Advanced Quantum Mechanics

Rajdeep Sensarma

sensarma@theory.tifr.res.in

Lecture #1

Symmetries and Quantum Mechanics

Ref : J. P. Elliot and P. G. Dawber, Symmetry in Physics
Sakurai, Modern Quantum Mechanics
Landau and Lifshitz, Quantum Mechanics
Michael Artin, Algebra
Serge Lang, Algebra

Basic Structure of QM

$\hbar = 1$

- An isolated quantum system at time t: $|\psi(t)\rangle$, a normalized vector in an abstract Hilbert space over complex no.s.

- Any observable (measurable quantity): a linear Hermitian operator in this Hilbert space. With a choice of basis they can be rep. by matrices.

- A special operator, the Hamiltonian, generates the time evolution of the state through the Schrodinger eqn.

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle$$

- The result of measurement of an observable cannot be predicted, but the possible values of the outcome and the probability of obtaining these values can be predicted if the state of the system is known.

The possible values of an observable are the eigenvalues of the corresponding operator and if an eigenvalue is obtained in a measurement, the state of the system right after the measurement is the corresponding eigenvector of the operator. The probability of obtaining this eigenvalue is

$$A|\lambda\rangle = \lambda|\lambda\rangle \qquad P(\lambda) = |\langle\psi|\lambda\rangle|^2$$

QM in practice

The Hamiltonian generates the dynamics ⟶ eigenstates of the Hamiltonian play imp. role in solving QM problems.

$$H|n\rangle = E_n|n\rangle$$ Expand the state in this basis $$|\psi(t)\rangle = \sum_n c_n(t)|n\rangle$$

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle \to i\dot{c}_n(t) = E_n c_n(t)$$ which gives $$c_n(t) = c_n(0)e^{-iE_n t}$$

A lot of effort is thus spent in finding and cataloguing the properties of Hamiltonian eigenstates

E.g.: If we know the matrix elements of an observable A between energy eigenstates, then the expectation of the observable is given by

$$A(t) = \langle\psi(t)|A|\psi(t)\rangle = \sum_{nn'} c_n^*(0)c_{n'}(0)e^{i(E_n - E_{n'})t}A_{nn'} \qquad A_{nn'} = \langle n|A|n'\rangle$$

Position basis and particle in external potential $\psi(x) = \langle x|\psi\rangle$ ⟶ Wave-function

$$\left[-\frac{\nabla^2}{2m} + V(x)\right]\psi(x) = E\psi(x)$$ ⟶ Schrodinger Wave Equation

QM in Real Systems

To solve a QM problem, we need 2 things: (a) Co-ordinates/Hilbert Space
(b) The Hamiltonian of the system

(a) The Hilbert Space depends both on the system and the things we are interested in

E.g.: A system of atoms can be described in different ways

- For thermal properties of a gas of atoms at low temp. -- neglect internal degrees of an atom and work with spatial co-ordinates of c.o.m. (i.e. free particles)

- For light absorption by atoms, -- neglect motion of atoms and work with the internal states (for H atom work with relative co-ord between e and p).

- For cooling the atoms by shining light on them, i.e. Laser Cooling, we need to worry about both the c.o.m. motion and the internal states of the atom.

E.g.: Seemingly different systems can be described by similar Hilbert space

- A spin 1/2 particle in a magnetic field can be described by a 2-state system.

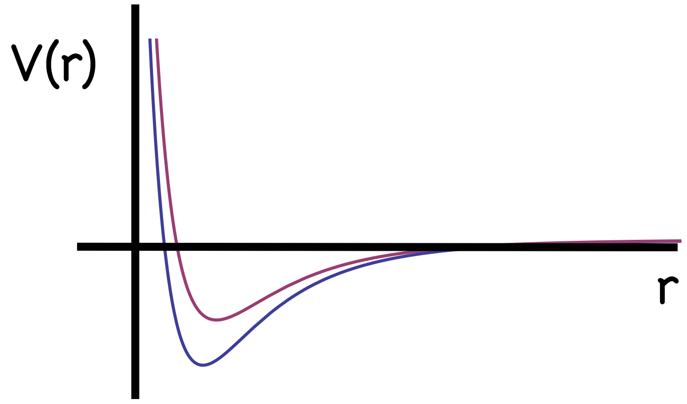
- A double quantum well can also be described by a 2 state system (if we only care about which well the electron is in and not about where it is in each well)

QM in Real Systems

(b) In most interesting cases, we do not know the exact Hamiltonian of the system

Elementary particles: The Standard model seems to describe them well, but people are looking for signatures of beyond Std. Model terms.

