# Lectures on Quantum Mechanics

## Part-B Time Dependent Schrodinger Equation

A course of lectures given at University of Hyderabad

A. K. Kapoor

`http://0space.org/users/kapoor`

akkapoor@cmi.ac.in; akkhcu@gmail.com

# Contents

# §1  Postulates of Quantum Mechanics

## 1  States of physical system

*The state of a quantum mechanical system is represented by a vector in a complex vector space with inner product (Hilbert Space).*

The null vector does not represent any state. Two non-null vectors represent the same state if and only if they are linearly dependent. Thus $|\psi_1\rangle$ and $|\psi_2\rangle$ represent the same state if there exists a complex number $c$ such that

$$|\psi_2\rangle = c|\psi_1\rangle \tag{1}$$

A vector that represents state of physical system will be called state vector. The quantum mechanical states represented by vectors in Hilbert space are called pure states. There are other possible states which are called mixed states. These are represented by a density matrix $\rho$. The density matrix is an operator having properties that it is hermitian and that its eigenvalues are between 0 and 1. A density matrix $\rho$ corresponds to a pure state if and only if $\rho^2 = \rho$.

| For a point particle | the states are represented by a square integrable function $\psi(\vec{r})$ *i.e.* by a function which obeys |
|---|---|

$$\int_{-\infty}^{\infty} |\psi(\vec{r})|^2 \, d^3r < \infty$$

The set of all square integrable function is a Hilbert space. All functions in the Hilbert space except function which is zero everywhere represent a possible state of a point particle.

## 2  Dynamical variables

*The dynamical variables of a physical system are represented by linear operators in the vector space.*

A linear operator representing a dynamical variable must have real eigenvalues and their eigenvectors must form a complete set. These properties are satisfied by self adjoint operators (hermitian operators). So we demand that the dynamical variables be represented by self adjoint operators in Hilbert space. An operator representing a dynamical variable will also be called an observable.

## 3  Probability and average value

*If the system is in a state $|\psi\rangle$, a measurement of dynamical variable $A$ will give one of its eigenvalues $\alpha_k$ with probability equal to $|\langle u_k|\psi\rangle|^2$, where $|u_k\rangle$ is normalised*

*eigenvector of $\widehat{A}$ corresponding to eigenvalue $\alpha_k$.* [1]

A result of any measurement of a dynamical variable is one of the eigenvalues of the corresponding operator. Conversely, every eigenvalue of an observable representing a dynamical variable is a possible result of a measurement of the dynamical variable.

As an example, let $|u_1\rangle, |u_2\rangle, \cdots, |u_n\rangle$ represent the eigenvectors of an observable $\hat{A}$. If the state vector of a physical system, $|u_i\rangle$, is an eigenvector of an operator $\hat{A}$ representing a dynamical variable $A$, a measurement of the dynamical variable gives value $\alpha$ with probability 1. Here $\alpha$ is the eigenvalue of $\hat{A}$ corresponding the eigenvector $|u_i\rangle$. Conversely, if the measurement of $A$ gives the value $\alpha$ with probability 1, the state of system will be represented by a vector which will be eigenvector of the operator $\hat{A}$ corresponding to the eigenvalue $\alpha$.

In general state vector $|\psi\rangle$ will not be an eigenvector of the given dynamical variable. In such a case a measurement of the variable $A$ willIn general state vector $|\psi\rangle$ will not be an eigenvector of the given dynamical variable. In such a case a measurement of the variable $A$ will results in values $\alpha_1, \alpha_2, \cdots, \alpha_n$ with probabilities $c_1|\alpha_2\rangle, c_1|\alpha_2\rangle, \cdots, c_n|\alpha_n\rangle$ where $c_1, c_2, \cdots, c_n$ are the coefficients in the expansion of the state vector $|\psi\rangle$

$$|\psi\rangle = \sum_k c_k |u_k\rangle \tag{2}$$

in terms of eigenvectors of $\hat{A}$. results in values $\alpha_1, \alpha_2, \cdots, \alpha_n$ with probabilities $c_1|\alpha_2\rangle, c_1|\alpha_2\rangle, \cdots, c_n|\alpha_n\rangle$ where $c_1, c_2, \cdots, c_n$ are the coefficients in the expansion of the state vector $|\psi\rangle$

$$|\psi\rangle = \sum_k c_k |u_k\rangle \tag{3}$$

in terms of eigenvectors of $\hat{A}$.

