Lecture 7/ Group theory in quantum mechanics

Literature:

M. S. Dresselhaus, G. Dresselhaus, and A. Jorio

Group Theory: Applications to the physics of condensed matter (available online)

D. Vvedensky, Group Theory, lecture notes of a course at the Imperial College London

www.cmth.ph.ic.ac.uk/people/d.vvedensky/courses.html

Symmetries play important role in quantum mechanics. They provide good "quantum numbers". They may be responsible for level degeneracies.

A standard example is a particle in a centrally symmetric potential. Then the states can be classified according to their angular momentum. For solid state we are interested in the symmetries of the crystal lattice

Group theory

A group is a set of elements with a multiplication operation.

1. If A and B belong to the group then $A \circ B$ also belongs to the group
2. Associativity $(A \circ B) \circ C = A \circ (B \circ C)$
3. Unit element $1 \circ A = A \circ 1 = A$
4. Inverse element: for every A there is A^{-1}: $A \circ A^{-1} = A^{-1} \circ A = \mathbb{1}$

A subgroup is a group within a group (with the same multiplication operation).

E.g. symmetry group of square has subgroup of 90° rotations.

A direct product of two groups G and H is a set of pairs (g, h) with $g \in G$, $h \in H$ and multiplication $(g_1, h_1) \circ (g_2, h_2) = (g_1 g_2, h_1 h_2)$

A group is said to be abelian if for all ellements $A \cdot B = B \cdot A$ and nonabelian otherwise
2 d rotations form an abelian group but
3 d rotations form a nonabelian group.

Conjugation

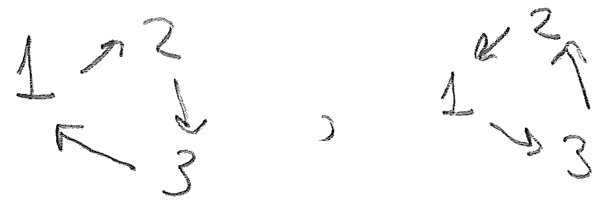
A is conjugate to B if $A = XBX^{-1}$
with some element X. Conjugation preserves the group multiplication: $(XAX^{-1})(XBX^{-1}) = X(AB)X^{-1}$
Thus it is a symmetry of the group

All elements related by conjugation form a class of conjugate elements. They are similar to each other. In 3d all rotations by given angle are conjugate to each other.

Example

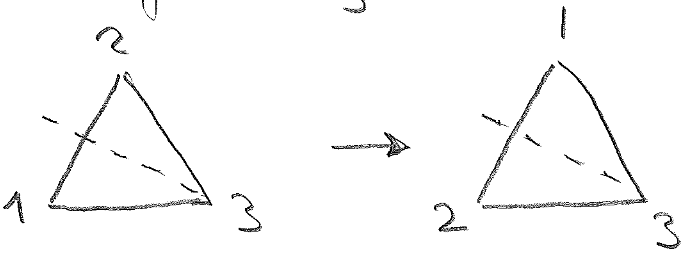
Permutation group for three numbers

It has 6 elements, identity I, pairwise permutations $1 \leftrightarrow 2$, $2 \leftrightarrow 3$, $1 \leftrightarrow 3$, cyclic permutations



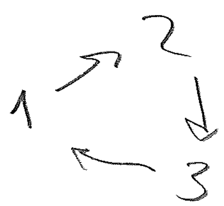
This group is <u>isomorphic</u> (has the same multiplication table) to the symmetry group of the equilatteral triangle D_3

$1 \leftrightarrow 2 \iff$



pairwise permutations $\iff$ 180° rotations about the height of the triangle $\iff$ mirror reflection

cyclic permutations $\iff$ 120° rotations



$\iff$

This group has 3 classes

1. I - identity
2. pairwise permutations
3. cyclic permutations

Indeed

$$(1\to 2)\,(2\to 3)\,(1\to 2)^{-1} = (1\to 2)(2\to 3)(1\to 2) =$$

$$= (1\to 2)(2\to 3)\{2,1,3\} = (1\to 2)\,\{2,3,1\} =$$

$$= \{3,2,1\} = (1\to 3)$$

$$(1\to 2)\,(1\to 2\to 3\to 1)\,(1\to 2)^{-1} = (1\to 2)(1\to 2\to 3\to 1)\{2,1,3\} =$$

$$= (1\to 2)\,\{3,2,1\} = \{2,3,1\} = (1\to 3\to 2\to 1)$$

Basis

Let $\psi_1(x,y,z)$ be some single valued function of x,y,z

Under the group transformation R $\psi_1(\vec{x})$ will go to $\psi_1(Rx) = \psi_2(x)$

If g is the order (number of elements) of the group G after making all g transformation we will get $\psi_1, \psi_2, \dots \psi_g$ functions

Not all of them are independent. For example if for symmetry group of square we will take $\psi_1 = x^2+y^2$ (or x^4+y^4) then we get the same ψ_1 for any symmetry operation

If we take $\psi_1 = x^2-y^2$ then for some operations $x \to -x \Rightarrow \psi_1 \to \psi_1$, but for $x \to y$, $y \to -x \Rightarrow \psi_1 = -\psi_1$. Here, however, we produce just multiplicative factors for ψ_1

In general, we will get some l linearly independent functions that transform through each other. For the same square symmetry functions $\psi_1 = x$, $\psi_2 = y$ form 2 dimensional set of these functions.

