Applications of Group Representation Theory

Introduction:

Amongst the most important and widespread applications are those involving

- normal modes of oscillation of discrete (eg molecules) and continuous (eg drumheads) classical mechanical systems, specifically the degeneracies of the frequencies of oscillations that arise from symmetries and their lifting (ie the reduction of degeneracy) due to symmetry-reducing perturbations
- stationary states of quantum mechanical systems (eg electrons in atoms), and the degeneracies (arising from symmetries) of the energy levels and the lifting of this degeneracy due to symmetry-reducing perturbations (eg external fields, crystal fields in solids)
- Selection rules in quantum mechanics — matrix elements of perturbations between (formerly) stationary states, and when they must vanish on symmetry grounds
- allowed forms and transformation properties of vectors (e.g magnetic and electric dipole moments) and tensors (e.g the electrical conductivity tensor, the elastic constant) of crystalline media.

See discussions in

Landau and Lifshitz, Quantum Mechanics, Sec's 96, 97

Mathews and Walker, Mathematical Methods of Physics, Sec. 16-5

Lomont, Applications of Finite Groups

Jones, H.F.

Cornwell, J.F.

Central ideas

Degeneracies almost always result from symmetries;
the theory of symmetry is group theory;
So how does group theory help us to understand degeneracy?

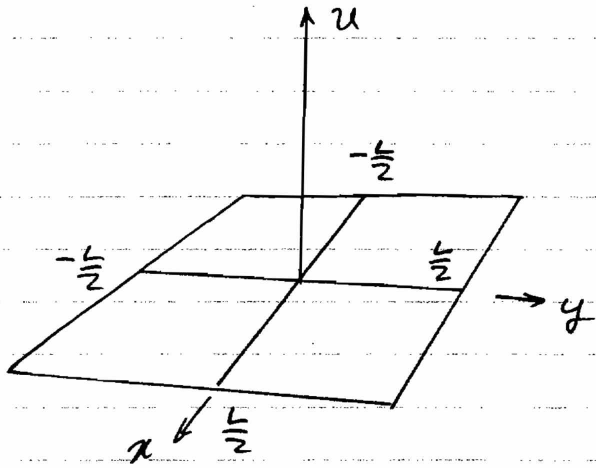
Irreducible representations and their dimensions govern (symmetry-originating) degeneracy patterns directly.

Eigenvectors* of physical matrices (Hamiltonians in quantum mechanics; spring constants in classical discrete systems) or differential operators are organised in degenerate sets (aka multiplets) that mix amongst themselves under symmetry transformations. Hence, eigenvectors* can be assigned to irreducible representations according to how they transform

* or Eigenfunctions (eg Schrödinger wave functions, or drumhead modes)

Example: The square drumhead (or the Schrödinger equation for a two-dimensional square well)

Displacement of the drumhead: $u(x,y,t)$



Wave equation: $$\frac{\partial^2 u}{\partial t^2} = c^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

Boundary conditions: $u = 0$ on $x = \pm L/2,\ y = \pm L/2$

Normal modes obey: $u(x,y,t) = \psi(x,y)\cos(\omega(t-t_0))$

Spatial patterns obey: $$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y) = -\frac{\omega^2}{c^2}\psi(x,y)$$

eigenfunctions

with $\psi(x,y) = 0$ on $x = \pm L/2,\ y = \pm L/2$

Separation of variables gives the following complete set of spatial patterns

$$\propto \begin{array}{c} \cos\,(2n_x+1)\pi\frac{x}{L} \\ \text{or} \\ \sin\,(2n_x)\pi\frac{x}{L} \end{array} \times \begin{array}{c} \cos(2n_y+1)\pi\frac{y}{L} \\ \\ \sin\,(2n_y)\pi\frac{y}{L} \end{array} \begin{array}{l} \leftarrow n = 0,1,2,\ldots \\ \\ n = 1,2,3,\ldots \end{array}$$

(*)

Call the collection $\psi^{a_x a_y}_{n_x n_y}$

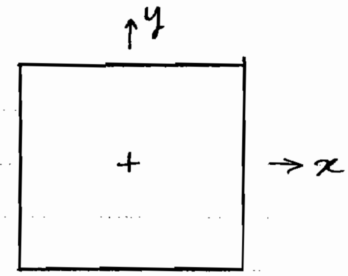
each s or c

integers (see *)

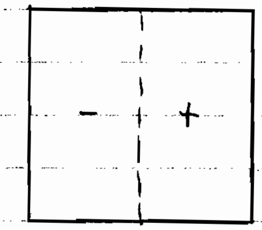
4/40

$\psi^{cc}_{00}(x,y) \propto \cos\frac{\pi x}{L} \cos\frac{\pi y}{L}$

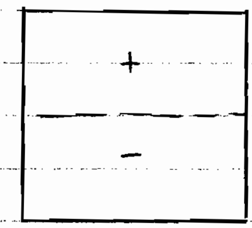
$$\frac{\omega^2}{c^2} = \frac{\pi^2}{L^2}(1^2+1^2)$$



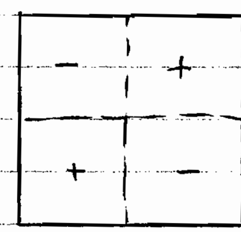
ψ^{sc}_{10} $\quad 2^2+1^2$



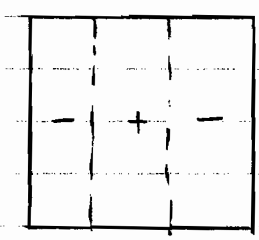
ψ^{cs}_{01} $\quad 1^2+2^2$



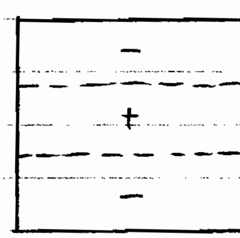
ψ^{ss}_{11} $\quad 2^2+2^2$



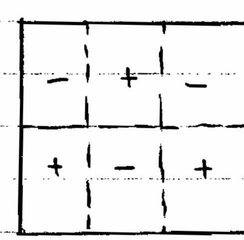
ψ^{cc}_{10} $\quad 3^2+1^2$



ψ^{cc}_{01} $\quad 1^2+3^2$



ψ^{cs}_{11} $\quad 3^2+2^2$



The symmetry group of the square is D_4

e : $(+x,+y) \to (+x,+y)$

b : $\to (+y,+x)$ ← mirror (not flip by π) because $u>0$ stays positive (4/18/01 – not convinced by this argument cf 3/135 rep A_2) eg diffusion w/ u as temp; does not transform like coords – diffusion in a 3D cube

bc : $\to (+x,-y)$

bc^2 : $\to (-y,-x)$

bc^3 : $\to (-x,y)$

c : $\to (-y,x)$

c^2 : $\to (-x,-y)$

c^3 : $\to (y,-x)$

$$D_4 = \{e, c, c^2, c^3, b, bc, bc^2, bc^3\} \qquad c^4 = b^2 = (bc)^2 = e$$

Recall how wave functions transform under symmetry operations

$$\psi(\underline{r}) \xrightarrow{R} \psi'(\underline{r}) = \psi(\underline{\underline{R}}^{-1}\cdot\underline{r})$$

