angle between the bonds would be 109° in the tetrahedron—see Week 7c excursion—but is modified to 104.5° in the isolated molecule.)

Considering the oxygen atom fixed, the symmetry and its analysis are identical to that for CO_2, but produce three active modes



Water vapour and carbon dioxide are greenhouse gases because they absorb infrared light emitted by the earth when exposed to sunlight, and heat up.

Given that water vapour has more active modes and at higher energies than carbon dioxide, it is likely to have a stronger greenhouse effect. Since aircraft emit water vapour in the high atmosphere, as condensation trails, as well as carbon dioxide, their greenhouse effect multiplies aircraft CO_2 emission by a couple of times.

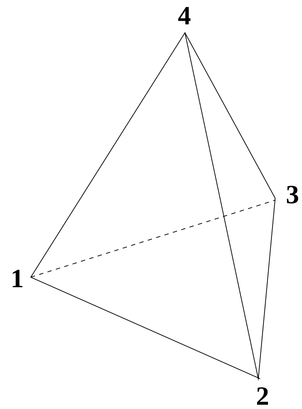
16. Tetrahedron. We mentioned tetrahedral symmetry in connection with ice and the four outer electrons of the oxygen atom. It is time to look at a more complicated group than that of the triangle. The tetrahedron is interesting because, just as the triangle group of $6 = 3!$ elements is also the group of all permutations of three objects, so the tetrahedral group is also the group of permutations of four objects.

Instead of the brute-force approach of working out all the elements of the tetrahedral group, let's see how much we can understand just using invariant sets and irreducible representations.

We should review what we have found out.

- The invariant sets are sets of group elements that are equivalent to each other in that they all have the same eigenvalues, and in particular they all have the same traces.
- A d-dimensional representation consists of one $d \times d$ matrix for each group element.
- The irreducible repesentations are orthogonal to each other in the sense that each vector constructed from the i, jth elements of each matrix for a given i, j is orthogonal to the vector

constructed from the i', j'th elements for i' different from i or j' different from j. Since these vectors are $\mid G \mid$ elements long, i.e., the size of the group G, it follows that the irreducible representations span a space of $\mid G \mid$ dimensions, and thus that $\mid G \mid =$ the sum of the squares d^2 of the dimensions of the irreducible representations.



Instead of trying to write down all the permutations that map the four vertices into one another, or, worse, the 3×3 matrices that transform the tetrahedron accordingly, let's try to find typical symmetry operations and also count how many of each there are.

First, there is one identity,

$$() \text{ or } \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}.$$

Second, there are two-fold (π radians or $180°$) rotations,

$$(12)(34) \text{ or } \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}.$$

There are three of these, corresponding to the three choices (including 2) we have for the vertex to write after 1 in the first cycle: (12)(34), (13)(24) or (14)(23). Or, geometrically, corresponding to the three pairs of opposite edges we can rotate into themselves: 1–2, 3–4 or 1–3, 2–4 or 1–4, 2–3. The matrix above does not have to be any one of these for this particular tetrahedron. It is a typical matrix: we can always choose axes so that the matrix given actually is a π-rotation.

Third, of course there are the three-fold rotations of each of the triangular faces,

$$(123) \text{ or } \begin{pmatrix} -1/2 & -\sqrt{3}/2 & \\ \sqrt{3}/2 & -1/2 & \\ & & 1 \end{pmatrix},$$

where the matrix is another typical matrix, this time of a $2\pi/3$ rotation in 3D.
There are four triangle faces and two threefold rotations on each, e.g., (123) and (132). (There are four ways to leave some vertex out of the three-cycle and two resulting 3-cycles for each vertex.) Thus, eight in all.

Fourth, we can reflect,

$$(12) \text{ or } \begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}.$$

There are six edges we can reflect into themselves, so six such operations. Or, 4!2 ("four choose two") = 6 ways of selecting two of the four vertices to put into the 2-cycle.

Fifth, we notice that there are no 4-cycles so far. These are a little hard to visualize on the tetrahedron, but we can calculate the product of (12)(34) with (24) to get (12)(34)(24) = (1234). Thus a reflection followed by a π-rotation gives a 4-cycle. A typical matrix is

$$\begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \begin{pmatrix} 1 & & \\ & -1 & \\ & & 1 \end{pmatrix} = \begin{pmatrix} -1 & & \\ & 1 & \\ & & 1 \end{pmatrix}.$$

(Watch out: this is a little slippery.)
There are six such 4-cycles, due to the $3! = 6$ permutations of the three vertices we can write after the 1 in the 4-cycle.

This gives a group of 24 elements. Since $24 = 4!$, the number of permutations of four vertices, we know we have not missed any.

We have at least five invariant sets as a result. No operation on the tetrahedron can convert any of the above five classes of operation into any other. For example, there is no way to get a three-fold rotation out of a two-fold rotation or a reflection. Of course, any of the five classes may break up into more than one invariant set: we would have to work out the elements and test ghg^{-1} for all pairs of elements g and h.

But let's start with the five classes and see if we can find irreducible representations based on them.

	1	3	8	6	6
	()	(12)(34)	(123)	(12)	(1234)
triv	1	1	1	1	1
3D	3	−1	0	1	−1

Here, we've written down the trivial representation and the **3D** representation, which is just the traces of the five matrices above.

Note that we did not write all 24 elements across the top of this table. We wrote only one representative of each invariant set (if these do turn out to be all the invariant sets). So we also wrote the counts, or size of each invariant set, across the top, so that we can multiply them by the traces when we are checking for orthogonality.