Here $|\psi\rangle$ and $|u_k\rangle$ are assumed to be normalized.

$$\langle\psi|\psi\rangle = 1; \qquad \langle u_k|u_k\rangle = 1, k = 1, 2, \ldots \tag{4}$$

In general, state vector $|\psi\rangle$ will not be an eigenvector of the given dynamical variable. In such a case a measurement of the variable $A$ will results in values $\alpha_1, \alpha_2, \cdots, \alpha_n$ with probabilities $c_1|\alpha_2\rangle, c_1|\alpha_2\rangle, \cdots, c_n|\alpha_n\rangle$ where $c_1, c_2, \cdots, c_n$ are the coefficients in the expansion of the state vector $|\psi\rangle$

$$|\psi\rangle = \sum_k c_k |u_k\rangle \tag{5}$$

---

[1]**Requires modification when eigenvalues of $A$ are degenerate.**

in terms of eigenvectors of $\hat{A}$.

<div style="border:1px solid black; display:inline-block; padding:2px;">Interpretation of Wave Function</div>

For a point particle describe by wave function $\psi(\vec{r})$, the probability of position being in a volume $d^3r$ at position $\vec{r}$, is given by $|\psi(\vec{r})\,d^3r|^2$.

## 4   Canonical quantization

*The operators corresponding to the generalized coordinates and momenta $\{q_k, p_k\}$ of a classical system satisfy*

$$\hat{q}_i\hat{q}_j - \hat{q}_j\hat{q}_i = 0 \tag{6}$$

$$\hat{p}_i\hat{p}_j - \hat{p}_j\hat{p}_i = 0 \tag{7}$$

$$\hat{q}_i\hat{p}_j - \hat{p}_j\hat{q}_i = i\hbar\delta_{ij} \tag{8}$$

The above relations are called **canonical commutation relations**.

| For a point particle | For a **point particle** the action of position and momentum operator on a wave function is given by |

$$\hat{x}_k\psi(\vec{x}) = x_k\psi(x); \qquad \hat{p}_k\psi(\vec{x}) = -i\hbar\partial_k\psi(\vec{x}).$$

## 5   Time evolution

*The time development of a system is governed by the Schrodinger equation*

$$i\hbar\frac{d}{dt}|\psi t\rangle = \hat{H}|\psi t\rangle \tag{9}$$

*where $|\psi t\rangle$ is the state vector of the system at time $t$ and $\hat{H}$ is the operator representing the Hamiltonian of the system.*

| For a point particle | The Hamiltonian operator for **a point particle** is given by |

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}).$$

and the time dependent Schrodinger equation is

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t)$$

# 6  Symmetrization postulate for identical particles

*For a system of identical particles, the state of the system remains unchanged under exchange of a pair of particles, it should be either symmetric or antisymmetric under an exchange of all the variables of the two identical particles.*[2]

---

For a System of Several Identical Point Particles

Let $(m_\alpha, \vec{r}_\alpha), \alpha = 1, 2, \ldots, n$, denote spin and position labels of $n$ identical point particles. Then under exchange of spin and position labels of every pair of pariticles, the wave function of the system must be completely symmetric (completely antisymmetric) for bosons (fermions).

---

[2]**T&C apply**

# §2    Time Dependent Schrodinger Equation

A derivation of Schrodinger equation is presented following Fermi's Lecture on Quantum Mechanics almost verbatim. This was the route taken by Schrodinger to arrive at his now famous equation.

Fermi begins with a comparison of variational principles for particles and waves.

| Point Particle | Waves |
|---|---|
| Mass Point | Wave packet |
| Trajectory | Ray |
| Velocity,$u$ | Group Velocity,$v_g$ |
| | Phase Velocity, (v) |
| Potential Energy $V(x)$ | Refractive Index, |
| | Function of position $n(x)$ |
| Energy $E$ | Frequency $\nu$ |
| | Dispersive medium, $n(\nu, x), v(\nu, x)$ |
| Maupertuis Principle: | Fermat Priniciple: |
| $\int \sqrt{E - V(x)} dx = \min$ | $\int \dfrac{ds}{v(\nu, x)} = \min$ |

**Remark** Note that,for a particle,$\int \sqrt{E - V(x)} dr$ =min,means $\int p dx = \min$ which, for $E = $ const, implies $\int (p dx - H dt) = \min$.