Let us see how our drumhead normal modes transform:

$$(e, c, c^2, c^3, b, bc, bc^2, bc^3)\,\psi^{cc}_{00}(x,y) = +\psi^{cc}_{00}(x,y)$$

This function transforms into itself under all operations of D_4. On physical grounds we expect that symmetry transformations of normal modes will produce normal modes with the same frequency, but they may or may not be new normal modes. In this case no new normal modes are obtained.

We say that the function ψ^{cc}_{00} forms the basis for a trivial representation of the group: if $\psi_j(\underline{r}) \to \psi_j(\underline{\underline{R}}^{-1}\cdot\underline{r}) = \sum_k D_{kj}\,\psi_k(\underline{r})$ then $D = 1$ (ie the 1×1 unit matrix) for all group elements.

Now let us look at how $\psi^{sc}_{10}(x,y) \propto \sin\frac{2\pi x}{L}\cos\frac{\pi y}{L}$ transforms (under the group elements):

$$(e, c^2, bc, bc^3): \psi^{sc}_{10}(x,y) \to (+,-,+,-)\,\psi^{sc}_{10}(x,y),$$

So no new degenerate eigenfunctions are generated, although the sign of the function obtained is not always as it was.

But under the remaining group elements we get a new function

$$(c, c^3, b, bc^2): \psi^{sc}_{10}(x,y) \to (-,+,+,-)\,\psi^{cs}_{01}(x,y).$$

So ψ^{sc}_{10} lives in a degenerate multiplet with one other eigenfunction, namely ψ^{cs}_{01} – together they form a basis for a two-dimensional representation of D_4

$$\begin{pmatrix}\psi^{sc}_{10}(x,y)\\ \psi^{cs}_{01}(x,y)\end{pmatrix} \longrightarrow D(g)\begin{pmatrix}\psi^{sc}_{10}(x,y)\\ \psi^{cs}_{01}(x,y)\end{pmatrix}$$

$$\begin{array}{ccccccccc} & e & c & c^2 & c^3 & b & bc & bc^2 & bc^3 \\ D(g) = & \begin{pmatrix}1&0\\0&1\end{pmatrix} & \begin{pmatrix}0&-1\\+1&0\end{pmatrix} & \begin{pmatrix}-1&0\\0&-1\end{pmatrix} & \begin{pmatrix}0&1\\-1&0\end{pmatrix} & \begin{pmatrix}0&1\\1&0\end{pmatrix} & \begin{pmatrix}1&0\\0&-1\end{pmatrix} & \begin{pmatrix}0&-1\\-1&0\end{pmatrix} & \begin{pmatrix}-1&0\\0&+1\end{pmatrix}\end{array}$$

We must end up with between 1 and $[g]$ functions; they are degenerate because they have been arrived at via symmetry operations.

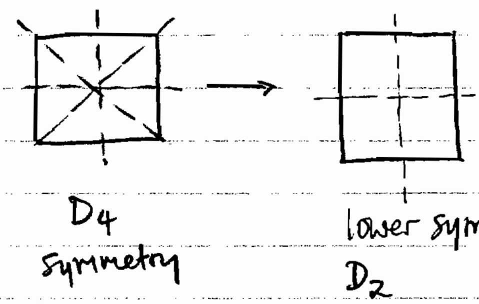
Barring accidental degeneracies (in which case the function we started with may be a linear combination of functions associated with distinct irreducible representations), the multiplet will form a basis for an irrep – the space it spans will not have any invariant subspaces and no further block diagonalisation is possible. So we see the central idea: the sizes of the irreps give the sizes of the degenerate multiplets.

Let us look at one more eigenfunction $\psi_{11}^{ss}(x,y) \propto \sin\frac{2\pi x}{L}\sin\frac{2\pi y}{L}$, which transforms as follows

$$(e, c, c^2, c^3, b, bc, bc^2, bc^3) : \psi_{11}^{ss}(x,y) \rightarrow (+,-,+,-,+,-,+,-)\,\psi_{11}^{ss}(x,y)$$

So no new functions are generated, and we have a one-dimensional, non-degenerate multiplet — but it does not live in the trivial/unit representation; instead it lives in another one-dimensional representation.

Later, we shall examine when and how symmetry-reducing perturbations lift the degeneracy of the degenerate multiplets. For example, suppose that we slightly distort the square rim



Diagonalising matrices that have symmetries
(see J. S. Lomont, p. 51 et seq, p. 100 et seq)

- Consider the matrix H_{jk} (Hermitian or real-symmetric) whose (real) eigenvalues and eigenvectors are of interest to us.
  $\{\varepsilon_\lambda\}$ $\{\psi_{\lambda j}\}$

E.g. H may be the Hamiltonian matrix for some quantal system in some basis

$$H_{jk} = \int d^3r\, \phi_j^*(\underline{r})\, \hat{H}\, \phi_k(\underline{r}) = \langle \phi_j | \hat{H} | \phi_k \rangle$$

- Let the group of matrices $\{D_{jk}(g) \mid g \in G\}$ constitute a matrix representation of the group G.