We can also guess there will be at least one more 1-D representation which we can call **parity**. This will be positive for rotations and negative for non-rigid motions of the tetrahedron such as reflections. Or, positive for permutations with even numbers of 2-cycles and negative for odd numbers of 2-cycles.

Here's a trick: multiply **parity** by **3D** to get **3D′**. This is OK since **parity** is 1-dimensional, i.e., its matrices are scalars.

	1	3	8	6	6
	()	(12)(34)	(123)	(12)	(1234)
triv	1	1	1	1	1
parity	1	1	1	−1	−1
3D	3	−1	0	1	−1
3D′	3	−1	0	−1	1

Now we have four representations. (Check that they are orthogonal. Remember to multiply by the counts, or else you will have to write out all 24 traces.)

To find out if anything is missing, sum the squares of the dimensions (i.e., of the traces of the identity): $1 + 1 + 9 + 9 = 20$. So we are short $4 = 2^2$, i.e., a 2-dimensional representations **2D**.

We could call this

	1	3	8	6	6
	()	(12)(34)	(123)	(12)	(1234)
2D	2	a	b	c	d

and solve four equations for these four unknowns: **2D** must be orthogonal to each of the other four. We finally get

	1	3	8	6	6
	()	(12)(34)	(123)	(12)	(1234)
triv	1	1	1	1	1
parity	1	1	1	-1	-1
2D	2	2	-1	0	0
3D	3	-1	0	1	-1
3D$'$	3	-1	0	-1	1

and we can check that they are all mutually orthogonal and the sum of squares of the dimensions is 24. It seems that we got the invariant sets correctly.

The trace of 2 for two-fold rotations in **2D** is a little puzzling. The only 2×2 matrix with a trace of 2 and whose square is the identity, is the identity itself. So this representation sees π-rotations as doing nothing. (The other traces in **2D** are consistent with 2×2 three-fold rotations, reflections, etc. in two dimensions.)

Two invariant subgroups can be assembled from these invariant sets: the only sums of counts that are divisors of 24 are 1+3 and 1+3+8. The first is called the Klein "vierergruppe" (German for "four-group") and has invariant subgroups formed by each element and the identity. The second is called the "alternating group" on four items, A_4, and is all the even 2-cycles, or all the rigid transformations, in the tetrahedron.

If we want to find modes of vibration of a tetrahedral molecule, we must eventually work out the matrices. But we can find out beforehand how they decompose. The representation we need is **motion**, the 12-dimensional tensor product of the 4-dimensional **perm** and the 3-dimensional **3D**.

	1	3	8	6	6
	()	(12)(34)	(123)	(12)	(1234)
perm	4	0	1	2	0
motion	12	0	0	2	0

To work out the group elements begins to need a computer program. Here is a quick and dirty MATLAB function which accepts the fewest possible matrices and generates the whole group of matrices.

```
% function group = groupgenMatrix(generator) THM 071102
% Finds closure of identity element and group elements in  generator
% E.g., generator = {[0,-1;1,0]}; rot4 = groupgenMatrix(generator); gives cell
%  array rot4: {[1,0;0,1],[0,-1;1,0],[0,1;-1,0],[0,-1;-1,0]}
% Uses brute force and
%   matColl = insertMatColl(element,matColl)
function group = groupgenMatrix(generator)
ng = size(generator); ng = ng(2);
sizmat = size(generator{1}); % all elements are square matrices of same size
group{1} = diag(diag(ones(sizmat(1)),0),0);
% unit matrix same size as generator mat
% insert the generator elements and their inverses
for k = 1:ng
  group = insertMatColl(generator{k},group);
  group = insertMatColl(generator{k}^-1,group);
```

```
end %for k = 1:ng
% repeat very inefficiently until group stops growing
sg1 = size(group);
while true
  sg = sg1;
  for k = 1:sg(2)
    for m = 1:sg(2)
      group = insertMatColl(group{k}*group{m},group);
      group = insertMatColl(group{m}*group{k},group);
    end %for m = 1:sg(2)
  end %for k = 1:sg(2)
  sg1 = size(group) % this takes a long time, so report size so far
  if sg1(2) == sg(2), break, end
end %while true
```

This code uses MATLAB *cell arrays*, `generator` and `group`, respectively to supply the generator elements and to collect the growing group. It explicitly (and redundantly) adds the identity element, then each generator element and its inverse. Then it starts finding products, both ways in case the elements are not commutative. It uses `insertMatColl(element,matColl)` to insert an element into a collection of matrices, relying on it to avoid inserting any element that is already there.

```
% function MatColl = insertMatColl(element,MatColl) THM 071102
% Uses
%   eqmat = equalmat(opmatrix1,opmatrix2)
% to find if the  element  is already in the cell  MatColl  and inserts if not
function MatColl = insertMatColl(element,MatColl)
sg = size(MatColl);
there = false;
for k = 1:sg(2)
  there = there | equalmat(element,MatColl{k});
  if there, break, end
end %for k = 1:sg(2)
if ~there
  MatColl{sg(2)+1} = element; % insert
end %if ~there
```

This in turn uses `equalmat(opmatrix1,opmatrix2)` to test two matrices for equality, which is an exercise (be careful when comparing real numbers).