Particles have dual nature, therefore consistency requires that both Maupertuis and Fermat principles should give the same answer. Therefore, we must have

$$\frac{1}{v(\nu, x)} = f(\nu)\sqrt{E - V(x)} \tag{10}$$

Velocity of a point mass is

$$u = \frac{p}{m} = \sqrt{2(E - V(x))/m}. \tag{11}$$

and group velocity, for waves, is given by

$$v_g = \frac{d\omega}{dk} = 1/(\frac{dk}{d\omega}) \tag{12}$$

Note that $v = \nu\lambda, \omega = 2\pi\nu$ and $k = 2\pi/\lambda$,

$$v_g = 1/\frac{d}{d\nu}(1/\lambda) = 1/\frac{d}{d\nu}(\frac{\nu}{v(\nu)}) \tag{13}$$

Thus, for velocity of a mass point, we get

$$\frac{1}{u} = \frac{d}{d\nu}(\frac{v}{v(v,x)}) \tag{14}$$

Velocity of a mass point $u$ corresponds to the group velocity $v_g$ of wave packet. Hence

$$\sqrt{\frac{m}{2}}\frac{1}{\sqrt{E - V(x)}} = \frac{d}{d\nu}(\nu f(\nu)\sqrt{E(\nu) - V(x)}) \tag{15}$$

$$= \frac{d}{d\nu}(\nu f(\nu))\sqrt{E(\nu) - V(x)} + \frac{\nu f(\nu)}{2}\frac{dE(\nu)}{d\nu}\frac{1}{\sqrt{E(\nu) - V(x)}} \tag{16}$$

This equation will be correct for all $x$ and all $V(x)$ if

$$\frac{d}{d\nu}(\nu f(\nu)) = 0 \text{ or } \nu f(\nu) = \text{const,K.} \tag{17}$$

and the coefficient of $\frac{1}{\sqrt{E-V(x)}}$ on both sides are equal:

$$\sqrt{\frac{m}{2}} = \frac{\nu f(\nu)}{2}\frac{dE(\nu)}{d\nu} = \frac{K}{2}\frac{dE(\nu)}{d\nu} \tag{18}$$

$$\Rightarrow \frac{dE(\nu)}{d\nu} = \text{const}, h \Rightarrow E = h\nu + \text{const.}, \tag{19}$$

Setting this last constant to zero gives

$$\boxed{E = h\nu} \tag{20}$$

and Eq.(10) determines the constant $K = \frac{\sqrt{2m}}{h}$. Also $\nu f(\nu) = K$ along with Eq.(1)implies

$$\frac{1}{v(\nu,x)} = \frac{K}{\nu}\sqrt{E(\nu) - V(x)} = \frac{\sqrt{2m}}{h\nu}\sqrt{E(\nu) - V(x)} \tag{21}$$

or

$$\frac{h}{\sqrt{2m(E(\nu) - V(x))}} = \frac{v}{\nu} = \lambda \tag{22}$$

This gives

$$\boxed{\lambda = \frac{h}{p}} \tag{23}$$

**Derivation of Schrdinger Equation** For monochromatic waves

$$\nabla^2 \psi - \frac{1}{v^2}\frac{d^2 \psi}{dt^2} = 0 \tag{24}$$

We set $\psi(x,t) = u(x)e^{-i\omega t}$, assuming $\omega$ to be fixed, using Eq. (13) we get

$$\nabla^2 u(x) + \frac{\omega^2}{v^2}u(x) = 0 \tag{25}$$

$$\Rightarrow \nabla^2 u(x) + \frac{4\pi\nu^2}{h^2\nu^2}(2m(E(\nu) - V(x))u(x) = 0 \tag{26}$$

$$\Rightarrow \nabla^2 u(x) + \frac{2m}{h^2}(E(\nu) - V(x))u(x) = 0 \tag{27}$$

For states with fixed energy, we have

$$E\psi = h\omega\psi \sim ih\frac{\partial\psi}{\partial t}, \tag{28}$$

giving the time dependent Schrdinger equation

$$ih\frac{\partial\psi}{\partial t} = -\frac{h^2}{2m}\nabla^2\psi + V(x)\psi \tag{29}$$

Clap!Clap!