Nuclear Physics: Lot of effort spent in getting parameters of nuclear interaction from scattering data.



Atomic Physics: It is usually impossible to know exact form of atom-atom interactions.

Condensed Matter Physics: It is impossible to work with all the details for 10^{23} particles. One uses simpler models to make the problem tractable.

How do we choose models? Are there guiding principles?

If we are interested in low-energy phenomena, some details of the original microscopic Hamiltonian are irrelevant. The formal way of finding out the relevant stuff is called RG, which we will not learn in this course.

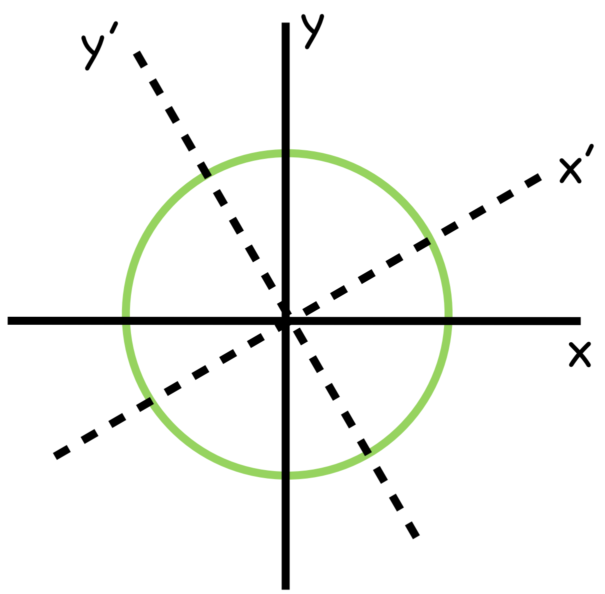
The second guiding principle is the concept of symmetries, which we will learn in some detail.

Shapes and Symmetry

(a) is more symmetric than (b), (c) which is more symmetric than (d)

(b) and (c) have the same symmetry

How do we formalize this?



The circle is defined by $x^2 + y^2 = a^2$

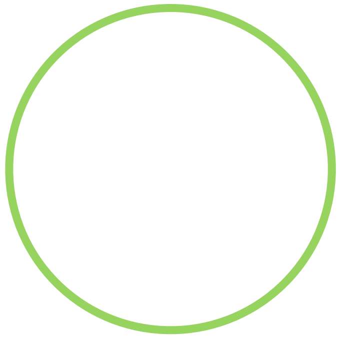
Let us choose new axes (x′,y′) rotated from (x,y) by angle θ

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Eqn. of circle in new co-ord: $x'^2 + y'^2 = a^2$

Core Idea of symmetry: There is a transformation of the ingredients (co-ord in this case) under which the form of something (eqn. defining the shape) remains unchanged. Such transformations would be called symmetry transformations or symmetries.

Shapes and Symmetry



- The circle looks the same under rotn. of axes, thus symmetries are about indistinguishability or about non-observables.
- Symmetries are very good at predicting if some quantity is 0. In this case, the eqn is independent of θ, which suggests (r, θ) as useful co-ord.
- Symmetries are not good for everything, e.g. area of circle etc. still needs to be computed. They are useful guides which constrain the possibilities.

- Rotation of co-ord axes by any angle is a symmetry of (a).
- (b) is symmetric only under rotations by $\pi/2$. Thus symmetry transformations of (b) are subset of those of (a). In this sense (a) is more symmetric than (b).
- Convince yourself that (b) and (c) has same symmetries, i.e. rotn. of axes by $\pi/2$.
- (d) is not invariant under any of this transformations and has the least symmetry of all.

Symmetry and Physical Laws

The physical laws governing a system are usually written as a relation (eqn., diff. eqn. etc) between different quantities (position and time, Electric and Magnetic fields, which are themselves functions of position and time etc.)

An operation on the ingredients of this relation, which keeps the form of the relations invariant is called a symmetry transformation or a symmetry of the system.

This operation could act on position/time, giving rise to spatio-temporal symmetries.

E.g: Newton's laws (for time indep. forces) $\vec{F} = m\ddot{\vec{r}}$ are invariant under t --> -t

The harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$ is invariant under q --> -q

This operation could act on internal co-ordinates giving rise to internal symmetries.