It is handy to write another version of this code which represents group elements as cycles instead of as matrices. We can use strings to represent the cycles on input and output, so that the invocation to generate the tetrahedral group is

`group = groupgen(4,{'(12)(34)','(123)','(12)'})`

producing 24 elements `'()'`,`'(12)(34)'`,`'(123)'`,`'(1,3,2)'`,`'(12)'`,`'(2,4,3)'`,`'(1,3,4)'`, `'(1,4,3)'`,`'(2,3,4)'`,`'(3,4)'`,`'(1,3)'`,`'(2,3)'`,`'(1,4,2)'`,`'(1,2,4)'`,`'(1,4,3,2)'`,`'(1,2,3,4)'`, `'(1,2,4,3)'`,`'(1,3,4,2)'`,`'(1,4)(2,3)'`,`'(1,3)(2,4)'`,`'(2,4)'`,`'(1,3,2,4)'`,`'(1,4)'`,`'(1,4,2,3)'`

The first parameter, 4, is the number of items being permuted, The items are specified as integers from 1 to this number. (Note that this implementation of `groupgen(n,generator)` generally uses commas to separate the item numbers—so that `n` can exceed 9 if we wish—but is flexible in permitting commas to be omitted for brevity in the input when `n` < 10.)

The code in `groupgen()` is very similar to that for `groupgenMatrix()`, but is now only the tip of the iceberg. We need an internal representation for the permutations, which uses arrays. Thus the cycle `6,(1,2,5)(3,4)` becomes

```
2,5,4,3,1,6;
 1,1,2,2,1,0
```

where the second row of the array identifies the cycles: cycle 1 is `(1,2,5)` and cycle 2 is `(3,4)`. (0 labels any cycle of length 1.)

This is better seen with the array indices added as a top row.

```
1 2 3 4 5 6
2 5 4 3 1 6
1 1 2 2 1 0
```

Then we can see how to find the inverse (just swap the first two rows

```
2 5 4 3 1 6
1 2 3 4 5 6
0 1 2 2 1 0
```

and then rearrange), so the new array is

```
5,1,4,3,2,6;
 1,1,2,2,1,0
```

The procedure for finding the product is also easy.

$$\texttt{(125)(34)}\text{ then }\texttt{(2345)}\text{ is }\begin{matrix}123456\\254316\end{matrix}\text{ then }\begin{matrix}123456\\134526\end{matrix}$$

which combines to

```
1 2 3 4 5 6
2 5 4 3 1 6
3 2 5 4 1 6
```

but then we must regenerate the cycles for the final conversion back to string notation.

```
3,2,5,4,1,6;
 1,0,1,0,1,0
```

The tricky part is the conversions. `oparray = cyc2array(n,opcycles)` can be done with finite automata (Week 11). `opcycles = array2cyc(oparray)` can be done using the cycles rows in the arrays. These occupy the bulk of the code and their explanation will have to wait.

17. Hexa/Octahedra. The "hexahedron" is just the cube, with six faces, eight vertices and twelve edges. The octahedron is the diamond-like structure with eight faces, six vertices (they could be one unit each out from the origin, in both positive and negative directions, along the three axes in three dimensions) and, again, twelve edges.

These two regular polyhedra are "duals" of each other: mapping faces into vertices and vertices into faces converts cube to octahedron and vice-versa. That is why they have the same number of edges: the duality maps edges into edges (why?).

Duality means that they have the same symmetries, which we can easily specify.

- the identity;
- 6 rotations by $\pi/2$, each transforming one pair of edges into themselves, namely two edges on opposite sides of the origin from each other;

- 8 rotations by $\pi/3$, each preserving one opposite pair of octahedral faces or hexahedral vertices (note that the complementary rotations, by $2\pi/3$, are taken care of from the other side of the polyhedron);
- 6 rotations by $\pi/4$, each preserving one opposite pair of hexahedral faces or octahedral vertices (again, the $3\pi/4$ complements are automatically included);
- 3 rotations by $\pi/2$, each preserving the same square hexahedra face or fourfold octahedral vertex as the $\pi/4$ rotations;
- inversion, which combines with the above 24 elements to give 48 elements for the whole group.

The first 24 elements can be seen as the permutations of the four diagonals of the cube into each other, and so form the same group as S_4. This group of rigid symmetries of the cube thus has the same invariant sets, hence the same invariant subgroups and the same representations, as the symmetries of the tetrahedron.

18. Dodeca/Icosahedra. The dodecahedron and the icosahedron are duals, so we can look at either one to discover the symmetry operations.

The dodecahedron has 12 ("dodeca") pentagonal faces and 20 ("icosa") threefold vertices. The icosahedron has 20 ("icosa") triangular faces and 12 ("dodeca") five-fold vertices. They each have 30 edges ($V + F = E + 2$).
So the following rotations are allowed.

- the identity;
- 15 rotations by $\pi/2$, each rotation preserving an edge and the edge opposite it;
- 20 rotations by $\pi/3$, each rotation preserving an icosahedral triangular face or a dodecahedral threefold vertex (note that the complementary, $2\pi/3$, rotations are provided by the $\pi/3$ rotations of the opposite face or vertex);
- 12 rotations of $\pi/5$ and 12 more of $2\pi/5$ preserving a dodecahedral pentagon or an icosahedral five-fold vertex (again, the complementary, $3\pi/5$ and $4\pi/5$, rotations are provided by the opposite face or vertex).

These form a subgroup of 60 rotations, the alternating group, A_5. A really careful inspection of the dodecahedron will reveal five cubes, each with edges formed by pairs of connected dodecahedron edges. A_5 is the set of even permutations of these five cubes.

Plainly none of these sets can be transformed into any other by rotations, reflections or inversion, so the invariant sets cannot be larger than these sets. If these three are the invariant sets of A_5, we see immediately that A_5 can have no invariant subgroups, and hence no factor groups, because the sizes of the invariant subgroups would not divide 60: any subgroup contains the identity, and none of 1 + 15, 1 + 20 or 1 + 24 divide 60. Nor do 1 + 15 + 20, 1 + 15 + 24 or 1 + 20 + 24.