We can consider group elements as linear operators acting on sets ψ_i:

$$G\psi_i = \sum_k G_{ki}\psi_k$$

If we choose ψ_i to be orthogonal and normalized than G_{ki} are matrices

These matrices G_{ki} form a <u>representation</u> of the group.

A linear representation of a group G is a set of $n \times n$ matrices $D(G)$ which have the same multiplication table as the group itself. The <u>dimension</u> of representation is the size n of those matrices

If by appropriate change of basis

$$D' = U D U^{-1}$$

with same matrix U (the same for all elements of the group) we can bring a representation to a block-diagonal form

$$D'(G) = \begin{pmatrix} D_1'(G) & 0 \\ 0 & D_2'(G) \end{pmatrix}$$

then the representation is said <u>reducible</u>

$D(G)$ is decomposed to the sum $D_1'(G)$ and $D_2'(G)$

Otherwise, it is called <u>irreducible</u>.

In quantum mechanics physical symmetries are represented by unitary matrices

For any group, there exist a one-dimensional identity representation: matrices 1×1 numbers with $D(G) = 1$. Basis function is the one that does not change under symmetry operation.

Let's find other irreducible representations of $\mathcal{D}(3)$.

Consider a function which is invariant with respect to $120°$ rotation but changes sign under $180°$ flips.

$$\psi(x, y, z) = z$$

This basis function generates another 1d representation with

$$\mathcal{D}\,(\text{cyclic permutations}) = 1$$

$$\mathcal{D}\,(\text{pairwise permutations}) = -1$$

We can construct 2d representation by transforming vector x, y with the elements of the group

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \underset{(2\leftrightarrow 3)}{A} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \underset{(1\to 3)}{B} = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

$$\underset{(1\to 2)}{C} = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad \mathcal{D} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \qquad F = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

1 2 3

1 2 3

A <u>character</u> of a representation $D(G)$ is a trace of the matrix D

$$\chi_D(G) = \operatorname{tr} D(G)$$

Traces are invariant $\Rightarrow$

$\chi_D(G)$ is basis independent

$\chi_D(G)$ is the same for all elements of the class

$\chi_D(I)$ gives the dimension of representation

Unit element is represented by the unit matrix

The character of a sum of representations equals the sums of characters

Character table for D_3

	D_3	I	$2C_3$ $(1 \leftrightarrow 2)$	$3C_2$
1	A_1	1	1	1
z	A_2	1	1	-1
x, y	E	2	-1	0

basis functions

irreducible representation

characters

For any group there are orthogonality relations

<u>Orthogonality of rows</u>

$$\sum_{\alpha} n_\alpha \chi_k(\alpha) \chi^*_{k'}(\alpha) = g \; \delta_{kk'}$$

The sum is over the classes of conjugate elements, n_α - number of elements in the class, g is the total number of elements in the group, k, k' denote two (different or coinciding) representations

<u>Orthogonality of columns</u>

$$\sum_k \chi_k(\alpha) \, \chi_k(\alpha') = \frac{g}{n_\alpha} \delta_{\alpha\alpha'}$$

Here the sum is over irreducible representations

The number of irreducible representations is equal to the number of conjugacy classes.

The sum of squares of dimensions of irreducible representations is equal to the number of elements of the group

$$\sum_k \dim^2(k) = g$$

We do not prove all these relations, see the references.

Character table for the point group of square D_4

D_4		I	$C_2 = C_4^2$	$2C_4$	$2C_2'$	$2C_2''$
$x^2+y^2+\alpha z^2$	A_1	1	1	1	1	1
$xy(x^2-y^2)$	A_2	1	1	1	-1	-1
x^2-y^2	B_1	1	1	-1	1	-1
xy	B_2	1	1	-1	-1	1
(xz, yz) (x, y)	E	2	-2	0	0	0

Irreducible representations in quantum mechanics

If G is the symmetry group of a Hamiltonian H

then $GH = HG$ for all elements of the group

Suppose Ψ_n is an eigenstate of H with energy E_n

Then $G\Psi_n$ will be also an eigenstate with the same energy. Indeed

$$H(G\Psi_n) = GH\Psi_n = GE_n\Psi_n = E_n(G\Psi_n)$$

If we diagonalize the Hamiltonian then the eigenvectors corresponding to the same energy form a representation of G

Dimensionality of a given irreducible representation gives us immediately degeneracy of the corresponding energy level

1-d representations → non-degenerate levels

2-d representation → two-fold degeneracy

etc.

Lifting of degeneracy by perturbation

If $H = H_0 + H_1$

symmetry of the perturbation H_1 is lower than symmetry of H_0

Decomposing representations of H_1 into that of H_0

we find which degeneracy are lifted

Example cubic potential is stretched along the z axis to form tetragonal potential. Cubic group has three dimensional representation with basis functions (x, y, z). For tetragonal symmetry it splits to two-dimensional (x, y) and one-dimensional z. Thus 3 fold degenerate level is split into 2-fold and non degenerate.