- We say that H is invariant under the symmetry group G if

$[D(g), H] \equiv D(g)H - HD(g) = 0 \quad \forall g \in G$, or equivalently

matrix notation

$$D(g)HD(g)^{-1} = H \quad \forall g \in G.$$

One way to understand this is as follows:

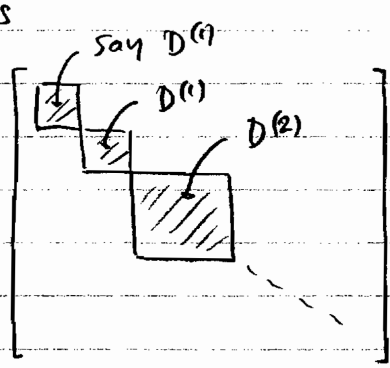
let ψ_λ be a complete orthonormal set of eigenvectors of H, ie,
$\Sigma_k H_{jk}\psi_{\lambda k} = \varepsilon_\lambda \psi_{\lambda j}$. (*)

Then, $\forall g \in G$, the vectors $\Sigma_k D_{jk}(g)\psi_{\lambda k}$ must also be eigenvectors of H with eigenvalue ε_λ: $\Sigma_{kl} H_{jk} D_{kl} \psi_{\lambda l} = \varepsilon_\lambda \Sigma_l D_{jl}\psi_{\lambda l}$

But, using (*) this is: $\Sigma_{kl} H_{jk} D_{kl} \psi_{\lambda l} = \Sigma_{kl} D_{jk} H_{kl} \psi_{\lambda l}$, and as this is true when acting on a complete orthonormal set ψ_λ it is true quite generally, ie, $\Sigma_k H_{jk} D_{kl} = \Sigma_k D_{jk} H_{kl}$.

- Now let us imagine that we have made a similarity transformation to a basis in which the representation $D(g)$ has been completely reduced, so that it has the explicit form of a direct sum of its constituent irreps

$D(g) =$



Remarks:
- We can always arrange the featuring irreps to be organised into clusters of $D^{(1)}$'s, of $D^{(2)}$'s etc.
- $D^{(\mu)}(g)$ and $D^{(\mu)}(g')$ need not commute with one another and cannot – in general – be simultaneously diagonalised.

- For the sake of illustration, suppose we find that $D(g)$ contains just two irreps and that they are distinct

$$D = D^{(\mu)} \oplus D^{(\nu)} \qquad (\mu \neq \nu)$$

Then, by the symmetry of H we have

$$\left(\begin{array}{c|c} D^{(\mu)} & 0 \\ \hline 0 & D^{(\nu)} \end{array}\right)\left(\begin{array}{c|c} H_{11} & H_{12} \\ \hline H_{21} & H_{22} \end{array}\right) = \left(\begin{array}{c|c} H_{11} & H_{12} \\ \hline H_{21} & H_{22} \end{array}\right)\left(\begin{array}{c|c} D^{(\mu)} & 0 \\ \hline 0 & D^{(\nu)} \end{array}\right)$$

ie block by block we have, $\forall g \in G$,

$$\left.\begin{array}{ll} 11: & D^{(\mu)} H_{11} = H_{11} D^{(\mu)} \\ 22: & D^{(\nu)} H_{22} = H_{22} D^{(\nu)} \end{array}\right\} \Rightarrow \text{(via Schur I)} \quad \begin{array}{l} H_{11} \propto \text{identity} \\ H_{22} \propto \text{identity} \end{array}$$

$$\left.\begin{array}{ll} 12: & D^{(\mu)} H_{12} = H_{12} D^{(\nu)} \\ 21: & D^{(\nu)} H_{21} = H_{21} D^{(\mu)} \end{array}\right\} \Rightarrow \text{(via Schur II)} \quad \begin{array}{l} H_{12} = 0 \\ H_{21} = 0 \end{array}$$

So we see what we have said a number of times already:

- the eigenvalue spectrum is organised into degenerate multiplets according to the sizes of the irreps of G

- the eigenfunctions/eigenvectors of a degenerate multiplet form (barring accidental* degeneracies) the basis for an irrep of G; they form an invariant subspace of states that transform into one another under the group transformations

- accidental degeneracy — when two irreducible multiplets share a common eigenvalue not owing to any symmetry but just via an accident of the parameters of the problem

- usually what at first sight appears as accidental degeneracy is in fact due to additional symmetries that we originally missed; higher symmetry usually means more degeneracy (because there are now more group elements available to connect states; irreducible representations get bigger)

Example: the hydrogen atom has quantum numbers n, l, m, s

$n = 1, 2, \ldots$; $l = 0, 1, \ldots n-1$; $m = -l, -l+1, \ldots, +l$; $s = \pm\frac{1}{2}$

The energy levels are labelled by n
but not l, m, s

no obvious symmetry reason for this } but in fact (Fock) there is an $O(4)$ not just an $O(3)$ symmetry that enforces this extra – not accidental – degeneracy

Summary:

- Eigenvectors are "assigned" to irreps, which specify how they transform (ie with whom they mix under symmetry operations)

$$\psi_j \rightarrow \psi_r^{(\mu)}$$

μ: which irrep – an irrep may feature more than once

r: which basis vector in the irrep

ψ_j: old indexing; $\psi_r^{(\mu)}$: new labelling

Then $\psi_r^{(\mu)} \longrightarrow \sum_{r'} S_{rr'}^{(\mu)} \psi_{r'}^{(\mu)}$ (μ: irrep.) perhaps should write $D_{rr'}^{(\mu)}$

- Highly symmetric states (eg H-atom s states) transform trivially; less symmetric states (eg H-atom p states) mix

- States in an irrep. form a basis for that irrep.

- Can think of irreps as being generated by symmetry operations as follows:
  - take one eigenvector
  - generate $\leq [g]$ others from it
  - all vectors thus generated are eigenvectors
  - any orthonormal set drawn from the space spanned by the generated vectors is a basis for the irrep.

Symmetry-reducing perturbations and the lifting of degeneracy 4/12

See Landau and Lifshitz, Quantum Mechanics, Sec. 96
H.F. Jones, Sec. 5.3

Typical setting – electrons in the d and f shells of atoms interact only slightly with the surrounding atoms in a crystal. What effect does this have on the atomic spectrum?

Another – an isotropic circular drumhead is perturbed so as to become 4-fold symmetric (see below for details). What is the impact on the frequencies of the normal modes of oscillation?