Inversion provides the extra symmetry operator that gives the 120-element symmetry group of the dodecahedron and the icosahedron.

19. Infinite groups
20. 1D crystals
21. 2D crystals
22. 2D waves
23. Brillouin zone.
24. Non-translational crystal symmetries.
25. Wallpaper groups.
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. I often find it useful to have three different texts open at the same topic when I am learning new ideas. So I should recommend two other texts on symmetry. They are Howard Georgi's *Lie Algebras in Particle Physics* [Geo82] and Elliott and Dawber's two-volume *Symmetry in Physics* [ED79a, ED79b]. Look them up, read them alongside these Notes, and use them to go further.

2. Apply each matrix operation in Note 1 to the set of vertices

$$\left\{ \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} \sqrt{3}/2 \\ 1/2 \end{pmatrix}, \begin{pmatrix} -\sqrt{3}/2 \\ 1/2 \end{pmatrix} \right\}$$

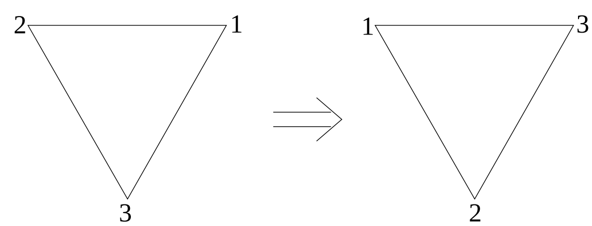
   and confirm that each gives back the same set.

3. Do enough of the matrix multiplications in the table in Note 2 to be sure that you understand how the table was constructed.

4. Confirm that the table in Note 3 is an accurate translation of the table in Note 2. Alternatively, try composing the cycles directly from the notation. For example (remembering that the first operator is on the right)

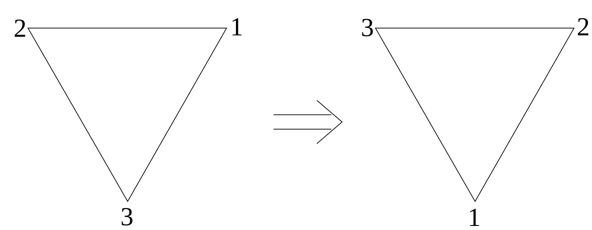
$$(123)(132) \Rightarrow \begin{array}{c} 1 \to 3 \to 1 \\ 3 \to 2 \to 3 \\ 2 \to 1 \to 2 \end{array} \Rightarrow ()$$

5. Note that two interpretations may be made of cycles such as (123). We may consider the labels to be firmly attached to the triangle, in which case the counterclockwise rotation of the whole is



(123) means rotate

   Otherwise we could imagine the triangle to be fixed and the labels to change places according to the cycle. This would be exactly the same as the first interpretation but clockwise.



(123) means relabel

What are the analogous two interpretations of the matrix operators?

6. How many different symmetries can you find in automobile wheels and hubcaps? Here are five to start.

Find examples with and without reflection symmetry.

7. Discuss the following examples in terms of broken symmetries.



8. Check that the triangle symmetry operations satisfy the group axioms.

9. Check that $\{(), (123), (132)\}$ by itself also satisfies the group axioms: it is a *subgroup*. Show that $\{(), (12)\}$, $\{(), (23)\}$ and $\{(), (31)\}$ are also each subgroups.

10. Which group axiom implies that the entries in each row (or in each column) are all distinct. As a special case, show that each inverse is unique.

11. Of the group and subgroups of triangle symmetries, which are also *commutative*?

12. Show that the size of a subgroup divides the size of the group.

13. Of the six operators of the triangle group, find two that can generate all the others using composition alone. How many such pairs of *generators* are there?

14. Write down a third form of the triangle group composition table using (arbitrarily chosen) single letters for each operator, say e for the identity, c and h for the rotations, and i, k and r for the reflections.
This table is getting so lean by now that we should start calling the operators by a simpler (and more general) name. We'll call them *elements* of the group.

15. Use the composition table to confirm that $f'f(f')^{-1}$ is a reflection if f and f' are any reflections in the triangle group.

16. Show that $\{(), (123), (132)\}$ is an invariant set of the triangle group.

17. Is $\{(), (12)\}$ an invariant subgroup of the triangle group?

18. How does the second composition table of Note 3 show that $gHg^{-1} \neq H$? (H here is $\{(), (12)\}$.)

19. How does the second composition table of Note 3 show that $gH \neq Hg$? (H here is $\{(), (12)\}$.)

20. How does the determinant being the product of the eigenvalues relate to the physical meaning of the determnant discussed in Week 3?

21. To show that the sum of the eigenvalues equals the sum of the diagonal elements for a general $n \times n$ matrix, we must compare two polynomials.
First, if we knew all the eigenvalues $\lambda_1, \lambda_2, ...\lambda_n$ then any eigenvalue λ satisfies

$$(\lambda - \lambda_1)(\lambda - \lambda_2)...(\lambda - \lambda_n) = 0$$

Second, any eigenvalue λ satisfies $Av = \lambda v$ for an eigenvector v, i.e., $(\lambda I - A)v = 0$, which can only happen if

$$\begin{aligned} 0 &= \det(\lambda I - A) = \begin{vmatrix} \lambda - a_{11} & -a_{12} & .. & -a_{1n} \\ -a_{21} & \lambda - a_{22} & .. & -a_{2n} \\ \vdots & & & \\ -a_{n1} & -a_{n2} & .. & \lambda - a_{nn} \end{vmatrix} \\ &= (\lambda - a_{11})(\lambda - a_{22})...(\lambda - a_{nn}) + \text{ terms involving } \lambda^k,\ k < n-1 \end{aligned}$$

so these two polynomials are

$$\begin{aligned} 0 &= \lambda^n - (\lambda_1 + \lambda_2 + ... + \lambda_n)\lambda^{n-1} + .. \\ \text{and} & \\ 0 &= \lambda^n - (a_{11} + a_{22} + ... + a_{nn})\lambda^{n-1} + .. \end{aligned}$$

See if this argument works for some particular 3×3 matrix.