E.g: Maxwell's equations, written in terms of a vector potential A, are invariant under $\vec{A} \to \vec{A} + \nabla\lambda$

Symmetry and Physical Laws

The physical laws governing a system are usually written as a relation (eqn., diff. eqn. etc) between different quantities (position and time, Electric and Magnetic fields, which are themselves functions of position and time etc.)

An operation on the ingredients of this relation, which keeps the form of the relations invariant is called a symmetry transformation or a symmetry of the system.

This operation could be global (i.e. the same operations act on ingredients at all space-time). The corresponding symmetries are called global symmetries

E.g: The Heisenberg model of interacting spins on a lattice $H = -J\sum_{ij} \vec{S}_i \cdot \vec{S}_j$ is invariant under all rotation of all spins by same angle

This operation could be local (i.e. different operations act on ingredients at different space-time). The corresponding symmetries are called gauge symmetries

E.g: Maxwell's equations, written in terms of a vector potential A, are invariant under $\vec{A} \to \vec{A} + \nabla\lambda$

This is a gauge symmetry as different things are added to A at different positions

Symmetry and Physical Laws

The physical laws governing a system are usually written as a relation (eqn., diff. eqn. etc) between different quantities (position and time, Electric and Magnetic fields, which are themselves functions of position and time etc.)

An operation on the ingredients of this relation, which keeps the form of the relations invariant is called a symmetry transformation or a symmetry of the system.

This operation could be discrete.The corresponding symmetries are called discrete symmetries.

E.g: Newton's laws (for time indep. forces) $\vec{F} = m\ddot{\vec{r}}$ are invariant under t --> -t

The harmonic oscillator $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$ is invariant under q --> -q

These operations cannot be carried out in a smooth way.

This operation could be continuous, i.e. the transformations on either space-time or gen. co-ord can be characterized by a set of parameters, which vary continuously. The operations are usually differentiable wrt these parameters.

E.g: Maxwell's equations, written in terms of a vector potential A, are invariant under $\vec{A} \to \vec{A} + \nabla\lambda$

This is a continuous symmetry as $\nabla\lambda$ is characterized by its 3 components, which vary continuously as fn. of space-time.

Symmetry and Quantum Mechanics

*mostly .... see time reversal later

In QM, the eqn. of motion is obtained from the Hamiltonian

$$i\partial_t|\psi\rangle = H|\psi\rangle$$

Transformations that leave the QM Hamiltonian invariant are symmetries of the system.*

- How do symmetry transformations manifest themselves in the Hilbert space?
- How does a state change under a symmetry transform?
- How does a generic QM operator change under a symmetry transform?

We will see that symmetries:

- Predict conserved quantities and provide quantum numbers.
- Predict degeneracies of eigenstates.
- Break up the large Hamiltonian matrix into block-diagonal form.
- Predict that some matrix elements of operators are 0 without calculating them.
- On breaking symmetries perturbatively, predict how the degeneracies will split.

Rather than studying effects of individual symmetries, we will systematically study the relation between symmetries and QM using the language of groups and representation of groups.

Basics of Group Theory

Set: A Set is a collection of objects or entities (no repetition allowed). It is often denoted by S={ a,b,c,...n}. Members of a set are called its elements and this is written as $a \in S$

Eg: Set of students in this class, set of integers, set of students whose name start with A, {Schrodinger, Heisenberg, Bohr, Pauli}, set of all 2 X 2 matrices ....

Group: A Group is a set G together with a binary operation $\circ$, which satisfies:

Closure: If $G_a \in G$ and $G_b \in G$ then $G_c = G_a \circ G_b \in G$

Associativity: $(G_a \circ G_b) \circ G_c = G_a \circ (G_b \circ G_c)$

Identity: There is one element of G, often denoted by E, $G_a \circ E = E \circ G_a = G_a \quad \forall G_a \in G$

This element is called the identity element of the group

Inverse: The inverse of an element is defined by $G_a \circ G_a^{-1} = G_a^{-1} \circ G_a = E \quad \forall G_a \in G$

For all elements, the inverse of the element is in G

- The number of elements in the set, G, is called the order of the group.
- If $G_a \circ G_b = G_b \circ G_a$ the group is called Abelian, otherwise it is called Non-Abelian

Basics of Group Theory

Group: Examples

The following are groups:

- The set {1,-1} with multiplication as combination rule Z_2
- The set {0,1} with a+b (mod 2) as combination rule
- Rotation by 0 and π around a given axis, combination rule is to apply one after the other C_2
- Inversion and doing nothing, these two transformations
- Permutation of 2 objects. The set elements are the specific permutations and not the objects
- The set {i,-i,1,-1} with multiplication as combination rule Z_4
- The set $e^{i\theta}$ with multiplication as combination rule U(1)

Abelian

- Set of all rotations in 3D
- Set of all symmetry operations of an equilateral triangle
- The set of all unitary N X N matrices U(N)
- The set of all orthogonal N X N matrices O(N)
- The set of all unitary N X N matrices with unit Determinant SU(N)
- The set of all orthogonal N X N matrices with unit Determinant SO(N)

Non-Abelian

Basics of Group Theory

Group: Examples

The following are NOT groups:

- The set of all integers forms a group with respect to addition, but not wrt multiplication. The inverse, wrt multiplication is a rational fraction, which is not an integer.