Basic ideas (couched in the language of quantum mechanics in some matrix representation – but the ideas are more general):

- Consider a system governed by the Hamiltonian H_0 (a matrix, but I shall only write the indices when necessary). The symmetry group of H_0 is denoted G_0 – then

  $$[D_0(g), H_0] = 0 \quad \forall\, g \in G_0,$$

  where $D_0(g)$ is the matrix representation of $g \in G_0$ in the same basis as H_0

- As we have discussed, the eigenvectors of H_0 form degenerate multiplets that constitute bases for irreps of G_0

Block diagonalise D_0 and pick one irrep, $\mu\, r$ — μ: which irrep; r: which "version" of μ

$D^{(\mu)}(g)$ for a typical g

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \\ & & \ddots \end{pmatrix} \mathcal{E}^{(\mu r)}$$

H_0 in the basis $\psi^{(\mu r a)}$ — a: which basis vector

- Now perturb the system: $H_0 \to H_0 + H_1$
  and denote by G_1 the symmetry group of H_1

  (ie, $[D_1(g), H_1] = 0 \quad \forall g \in G_1$ where $D_1(g)$ is the matrix representation of $g \in G_1$).

  i) If H_1 has higher symmetry than H_0 (or the same symmetry)
  (i.e., G_0 is a subgroup of G_1)
  then the symmetry of H is the lower of G_0 and G_1 (ie, G_0) and the irreps (and hence degeneracy structure) are unchanged by the perturbation – the perturbation does not lift any of the (symmetry-originating) degeneracy

  ii) If, on the other hand, H_1 has strictly lower symmetry (i.e., G_1 is a subgroup of G_0 and not G_0 itself) then the symmetry of H is the lower of G_0 and G_1 (ie, G_1) and the irreps (and hence degeneracy structure) are modified – the perturbation may or may not lift various degeneracies, depending on whether the corresponding irreps become reducible now that the symmetry is lower (i.e., now that some of the elements of the group are deleted).

- Why might lowering the symmetry lead to the reducibility of what used to be an irrep?

  Well, in an irrep, the symmetry elements connect all states to one another. But now that some elements are deleted, what used to be an invariant subspace may fall into two or more invariant fragments.

Said another way, if we stack the matrices of an irrep on top of one another, make the nonzero elements opaque, and try to peer through, then in no basis will there be any transparent off-diagonal blocks. But if we remove some of the "sheets", as we must do when we replace G_0 by its subgroup G_1, then the situation may change.

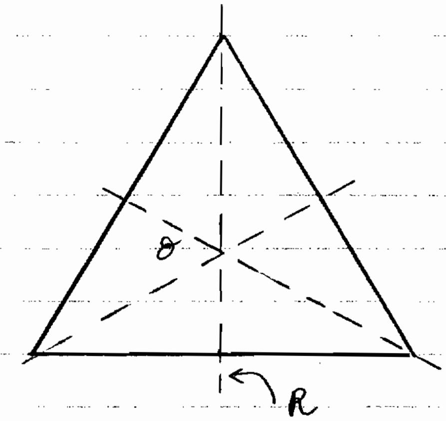
• So, how do we proceed? We take our formerly degenerate multiplet μ, r and use its basis vectors to construct a representation of the smaller group G_1 — this simply amounts to deleting the matrices from the old irrep that correspond to group elements that are no longer present. (In practice, we often work with characters.) We then use information about the irreps of G_1 (usually its character table) to express our rep of G_1 as a direct sum of irreps.

If decomposition occurs then the degeneracy is lifted from its old value, and the multiplet splits into pieces, each of degeneracy corresponding to the sizes of the irreps of G_1 contained in our rep.

Moreover, what was an invariant subspace splits into two or more invariant subspaces, each spanned by eigenvectors from the corresponding irrep of G_1

Example: Consider a quantum mechanical particle confined to the interior of an equilateral triangle

(Our analysis applies equally to the normal modes of a drumhead.)
Schrö. eq → wave eq.



C: rotate by $2\pi/3$ about O
b: reflect in R

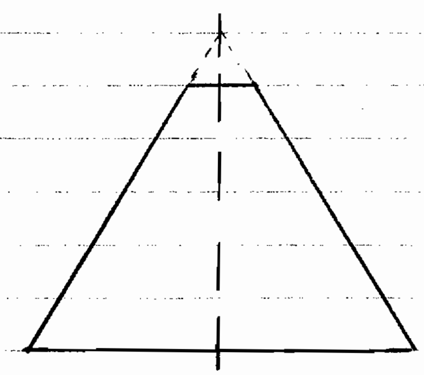
The symmetry group G_0 is $D_3 = gp\{e, c, b\}$, $c^3 = b^2 = (bc)^2 = e$

The character table is

D_3	E (e)	$2C_3$ (c, c^2)	$3C_2$ (b, bc, bc^2)	
A_1	1	1	1	
A_2	1	1	−1	z
E	2	−1	0	x, y

↑ basis functions of the vector rep

Now perturb the system by truncating a vertex in a way that preserves the reflection symmetry



The symmetry group becomes $G_1 = C_2 = gp\{e, b\}$, $b^2 = e$

The character table is

	E	C_2
C_2	(e)	(b)
A_1	1	1
A_2	1	-1
χ	2	0

possibly reducible rep of C_2 in the E basis of D_3

use orthogonality theorem here

Now, let us consider a pair of degenerate states in the unperturbed system that transform according to the rep E

The corresponding characters of this rep of D_3 are

	E	$2C_3$	$3C_2$
	(e)	(c, c^2)	(b, bc, bc^2)
E	2	-1	0

This basis also provides a rep of G_1 (ie C_2) – we retain the group elements e and b, so the characters for this rep of C_2 are 2 and 0 (see the line χ in the
(e) (b) C_2 character table)

Then we write $\chi(g) = a_{A_1}\chi^{(A_1)}(g) + a_{A_2}\chi^{(A_2)}(g)$
$\forall g \in G_1 (= C_2)$
and by orthogonality we have

$$a_{A_1} = \langle \chi^{(A_1)}, \chi \rangle = \frac{1}{[g]} \sum_{\alpha} \chi_{\alpha}^{(A_1)*} \chi_{\alpha} k_{\alpha}$$

conjugacy class its multiplicity

$$= \frac{1}{2}\left[(1\cdot 2)\cdot 1 + (1\cdot 0)\cdot 1\right] = 1$$

$$a_{A_2} = \langle \chi^{(A_2)}, \chi \rangle = \frac{1}{2}\left[(1\cdot 2)\cdot 1 + (-1\cdot 0)\cdot 1\right] = 1$$

So we learn that $D = D^{(A_1)} \oplus D^{(A_2)}$ and hence that the degeneracy is lifted by the perturbation.

our rep of C_2 in the basis of the irrep E of D_3

Example : A spherically symmetric atom is placed at the centre of a weakly tetrahedral environment. Examine the splitting of an angular momentum 2 multiplet.