22. In Note 9 we observed that the sum of the squares of the dimensions of the irreducible representations equalled the size of the group. Use the following thoughts to see why.
Consider the vectors made up from each *matrix element* of the irreducible representations.

rep.	()	(123)	(132)	(12)	(23)	(31)
triv	1	1	1	1	1	1
direc	1	1	1	-1	-1	-1
2D11	1	$-1/2$	$-1/2$	-1	$1/2$	$1/2$
2D12	0	$-\sqrt{3}/2$	$\sqrt{3}/2$	0	$\sqrt{3}/2$	$-\sqrt{3}/2$
2D21	0	$\sqrt{3}/2$	$-\sqrt{3}/2$	0	$\sqrt{3}/2$	$-\sqrt{3}/2$
2D22	1	$-1/2$	$-1/2$	1	$-1/2$	$-1/2$

Show that these are mutually orthogonal.
Hence the 6 vectors completely span the 6-D space of vectors of length 6. Show that this implies that the sum of squares of representation dimensions equals the size of the group.

23. Try block-diagonalizing **perm** (Note 9) with the Fourier transform (Week 9)

$$S = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}$$

where $\omega = e^{2\pi i/3}$, one of the 2-number cube roots ("complex cube roots") of 1. What are the resulting matrices and their traces?

24. Do the matrix-vector multiplications

$$R(g_1) \mid g_2 >=\mid g_1 g_2 >$$

to confirm that the matrices for the regular representation are correct in Note 11.

25. Check $R(\ ()\ ), R(\ (123)\ )$ and $R(\ (12)\ )$ in Note 11 and work out the other three matrices of the regular representation.

26. Show that the projection operators for the regular representation of the triangle group in Note 11 give the subspaces claimed: normalize the vectors, postmultiply by the transposes (to give 6×6 matrices) and, for the 4-dimensional subspace, sum the four matrices.

27. In Note 11 find S^{-1} for the block-diagonalization of the regular representation, check that $SS^{-1} = I$ and that $SR(g)S^{-1}$ is block diagonal (1+1+4) for each matrix $R(g)$ in the regular representation. (Use MATLAB.)

28. How would you decompose the 4×4 blocks of the block-diagonalized regular representation in Note 11 to two 2×2 blocks?

29. Find the irreducible representations of Z_2 in Note 12.

30. Check the projection matrices for representation **molec** in Note 13.

31. a) Rotate each pair of (x,y) coordinates in the vector a of Note 13, using the 2×2 matrix for $2\pi/3$, to get c of Note 13.
b) Draw the motion vectors for the system in the vibration mode given by c.

32. a) Show that the component of a two-dimensional vector $u = xe_1 + ye_2$ that is orthogonal to a normalized vector $v = ce_1 + se_2$, $c^2 + s^2 = 1$, is

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

using Clifford algebra (interval algebra: Week 7c).
b) On the way to this result you will probably find the component of u that is parallel to v as

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

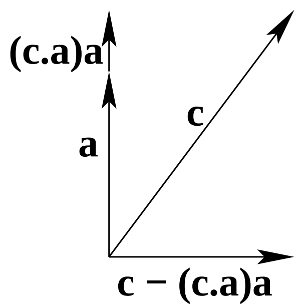
Show that, dropping the (e_1, e_2), this equals

$$(cx + sy) \begin{pmatrix} c \\ s \end{pmatrix} = (c, s) \begin{pmatrix} x \\ y \end{pmatrix} \begin{pmatrix} c \\ s \end{pmatrix}$$

c) $(c, s)\begin{pmatrix} x \\ y \end{pmatrix}$ gives the *dot product* (or *inner product*), $\vec{v}.\vec{u}$, of $\vec{v}$ with $\vec{u}$, obtained by summing the products of the coordinates. Summing the products of the coordinates has the same significance in higher dimensions, so we can, in 6D, find the component of c orthogonal to a. Show that

$$c - (c.a)a$$

gives this, and, when normalized, gives b of Note 13. (Use MATLAB.)



33. Construct transformation matrix S for the six projection vectors of Note 13 in such a way that SgS' is 2×2 block-diagonal for each 6×6 group element matrix in the triangle group. Show that the results are as given in Note 13.

34. Note 13 argues that the 2×2 blocks in the block-diagonalization of the group operators require that the frequencies be the same for the modes mixed by each 2×2 block. Why does this argument not apply to the 6×6 matrix before block-diagonalization, implying that *all* frequencies must be the same?

35. Why will a molecule of n atoms have $2n - 3$ modes of *vibration* in 2 dimensons? $3n - 6$ generally in three dimensions? What happens in 3 dimensions if the molecule is in the form of a straight line?