- The set of all integers is not a group wrt subtraction, as subtraction is not associative.

- The set of all Hermitian matrices do not form a group wrt matrix multiplication, since product of Hermitian matrices is not necessarily a Hermitian matrix (closure).

- Set of all N X N orthogonal matrices with Det=-1 (identity does not exist)

- Set of all N X N matrices do not form a group wrt matrix multiplication (Det may be 0 and hence inverse will not exist for all members).

- The set of positive integers is not a group wrt addition (Identity and inverse is not part of the set)

Symmetries and Groups

The set of all symmetry transformations of a Hamiltonian has the structure of a group, with group multiplication equivalent to applying the transformations one after the other

Let G be the set of symmetry transformations G_a which keeps the Hamiltonian invariant.

Closure: If G_a and G_b are transformations which keep H invariant, then applying them one after the other, $G_a G_b[H]=G_a[H]=H$. So $G_a G_b$ is a symmetry transformation of H

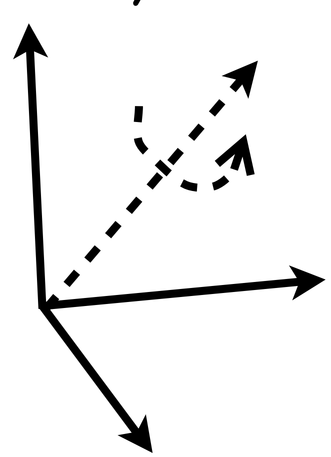
Associativity: Application of symmetry transformations are associative.

Identity: There is always a trivial transformation, where nothing is done to the original co-ordinates. This is the identity element of the group.

Inverse: As long as an inverse transformation exists, it is a symmetry transformation, i.e. it leaves the Hamiltonian invariant. Thus the inverse is part of the set G

Example: Consider a particle moving in a spherically symmetric potential. Rotation about any axis by any angle is a symmetry. The set of all such rotn.s form a group

- 2 rotations result in another rotation --- Closure
- Rotations are associative
- No rotation is the identity element.
- Inverse of a rotation is rotn. about same axis by $-\theta$



Basics of Group Theory

Group Tables

As far as group properties are concerned, individual elements do not matter, what matters is how they combine with each other, i.e. their inter-relations.

For small finite groups, a nice way to visualize this is through Group Multiplication Tables

	1	-1
1	1	-1
-1	-1	1

Group : {1,-1}

	E	R
E	E	R
R	R	E

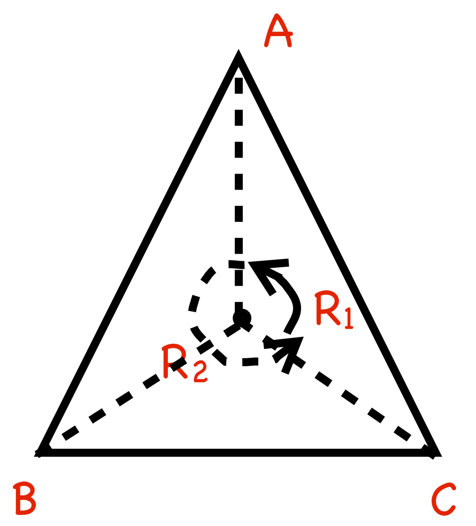
Group : {E,R} ,
E is rotn. by 0,
R is rotn. by π

- Rows and Columns corresponds to elements of the group.
- The entry in each square is the result of applying the column group element after the row group element.
- By convention, the first row/column belongs to the identity element.
- Abelian groups have symmetric multiplication tables