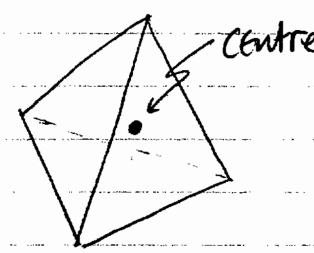
- G_0 is the rotation group $SO(3)$.
- Rotations through angle θ (regardless of axis) reside in the same conjugacy class.
- The irreps are labelled by total angular momentum $l = 0, 1, 2, \ldots$ and the irrep l is $2l+1$-dimensional; its basis is a $2l+1$-fold degenerate multiplet.
- Anticipating a result from the theory of continuous groups, the character of conjugacy class θ in irrep l is

$$\chi_\theta^{(l)} = e^{-il\theta} + e^{-i(l-1)\theta} + \cdots + 1 + e^{i\theta} + \cdots + e^{il\theta}$$

For $l=2$ this is $\quad 1 + 2\cos\theta + 2\cos 2\theta$

4 places to put vertex, 3 subsequent rotations

- The tetrahedral group $G_1 = T$ is a finite subgroup of $G_0 = SO(3)$, of order 12. Its elements fall into conjugacy classes of rotations through $0, \pi, 2\pi/3$ and $4\pi/3$



T	E	$3C_2$	$4C_3$	$4C_3^2$	
A	1	1	1	1	
E_1	1	1	ω	ω^2	$\leftarrow \omega = e^{2\pi i/3}$
E_2	1	1	ω^2	ω	
T	3	-1	0	0	
	0	π	$2\pi/3$	$4\pi/3$	$\leftarrow$ angle of rotation, θ
$\chi_\theta^{(2)}$	5	1	-1	-1	$\leftarrow$ rep of T in old basis

Decomposition is certain – there are no irreps of T of dimension 5; but what is the precise decomposition?

$\ell=2$ irrep. of $SO(3)$

$$\chi^{(2)}_{\alpha} = \sum_{\mu} a_{\mu}\, \chi^{(\mu)}_{\alpha}$$ ← labels irreps of T 4/180

Conjugacy class of T

Orthogonality yields $a_{\mu} = \langle \chi^{(\mu)}, \chi \rangle$ i.e.

$$
\begin{aligned}
a_A &= \tfrac{1}{12}\left[1(1\cdot 5) + 3(1\cdot 1) + 4(1\cdot(-1)) + 4(1\cdot(-1))\right] &&= 0 \\
a_{E_1} &= \tfrac{1}{12}\left[1(1\cdot 5) + 3(1\cdot 1) + 4(\omega(-1)) + 4(\omega^2(-1))\right] &&= 1 \\
a_{E_2} &= \tfrac{1}{12}\left[1\cdot(1\cdot 5) + 3(1\cdot 1) + 4(\omega^2(-1)) + 4(\omega(-1))\right] &&= 1 \\
a_T &= \tfrac{1}{12}\left[1\cdot(3\cdot 5) + 3(-1\cdot 1)\right] &&= 1
\end{aligned}
$$

(Note $1 + \omega + \omega^2 = 0$.)

So we learn that $D = D^{(E_1)} \oplus D^{(E_2)} \oplus D^{(T)}$

our rep of G_1 in our irrep of G_0

sometimes we write simply

$E_1 \oplus E_2 \oplus T$

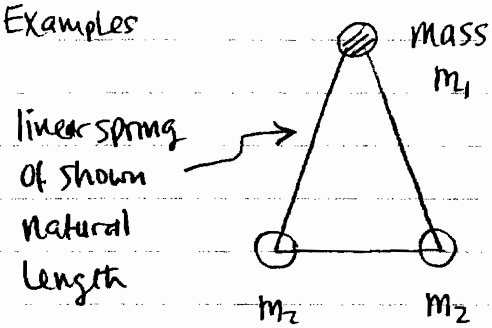
dim: 1 1 3

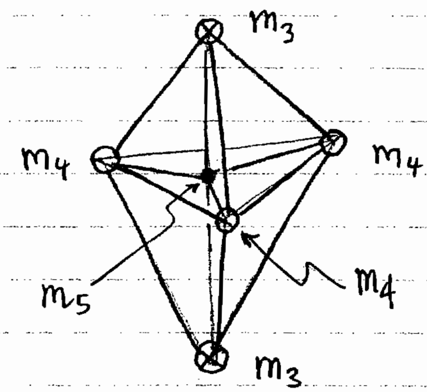
So our formerly degenerate multiplet of 5 states spans 3 irreps.
The degeneracy will be lifted from 5 to 1, 1, 3

Normal modes of oscillation for a discrete system

Envisage a system of "balls and springs" ie a discrete classical mechanical system.

Examples





These systems certainly have symmetries, and we would like to exploit these symmetries in order to classify the normal modes of oscillation via irreps.

Let us start with the Lagrangian for the system expressed in terms of N generalised coordinates $\{\tilde{q}_j\}_{j=1}^{N}$. (Quite generally, the symmetry analysis of physical systems is more transparent at the level of the Lagrangian or Hamiltonian (scalar entities) than it is at the level of equations of motion (eg vector entities).)

$$L = \frac{1}{2} \sum_{jk=1}^{N} \dot{\tilde{q}}_j \, \underset{(*)}{a_{jk}}(\tilde{q}) \, \dot{\tilde{q}}_k - V(\underset{\text{the collection of } \tilde{q}\text{'s}}{\tilde{q}})$$

To study small oscillations we need to

i) determine configurations $\tilde{q}_0$ of mechanical equilibrium

ii) expand around them to obtain an approximate Lagrangian quadratic in the departures from equilibrium $q_j \equiv \tilde{q}_j - \tilde{q}_{0j}$ and their velocities $\dot{q}_j = \dot{\tilde{q}}_j$.

(*) Note – a_{jk} can be taken to be symmetric, i.e., $a_{jk}(\tilde{q}) = a_{kj}(\tilde{q})$

The equations of motion, $\frac{d}{dt}\frac{\partial L}{\partial \dot{\tilde{q}}_j} - \frac{\partial L}{\partial \tilde{q}_j} = 0$, (#)

read $\frac{d}{dt}\sum_k a_{jk}(\tilde{q})\,\dot{\tilde{q}}_k = -\frac{\partial V}{\partial \tilde{q}_j}$

At equilibrium, $\tilde{q}_j(t) = \tilde{q}_{0j}$ ← constant, for which the lhs vanishes so $\tilde{q}_0$ obey

$$\partial V / \partial \tilde{q}_j \Big|_{\tilde{q}=\tilde{q}_0} = 0.$$

Suppose that we can find a solution $\tilde{q}_0$ and, furthermore, that it is stable with respect to small perturbations. (We will address neutral equilibria – eg associated with overall translations and rotations of a molecule – later.)