36. Why is it enough to consider CO_2 in 2D rather than 3D?

37. **Spring constants.** Since we modelled molecular bonds with springs in Notes 14 and 15, we might wonder how strong these springs are if we could squeeze them between our fingers. We can calculate this and compare it with the springs in a bathroom scale. Squeeze your bathroom scale and note how much you squeezed it (say 1 mm) and what it registered (say 50 kg).
Classical physics tells us that the force F required to squeeze a spring of constant k a distance x is $F = kx$, and that the force F exerted on a bathroom scale by somebody of mass m standing on it is $F = mg$ where $g \simeq 10$ m/sec^2 is the acceleration due to gravity at the Earth's surface. From the above data, show that k for the bathroom scale is $k \simeq 500$ kilo kg/sec^2.
To find k for the "springs" in the CO_2 molecule, use $m\omega^2 = 2k$ from Note 12, where ω is the angular frequency and m is a mass which we'll take to be that of one oxygen atom, m = 16Da, in Daltons (or "unified atomic mass units"), 1Da = $1/(1000N_A) = 1.66 \times 10^{-27}$ kg. (N_A is Avogadro's number, the number of molecules in a gram-mole of substance.)
(Using this formula for k and the oxygen mass for m is simplified guesswork, and we'll only get a ballpark result for k, but close enough to compare in general terms with the bathroom scale.)
We need to convert the wavenumbers, 2349/cm and 677/cm, to angular frequencies for light: $\omega = 2\pi f = 2\pi c/\lambda$ where $1/\lambda$ is the wavenumber and $c = 0.3$ giga m/sec is lightspeed. For $1/\lambda = 1000$/cm = 0.1 mega/m, $\omega = 0.188$ peta/sec.
Calculate k for the two modes of CO_2 and find out what fractions (or multiples) they are of your bathroom scale.

38. Work out the symmetry modes for H_2O vapour.

39. Work out the spring constant k for the three measured modes for H_2O.

40. Look up methane and ozone structure and work out their active modes. Look up the energies of these modes and calculate the spring constants.

41. Show that $(123) = (13)(12)$ and go on to show that any odd cycle can be written as a sequence of an even number of 2-cycles, and that any even cycle can be written as a sequence of an odd number of 2-cycles.

42. Show that the vierergruppe is commutative. What other group has four elements? Is it also commutative? Show that these are the only two groups of four elements. (Hint: why must no element occur more than once in any row or any column of the group composition table?)
What are the groups of 3, 2 or 1 elements?
Find all the invariant subgroups of all the above groups.
What is the smallest non-commutative group?

43. What is the factor group of the vierergruppe in the alternating group A_4?
What are the factor groups of the vierergruppe and of the alternating group in the tetrahedral group?

44. Show that the group of tetrahedral *rotations* has four invariant classes and four representations, of 1, 1, 1 and 3 dimensions, respectively. What are they? (Hint. Find a way of breaking the 2D representation of the full tetrahedral group into two 1-D representations using $e^{\pm 2\pi i/3}$.)

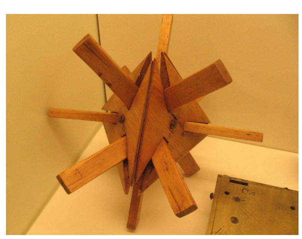
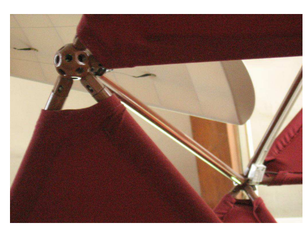
45. Find the invariant sets of the alternating group, A_4. (What happens to the 3-fold rotations in the absence of reflection?)
Find the four irreducible representations of A_4. (The **2D** representation of the tetrahedral group breaks down into two orthogonal one-dimensional representations involving $\omega = e^{2\pi i/3}$ and ω^2, the other two cube roots of 1. Find them. Note that their two rows add up to the row for **2D**. Explore the connection between the three-fold rotations and the cube roots of 1.)

46. In the tetrahedral group representations of Note 16, what are the irreducible representations composing **perm** and **motion**? Hint: what linear equation must be solved?
Characterize most of the modes of motion described by **motion**.

47. What are the invariant sets and the irreducible representation of the full 48-element symmetry group of the cube?

48. Show that the symmetry group of the icosahedron, i.e., A_5 augmented by inversion, is not the same group as S_5, the full permutation group on 5 elements.

49. What is the symmetry of the following (three different versions shown)?

(Photos of kite connectors from the Alexander Graham Bell National Historic Site of Canada, Baddeck, Nova Scotia, shown by kind permission of Parks Canada. The assembled kite on the right was designed for the exhibition; the connectors on the left and in the middle are original artifacts.)

50. Here is a "BuckyBall" (named after Buckminster Fuller). How many 5-fold and how many 6-fold axes does it have? What is the ratio of radii of the smaller circles to the larger circles? How many 3-fold axes does it have?

51. What is the (approximate) symmetry of the following?

52. Show that the following are the full sets of irreducible representations of their respective groups (the full group of permutations of five things, and the alternating subgroup—even number of swaps, or all the rigid rotations of a dodecahedron or icosahedron).

	1	10	20	30	24	15	20
S_5	()	(12) (123)	(1234)	(13452)	(12)(34)	(12)(345)	
U	1	1	1	1	1	1	1
U′	1	-1	1	-1	1	1	-1
V	4	2	1	0	-1	0	-1
V′	4	-2	1	0	-1	0	1
W	5	1	-1	-1	0	1	1
W′	5	-1	-1	1	0	1	-1
	6	0	0	0	1	-2	0

	1	20	15	12	12
A_5	()	(123)	(12)(34)	(12345)	(13452)
U	1	1	1	1	1
Y	3	0	-1	$(1+\sqrt{5})/2$	$(1-\sqrt{5})/2$
Z	3	0	-1	$(1-\sqrt{5})/2$	$(1+\sqrt{5})/2$
V	4	1	0	-1	-1
W	5	-1	1	0	0

What is the significance of the golden ratio (excursion, Week ii) here?