Basics of Group Theory

Group D_3: Symmetries of Equilateral Triangle

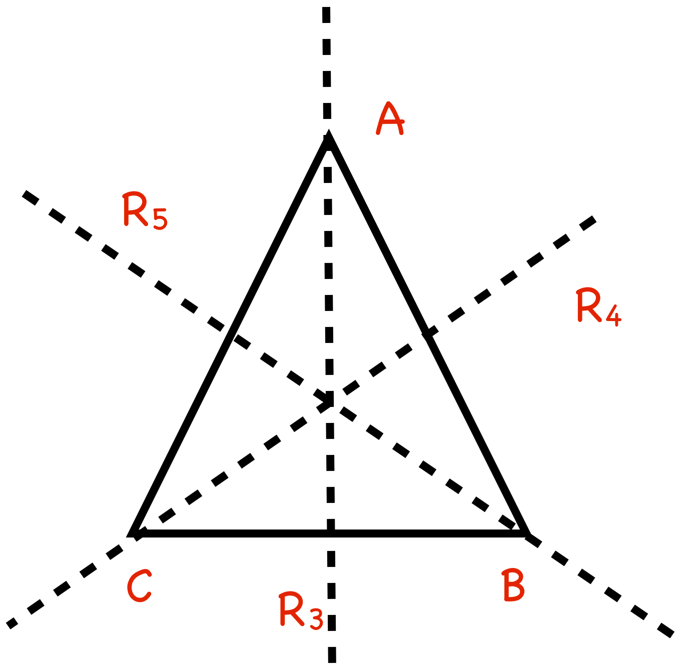
R_1, R_2: rotn. by $2\pi/3$ and $4\pi/3$ about z axis



R_1: A –> B, B –> C, C –> A

R_2: A –> C, B –> A, C –> B

R_3,R_4,R_5: rotn. by π about axes shown through the centroid



R_3: A –> A, B –> C, C –> B

R_4: A –> B, B –> A, C –> C

R_5: A –> C, B –> B, C –> A

Group Tables

	E	R_1	R_2	R_3	R_4	R_5
E	E	R_1	R_2	R_3	R_4	R_5
R_1	R_1	R_2	E	R_4	R_5	R_3
R_2	R_2	E	R_1	R_5	R_3	R_4
R_3	R_3	R_5	R_4	E	R_2	R_1
R_4	R_4	R_3	R_5	R_1	E	R_2
R_5	R_5	R_4	R_3	R_2	R_1	E

$$\{E, R_1, R_2, R_3, R_4, R_5\} = \{R_1^3, R_1, R_1^2, R_3, R_1R_3, R_3R_1\}$$

Could have generated D_3 from R_1 and R_3

Basics of Group Theory

Isomorphism

The important thing about a group is how the elements combine, not what the elements are. This is expressed through the ideas of isomorphism and homomorphism:

If there is a mapping between elements of two groups which preserves group multiplication

$$G_a \to H_a \quad G_b \to H_b \quad G_a G_b = G_c \quad G_c \to H_c \quad H_a H_b = H_c$$

for all pairs of group elements, then the two groups are called isomorphic if the mapping is one-on one and homomorphic if the mapping is not one-on one. Isomorphic groups can be treated as the same group.

Examples of groups which are isomorphic to each other:

All groups with 2 elements are isomorphic to each other (Z_2, inversion, permutation of 2 objects)

The group of 2D rotations and the group U(1)

The group D_3 and the group of permutations of 3 objects (try to show this)

	I	-I
I	I	-I
-I	-I	I

	E	R
E	E	R
R	R	E

If you can show 2 groups are isomorphic then you can translate properties of one to the other

Basics of Group Theory

Subgroups

Subgroup: If G is a group and H is a subset of G, which forms a group with the same group multiplication rule as in G, then H is called a subgroup of G

Examples:

- Z_2 {1,-1} is a subgroup of Z_4 {i,-i,1,-1}
- Z_4 is a subgroup of U(1)
- Set of rotations about the z axis is a subgroup of the set of all rotations
- The symmetries of a square is a subgroup of symmetries of a circle
- Symmetries of a 1D lattice is a subgroup of translation invariance

If a symmetry is broken, say rotational invariance is broken by presence of a lattice, then some symmetries may be left intact. They form a subgroup of the original symmetry group

Direct Product Group: If G and H are two groups whose elements commute, i.e. $G_aH_b=H_bG_a$, and if K is another group whose elements can be uniquely written as $K_a=G_aH_a$, then K is called a direct product group of G and H, K = G X H

If a group is a direct product of other groups, then one can study the properties of the individual symmetry groups and translate this to the properties of the direct product group easily.

e.g. The group O(3) is a direct product of the groups SO(3) (rotations) and inversion. This is also what one means when one says that the standard model has SU(3) X SU(2) X U(1) symmetry