Then we may assume that small motions remain small and we may expand to quadratic order:

$$L = \frac{1}{2}\sum_{jk} \dot{q}_j\, a_{jk}(\tilde{q}_0 + q)\, \dot{q}_k - V(\tilde{q}_0 + q)$$

$$\approx \frac{1}{2}\sum_{jk} \dot{q}_j\, \underbrace{A_{jk}}_{a_{jk}(\tilde{q}_0)}\, \dot{q}_k - \underbrace{\cancel{V(\tilde{q}_0)}}_{\text{Const: irrelevant}} - \sum_j \overbrace{\cancel{\frac{\partial V}{\partial \tilde{q}_j}\Big|_{\tilde{q}_0}}}^{0 \text{ at eqm}} q_j$$

$$- \frac{1}{2}\sum_{jk} q_j\, \underbrace{B_{jk}}_{\frac{\partial^2 V}{\partial \tilde{q}_j \partial \tilde{q}_k}\Big|_{\tilde{q}=\tilde{q}_0}}\, q_k + \text{cubic and higher order terms}$$

← ie, a system of coupled linear oscillators

This is the Lagrangian that we shall work with. The transformation from $\tilde{q}$ to q is a simple shift, so the form of the Euler–Lagrange equation is preserved (#) and the equation of motion becomes

(in matrix notation) $\underline{\underline{A}} \cdot \ddot{\underline{q}} = -\underline{\underline{B}} \cdot \underline{q}$

(i.e. $\sum_k A_{jk} \ddot{q}_k = - \sum_k B_{jk} q_k$), a system of coupled linear oscillators.

Now let us seek normal modes of oscillation, ie, motions of the form

$$\underline{q}(t) = \alpha \, \underline{Q} \cos \omega (t - t_0).$$

sets phase

amplitude — a normalised vector — frequency

Insertion into the equations of motion gives

$$\underline{\underline{B}} \cdot \underline{Q} = \omega^2 \underline{\underline{A}} \cdot \underline{Q}$$

makes this a generalised eigenproblem

only has solutions for characteristic values of ω^2

Now $\underline{\underline{A}}$ is symmetric ($\underline{\underline{A}} = \underline{\underline{A}}^T$) and positive-definite (all eigenvalues are positive) — in fact, in many settings

$$\underline{\underline{A}} = \text{diag}(\text{masses of the particles}) \; —$$

positive

This means that we can find a "squashing of the coordinates" transformation under which $\underline{\underline{A}} \to \underline{\underline{I}}$ (the identity):

$$\underline{\underline{S}} = \text{"}\underline{\underline{A}}^{-1/2}\text{"} \quad \text{means} \quad \underline{\underline{R}} \; \underbrace{\underline{\underline{R}}^{-1} \underline{\underline{A}} \, \underline{\underline{R}}} \; \underline{\underline{R}}^{-1}.$$

$(= \underline{\underline{S}}^T)$

suitable orthogonal transformation

is diagonal; replace diagonal entries m_α by $1/\sqrt{m_\alpha}$

(Eg. if $\underline{\underline{A}} = \text{diag}(\text{masses})$ then $\underline{\underline{S}} = \text{diag}(1/\sqrt{\text{masses}})$.)

Then $\underline{\underline{S}}^T \cdot \underline{\underline{A}} \cdot \underline{\underline{S}} = \underline{\underline{I}}$.

We use this transformation as follows

inserts

$$\underbrace{\underline{\underline{S}}^T \, \underline{\underline{B}} \, \underline{\underline{S}}}_{\equiv \underline{\underline{B}}'} \, \underbrace{\underline{\underline{S}}^{-1} \, \underline{\underline{Q}}}_{\equiv \underline{\underline{Q}}'} = \omega^2 \, \underbrace{\underline{\underline{S}}^T \, (\underline{\underline{S}}^T)^{-1}}_{= \underline{\underline{I}}} \, \underbrace{\underline{\underline{S}}^T \, \underline{\underline{A}} \, \underline{\underline{S}}}_{\equiv \underline{\underline{A}}'} \, \underbrace{\underline{\underline{S}}^{-1} \, \underline{\underline{Q}}}_{\equiv \underline{\underline{Q}}'}$$

to arrive at the conventional eigenproblem form : $\underline{\underline{B}}' \cdot \underline{\underline{Q}}' = \omega^2 \underline{\underline{Q}}'$.

The characteristic equation for the normal mode frequencies is then, as usual,

$$\det(\underline{\underline{B}}' - \omega^2 \underline{\underline{I}}) = 0 .$$

In terms of $\underline{\underline{A}}$ and $\underline{\underline{B}}$ this reads

$$\det\left(\underline{\underline{S}}^T \cdot (\underline{\underline{B}} - \omega^2 \underline{\underline{A}}) \cdot \underline{\underline{S}} \right) = 0$$

or
$$\det(\underline{\underline{S}}\,\underline{\underline{S}}^T) \cdot \det(\underline{\underline{B}} - \omega^2 \underline{\underline{A}}) = 0 .$$

$\neq 0$ (by positive definiteness of $\underline{\underline{A}}$)

So this factor must vanish

Now on to symmetry considerations

Imagine transforming the coordinates and velocities

$$\underline{q} \to \underline{\underline{D}}(g)\cdot\underline{q},$$
$$\dot{\underline{q}} \to \underline{\underline{D}}(g)\cdot\dot{\underline{q}},$$

where the matrix $\underline{\underline{D}}(g)$ is a representation of the element g of a group G.

If the Lagrangian L is invariant under such a transformation, ie if

$$L(\underline{q},\dot{\underline{q}}) \to L(\underline{\underline{D}}(g)\cdot\underline{q}, \underline{\underline{D}}(g)\cdot\dot{\underline{q}}) = L(\underline{q},\dot{\underline{q}}),$$

$\forall g\in G$ then we say that the Lagrangian (and hence the system) has the symmetry group G.