53. **Symmetric field trip: Galois and the quintic** This excursion depends on the excursions in Week 4 labelled "Field trip", "Symmetric polynomials" and "Roots of unity".
a) We saw in "Field trip" that polynomials have coefficients in some field, although some roots of some polynomials may not be in the field. This field is the context of the following. In "Symmetric polynomials" we saw that the coefficients of any polynomial are symmetric expressions of its roots. If the polynomial can be factored in the field, the coefficients of any factor polynomial are therefore symmetric expressions of the roots of the factor, i.e., of *some* of the roots of the original polynomial. This led Galois to the *subgroup* of S_n, the permutation group on all n roots of the original polynomial, that preserves *all* polynomials that yield an element of the field when evaluated using a root of the original polynomial.
(Instead of working with "polynomials that yield an element of the field" we can work with polynomials that yield 0, simply by subtracting said "element of the field" from the constant coefficient of such a polynomial to get the equivalent 0-valued polynomial. This 0-valued polynomial must be a factor of the original polynomial because it goes to 0 when evaluated using a root of the original polynomial—but see part (g) for a subtlety.)
For example, $x^3 + x^2 + x + 1 = (x + 1)(x^2 + 1)$ and its roots are -1, $\surd$ and $-\surd$ (using the notation, from "Field trip", $\surd$ for $\sqrt{-1}$). Verify that the coefficients of the original polynomial, $x^3 + ax^2 + bx + c$, are the symmetric expressions $a = -(-1 + \surd + (-\surd))$, $b = (-1) \times \surd + \surd \times (-\surd) + (-1) \times (-\surd)$ and $c = -((-1) \times \surd \times (-\surd))$
Verify that the coefficients of the quadratic factor, $Ax^2 + Bx + C$, are the symmetric expressions $B = A \times (-(\surd + (-\surd)))$ and $C = A \times \surd \times (-\surd)$
Over all the roots, what is the permutation group that does not change the original polynomial, $x^3 + x^2 + x + 1$? What is the permutation group that does not change *any* of the three polynomials above (including the original)? What field operations $(+, -, \times, /)$ on the roots give the latter group?
b) Moving on to the more complicated polynomial

$$x^5 + x^2 + x + 1 = (x^3 - x + 1)(x^2 + 1)$$

let's work in F_3, the field of arithmetic modulo 3 from "Field trip", to keep things manageable. In F_3, neither of these factors can be factored further: the first has roots $r_1 = r$, $r_2 = r + 1$ and $r_3 = r - 1$ where r satisfies the equation $r^3 - r + 1 = 0$; the second has roots $r_4 = \surd$ and $r_5 = -\surd$. What are the permutations of these roots that leave all three polynomials invariant?
Of the six permutations of the three things that could be the roots of $x^3 - x + 1$, only three are valid. These correspond to the field operation of adding 1 (in the field F_3): $1 + [r, r+1, r-1] = [r+1, r-1, r]$. This corresponds to the permutation (123). We cannot map $r \to r + 1$ in any way that leaves $r - 1$ unchanged: $r - 1 \to r + 1 - 1 = r$. So there is no permutation (12). Only the subgroup {(),(123),(132)} applies.
c) Over the field of rational numbers, $x^3 - x + 1$ is a special case of $x^3 + px + q$. Show that $r_1 = u_+ + u_-$ is a root ($x - u_+ - u_-$ is a factor) where

$$u_\pm = \sqrt[3]{-\frac{q}{2} \pm \sqrt{\frac{q^2}{4} + \frac{p^3}{27}}}$$

Show that $u_+u_- = -p/3$ and that $u_+^3 + u_-^3 = -q$. Finally, show that $r_2 = \omega u_+ + u_-/\omega$ and $r_3 = u_+/\omega + \omega u_-$ are also roots, where $\omega = e^{2\pi i/3}$ or $= e^{-2\pi i/3}$ is a primitive cube root of unity.
With these properties established, you can see that both (123) and (23) permutations of the roots of $x^3 + px + q$ can be generated by operations from the field $(+, -, \times, /)$: (123) comes from multiplying any root by ω, and (23) comes from swapping u_+ with u_-, i.e., from dividing either of them into $-p/3$.

From (b) and (c) we have two different groups for $x^3 - x + 1$, depending on whether it is considered over field F_3 or field Q (the usual notation for the field of rational numbers): for F_3 the group is $\{(), (123), (132)\}$ while for Q it is the full permutation group of three roots, $S_3 = \{(), (123), (132), (23), (31), (12)\}$. (It is a standard convention to write S_n for the permutation group on n items, because S_n is called the "symmetric" group on n items. This is dumb, because any group describes symmetries. The only groups that should be called "symmetric" would be those such as the vierergruppe, $\{1, a, b, c\}$, which is unchanged by any permutation of the elements a, b or c. But, then, any group also describes permutations, so "permutation" group is also ambiguous, pertaining either to the full permutation group or to some subgroup of permutations.)

d) Now return to the three polynomials of (b) and to field F_3. $x^5 + x^2 + x + 1$ factored into $x^3 - x + 1$ and $x^2 + 1$ and we must consider both factors to find the Galois group of $x^5 + x^2 + x + 1$. The group for $x^3 - x + 1$ we have seen to be the (cyclic) group $C_3 = \{()$, $(123), (132)\}$ (in F_3). The group for $x^2 + 1$ is just $S_2 = C_2 = \{(), (45)\}$, where (45) swaps roots $r_4 = \surd$ with $r_5 = -\surd$, i.e., negates them. (C_n is the notation for the group that cycles n items. Show that S_2 and C_2 are the same group.)

The group for $x^5 + x^2 + x + 1$ is the "product group" $C_3 \times S_2 = \{(), (123), (132), (45)$, $(123)(45), (132)(45)\}$. Work out the composition (multiplication) table for $C_3 \times S_2$ and see how product groups and factor (quotient) groups complement each other.

What is the Galois group of $x^5 + x^2 + x + 1$ in field Q? Work out the product group in this case.

e) We can relate the Galois group of a polynomial to the extensions to the field needed to contain its roots. For finite fields, each field extension must correspond to a cyclic group. For example, to solve $x^5 + x^2 + x + 1$ in field F_3, we can extend F_3 first to $F_3[\surd]$ to accommodate the $x^2 + 1$ factor, and then to $F_3[\surd][r]$ to contain the roots of $x^3 - x + 1$. (Or $F_3[r][\surd]$.) The group corresponding to each extension is cyclic.

Mathematicians speak, more generally, of commutative groups. Show that any cyclic group is commutative. Show that every element of any commutative group is an invariant set and hence that any commutative group has a chain of cyclic factor groups. Hence any chain of commutative factor groups corresponds to a chain, no shorter, of cyclic factor groups. So "commutative factor groups" can replace "cyclic factor groups" in all of this discussion. (If the group composition table is available, commutativity is easy to check: the composition table is symmetric.)

To solve $x^5 + x^2 + x + 1$ in field Q, we must extend to $Q[u_+, \omega] = Q[u_+][\omega]$ or $Q[\omega][u_+]$.

f) The full permutation groups S_2, S_3 and S_4 all have cyclic chains of factor groups, so all Galois groups for polynomials of degrees 2, 3 and 4 can be factored into a sequence of cyclic groups. This means that we can always find a sequence of extensions of the field that provides the polynomial coefficients, which involve only root extraction : "radical extensions".

For S_5, A_5 is invariant and gives a cyclic factor group, but, as we saw in Note 18, A_5 has no proper invariant subgroups. Nor is A_5 even commutative, let alone cyclic. So there may be quintic polynomials (degree 5) which cannot be factored in any radical extension of any radical extension of .. of the field of its coefficients. An example of a quintic whose Galois group is the full S_5 is $x^5 - x - 1$.

g) The Galois group need not be the full permutation group even if the polynomial has no factors in the field. For instance, $x^4 - 2x^3 + 4x + 2$ in Q has roots $r_1 = u + \sqrt{v}, r_2 = u - \sqrt{v}$ and r_3, r_4 are 2-number conjugates ("complex conjugates") of these, where $u = (1+i)/2$ and $v = 1 + 3i/2$. Show that

$$\begin{aligned}
r_1 r_2 + r_3 r_4 &= -2 \\
(r_1 + r_2)(r_3 + r_4) &= 2 \\
r_1 r_2 (r_3 + r_4) &= 2 \\
(r_1 + r_2) r_3 r_4 &= 2
\end{aligned}$$

so that there are symmetric expressions in the field which do not change under (12), (34) or

(13)(24). Hence the Galois group has no more than 8 elements instead of the 24 elements of S_4.
What does this mean in terms of extending the field to factor $x^4 - 2x^3 + 4x + 2$?
Find at least one 0-valued polynomial of degree less than 4 involving these roots but which is not a factor of the original, degree-4 polynomial.
h) This raises the question of how to find Galois groups when we do *not* know the roots of the polynomial. (In everything above we worked from the roots.) Chebotaryov proved a "density theorem" saying that the proportion of all finite fields in which a given polynomial (of degree n) factors tends eventually to the reciprocal of the size of the Galois group of that polynomial. So we can write a program which, by brute force, tries several hundred or a few thousand finite fields, F_p, and finds in what proportion of them the polynomial factors. Then we get an idea of the size of the Galois group, and can figure out which (sub)group of S_n it must be.
This is not a pretty procedure in the eyes of mathematicians. Nor is it very useful, ultimately, since the whole discussion of this excursion is not very practical. To find roots of any polynomial to accuracy good enough for any scientific need, we can use a graphing calculator or program to find them to one or two significant figures, and then use a method Newton invented to find them to any further desired accuracy.
But utility is not the only criterion for mathematics or anything else. A pencil is useful. A Beethoven sonata is not. Which is the more significant achievement?
Do we eat to live or do we live to eat? Discuss, in terms of utility, economic advantage and Galois theory.
i) In the above I have attempted to sketch the intuitions that may have occurred to Galois, of which the most significant are the importance of the symmetries of *all* 0-valued polynomials ((a) above) and the need for commutative extensions ((e) above). These intuitions are not proofs. Modern Galois theory is much more abstract, facilitating the proofs, but neglecting to give beginners experience with the abstractions.
The first proof of the general insolubility of the quintic was a given by Abel, who showed a contradiction if the quintic were supposed to be generally solvable. Abel used commutative groups in this proof, hence these are usually known as "Abelian groups".
j) Look up Nikolai Grigorievich Chebotaryov (also called Cebotarev) 1894–1947, Emil Artin 1889–1962, Niels Henrik Abel 1802–29 and the regrettably romantic life of Evariste Galois 1810–31. For the general solutions of cubics and quartics, look up Niccolo Tartaglia 1499–1557, Girolamo Cardano 1501–76 and Ludovico Ferrari 1522–65 (the quadratic solution was known in Babylonian times).
k) The last chapter of [Saw55] concretely discusses some crucial aspects of Galois theory. Use it to supplement this Excursion. Find out how Galois' theory of algebraic equations bears on differential equations.

54. What two groups are contained in any field? (If the field has n elements, one group also has n elements, and the other has $n - 1$.)

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

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