Under what circumstances does our quadratic Lagrangian have such symmetry? We must have

$$\tfrac{1}{2}\dot{\underline{q}}\cdot\underline{\underline{D}}(g)^T\cdot\underline{\underline{A}}\cdot\underline{\underline{D}}(g)\cdot\dot{\underline{q}} - \tfrac{1}{2}\underline{q}\cdot\underline{\underline{D}}(g)^T\cdot\underline{\underline{B}}\cdot\underline{\underline{D}}(g)\cdot\underline{q}$$
$$= \tfrac{1}{2}\dot{\underline{q}}\cdot\underline{\underline{A}}\cdot\dot{\underline{q}} - \tfrac{1}{2}\underline{q}\cdot\underline{\underline{B}}\cdot\underline{q}$$

ie
$$\left.\begin{aligned}\underline{\underline{D}}(g)^T\cdot\underline{\underline{A}}\cdot\underline{\underline{D}}(g) &= \underline{\underline{A}}\\ \underline{\underline{D}}(g)^T\cdot\underline{\underline{B}}\cdot\underline{\underline{D}}(g) &= \underline{\underline{B}}\end{aligned}\right\}\ \forall g\in G.$$

What would be the consequences of this symmetry?

Suppose that $\underline{Q}$ is a normal mode with frequency ω^2, i.e, $(\underline{\underline{B}}-\omega^2\underline{\underline{A}})\cdot\underline{Q}=\underline{0}$.

Then
$$(\underline{\underline{B}}-\omega^2\underline{\underline{A}})\cdot(\underline{\underline{D}}\cdot\underline{Q}) = \underline{\underline{D}}^{T-1}\underline{\underline{D}}^T(\underline{\underline{B}}-\omega^2\underline{\underline{A}})\cdot\underline{\underline{D}}\cdot\underline{Q}$$
$$= \underline{\underline{D}}^{T-1}(\underbrace{\underline{\underline{D}}^T\underline{\underline{B}}\,\underline{\underline{D}}} - \omega^2\underbrace{\underline{\underline{D}}^T\underline{\underline{A}}\,\underline{\underline{D}}})\cdot\underline{Q} = \underline{\underline{D}}^{T-1}(\underline{\underline{B}}-\omega^2\underline{\underline{A}})\cdot\underline{Q} = \underline{0}$$

ie, $\underline{\underline{D}}(g)\cdot\underline{Q}$ is also a normal mode with frequency ω^2.

What about the issue of degeneracy as a consequence of this symmetry?

Let us suppose that the symmetry is orthogonal, ie, $\underline{\underline{D}}(g)^T = \underline{\underline{D}}(g)^{-1}$.
Then our symmetry reads

$$\left.\begin{aligned} \underline{\underline{A}} \cdot \underline{\underline{D}}(g) &= \underline{\underline{D}}(g) \cdot \underline{\underline{A}} \\ \underline{\underline{B}} \cdot \underline{\underline{D}}(g) &= \underline{\underline{D}}(g) \cdot \underline{\underline{B}} \end{aligned}\right\} \quad \forall g \in G$$

By working in a basis that block-diagonalises $\underline{\underline{D}}(g)$ $(\forall g \in G)$ into irreps and then applying Schur's lemmas we see that in this basis $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are block diagonal, too, with blocks proportional to the identity:

a number

$$\underline{\underline{A}} \rightarrow \begin{pmatrix} a^{(1)} \underline{\underline{I}}^{(1)} & 0 & \cdots \\ 0 & a^{(2)} \underline{\underline{I}}^{(2)} & \\ 0 & 0 & \ddots \\ \vdots & \vdots & \end{pmatrix}$$

and similarly for $\underline{\underline{B}}$

appropriate identity

Thus the eigenproblem becomes block diagonal and algebraic in each block (ie each irrep)

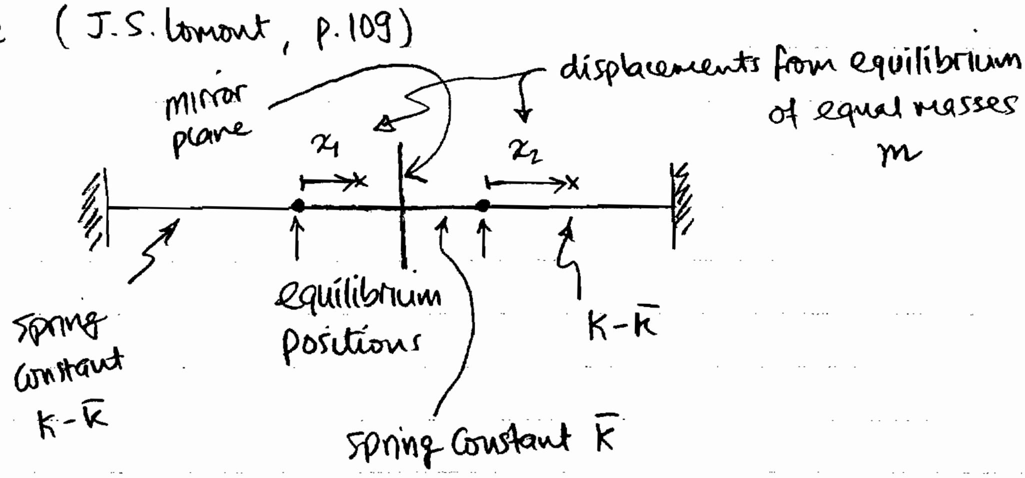
- the value of ω in irrep μ is given by the algebraic equation $b^{(\mu)} = \omega^2 a^{(\mu)}$

  $$\text{ie} \quad \omega^{(\mu)} = \sqrt{b^{(\mu)} / a^{(\mu)}}$$

- all vectors in the invariant subspace μ are eigenvectors (ie normal modes) with frequency $\omega^{(\mu)}$

- any linearly independent set (preferably orthonormal) is invariant subspace μ can be taken as basis eigenvectors (ie basis normal modes).

Example (J.S. Lomont, p.109)



Lagrangian $L = \frac{1}{2} m \dot{x}_1^2 + \frac{1}{2} m \dot{x}_2^2$
$$- \left[\tfrac{1}{2}(k-\bar{k})\, x_1^2 + \tfrac{1}{2}\bar{k}(x_2 - x_1)^2 + \tfrac{1}{2}(k-\bar{k})\, x_2^2 \right]$$

Symmetry: Under $\left.\begin{array}{l} x_1 \to -x_2 \\ x_2 \to -x_1 \end{array}\right\}$ we have $L \to L$

So, with $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \to \underline{\underline{D}}(g) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

we have $\underline{\underline{D}}(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\underline{\underline{D}}(r) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$.

reflection

Together, these form a faithful representation of the abelian group C_2: gp$\{r\}$ with $r^2 = e$

The character of our representation is $\chi(e) = 2$, $\chi(r) = 0$.

The character table for the (2) irreps of C_2 is

C_2	(e)	(r)
$\chi^{(1)}$	1	1
$\chi^{(2)}$	1	-1
χ	2	0

$\frac{1}{\sqrt{2}}(1,+1)$ antisymmetric mode

So $D = D^{(1)} \oplus D^{(2)}$

symmetric mode $\frac{1}{\sqrt{2}}(1,-1)$

no degenerate normal modes

Direct product representations and their decomposition

- Let us suppose that we have two representations of the group G:

$$\psi_j \to \sum_{k=1}^{d_1} D_1(g)_{jk}\,\psi_k \; ; \qquad \phi_j \to \sum_{k=1}^{d_2} D_2(g)_{jk}\,\phi_k$$

for all elements g of G.

Then we may form what is called a product representation, denoted $D_1 \otimes D_2$, which has elements

$$\underbrace{D_1(g)_{j_1 k_1}\; D_2(g)_{j_2 k_2}}_{\text{same element}}$$

which we denote $(D_1 \otimes D_2)(g)_{j_1 j_2,\, k_1 k_2}$

together these constitute the "first" index

the "second" index

Then under $g \in G$ the product basis element $\psi_{j_1}\phi_{j_2}$ transforms as follows

$$\psi_{j_1}\phi_{j_2} \to \sum_{k_1 k_2} (D_1 \otimes D_2)(g)_{j_1 j_2,\, k_1 k_2}\, \psi_{k_1}\phi_{k_2}$$

- As $D_1 \otimes D_2$ constitutes a representation of G (check this), we may ask the question: is this irreducible? In general, the answer is yes:

the irreps of G

$$D_1 \otimes D_2 = \sum_\mu{}^{\oplus} a_\mu\, D^{(\mu)}$$

0, 1, 2, etc

This decomposition is called the Clebsch-Gordan decomposition. It may be effected in the usual way, via orthogonality relations and characters. This idea underlies the theory of angular momentum addition in quantum mechanics.

- In the quantum mechanics setting we have two sources of angular momentum (eg the orbital and spin motion of one particle; two spins; two orbital motions). We have wavefunctions (including spinors) for each source and they transform according to the total angular momentum in each source. We form product wavefunctions to describe the motion of each source of angular momentum. By decomposing this product representation we learn the possibilities for the <u>total</u> angular momentum.

The general rule (ie Clebsch-Gordan series) reads

$$D^{(l_1)} \otimes D^{(l_2)} = \sum_{l=|l_1-l_2|}^{l_1+l_2 \,\oplus} D^{(l)}$$

ie one angular momentum irrep for each angular momentum between $|l_1-l_2|$ and l_1+l_2.

Eg $\quad 1 \otimes 1 = 0 \oplus 1 \oplus 2$

Eg. $\quad 2 \otimes 3 = 1 \oplus 2 \oplus 3 \oplus 4 \oplus 5$

Eg $\quad 1 \otimes (1 \otimes 1) = 1 \otimes (0 \oplus 1 \oplus 2)$

$$= 1 \oplus 0 \oplus 1 \oplus 2 \oplus 1 \oplus 2 \oplus 3 \qquad = (1 \otimes 1) \otimes 1$$

In practice, we almost always consider the decomposition into irreps of product reps themselves formed from irreps. (This is not necessary, but the extension to products formed by reducible reps is straightforward.)

cf Quantum mechanics, in which we usually consider the addition of angular momentum for states that have "sharp" individual angular momenta.

Characters of direct product reps:

The characters for a direct product rep are the products of the characters of the constituent reps

Why? $$\chi^{(D_1 \otimes D_2)} = \sum_{jk} (D_1 \otimes D_2)_{jk,jk}$$
$$= \sum_{jk} (D_1)_{jj} (D_2)_{kk} = \chi^{(D_1)} \chi^{(D_2)}$$

(for any element g of G)

So computing characters in product reps is especially simple.

Decomposition of product reps: the Clebsch-Gordan series:

Take two irreps μ and ν and form the product rep, denoted $D^{(\mu\times\nu)}$. Then we have $\chi^{(\mu\times\nu)}(g) = \chi^{(\mu)}(g)\,\chi^{(\nu)}(g)$.

Now, $D^{(\mu\times\nu)} = \sum_\sigma^\oplus a_\sigma D^{(\sigma)}$ ← the Clebsch-Gordan series

So $\chi^{(\mu\times\nu)} = \sum_\sigma^\oplus a_\sigma \chi^{(\sigma)}$

So, via orthogonality of characters,

$$a_\sigma = \frac{1}{[g]} \sum_{g\in G} \chi^{(\sigma)}(g)^* \, \chi^{(\mu\times\nu)}(g)$$
$$= \frac{1}{[g]} \sum_{g\in G} \chi^{(\sigma)}(g)^* \, \chi^{(\mu)}(g)\, \chi^{(\nu)}(g).$$

the computation of the amplitudes in the Clebsch-Gordan series.

Example: The dihedral group $D_3 = \{c, b\}$ with $c^3 = b^2 = (bc)^2 = e$

The character table is

D_3	E (e)	$2C_3$ (c, c^2)	$3C_2$ (b, bc, bc^2)
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Examples of product reps and their characters

$A_1 \otimes A_1$	$1^2 = 1$	$1^2 = 1$	$1^2 = 1$
$A_2 \otimes E$	$1 \cdot 2 = 2$	$1 \cdot (-1) = -1$	$(-1) \cdot 0 = 0$
$E \otimes E$	4	$+1$	0

By inspection:

$$A_1 \otimes A_1 = A_1$$
$$A_2 \otimes E = E$$

By orthogonality applied to $E \otimes E$:

$$a_{A_1} = \frac{1}{6}\left[(4 \cdot 1) + 2(1 \cdot 1) + 3(0 \cdot 1) \right] = 1$$

$$a_{A_2} = \frac{1}{6}\left[(4 \cdot 1) + 2(1 \cdot 1) + 3(0 \cdot (-1)) \right] = 1$$

$$a_E = \frac{1}{6}\left[(4 \cdot 2) + 2(1 \cdot (-1)) + 3(0 \cdot 0) \right] = 1$$

$$\Rightarrow \quad E \otimes E = A_1 \oplus A_2 \oplus E$$