## Remarks:

The highlight of this route is the derivation of de Broglie relation $\lambda = h/p$ and the Einstein relation $E = h\nu$ for point particles by demanding the action principles for matter and waves give the same result.
I thank Bindu Bambah for providing Fermi's Chicago University lecture notes to me. I wish Fermi's Lecture Notes were available to the present generation of students.

# §3   Probability Conservation

## 1   Recall and Discuss

1. Charge conservation in electrodynamics

2. Equation of continuity and local conservation of charge

See Feynman Lectures on Physics Vol-II.

## 2   Point Particle in a Potential Well

We shall discuss some aspects of the Schrodinger equation using the coordinate representation for a particle in a potential $V(\vec{r})$. The classical Hamiltonian, $H_{cl}$, is

$$H_{cl} = \frac{\vec{p}^2}{2M} + V(\vec{r}) \tag{30}$$

The corresponding quantum mechanical operator, $\hat{H}$, in the coordinate representation is obtained by replacement $\vec{p} \to -i\hbar\nabla$ in the classical Hamiltonian. So we have

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 + V(\vec{r}). \tag{31}$$

The Schrodinger equation assumes the form

$$-i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \hat{H}\psi(\vec{r},t) \tag{32}$$

or

$$-i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = \frac{1}{2M}\nabla^2\psi(\vec{r},t) + V(\vec{r},t)\psi(t). \tag{33}$$

## 3   Equation of Continuity

Consider motion of a particle in a potential well $V(\vec{r})$. The time dependent Schrödinger equation is

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi(\vec{r},t) \tag{34}$$

Taking complex conjugate we get (assuming the potential to be real $V(\vec{r})^* = V(\vec{r})$

$$-i\hbar\frac{\partial\psi^*(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^*(\vec{r},t) + V(\vec{r})\psi^*(\vec{r},t) \tag{35}$$

If we multiply Eq.(34) by $\psi^*(\vec{r},t)$ and Eq.(35) by $\psi(\vec{r},t)$ and subtract, the potential terms cancel, and we get

$$i\hbar\psi^*(\vec{r},t)\frac{\partial}{\partial t}(\vec{r},t) + i\hbar\psi(\vec{r},t)\frac{\partial}{\partial t}\psi^*(\vec{r},t) = -\frac{\hbar^2}{2m}[\psi^*(\vec{r},t)\vec{\nabla}^2\psi(\vec{r},t) - \psi(\vec{r},t)\vec{\nabla}^2\psi^*(\vec{r},t)] \tag{36}$$

Eq.(36) can be written as

$$i\hbar\frac{\partial}{\partial t}\{\psi^*(\vec{r},t)\psi(\vec{r},t)\} = -\frac{\hbar^2}{2m}\vec{\nabla}[\psi^*(\vec{r},t)\vec{\nabla}\psi(\vec{r},t) - \psi(\vec{r},t)\vec{\nabla}\psi^*(\vec{r},t)] \qquad (37)$$

To see this expand, the right hand side of Eq.(37). It will give four terms, two of which cancel giving the right hand side of Eq.(36). We define

$$\rho = \psi^*(\vec{r},t)\psi(\vec{r},t) = |\psi(\vec{r},t)|^2 \qquad (38)$$

$$\vec{j} = -\frac{i\hbar}{2m}\left(\psi^*(\vec{r},t)\vec{\nabla}\psi(\vec{r},t) - \psi^*(\vec{r},t)\vec{\nabla}\psi(\vec{r},t)\right) \qquad (39)$$

With $\rho$ and $\vec{j}$ defined as in (38) and (39), Eq.(37) can be written as

$$\frac{\partial\rho}{\partial t} = -\vec{\nabla}.\vec{j} \qquad (40)$$

or

$$\frac{\partial\rho}{\partial t} + \vec{\nabla}.\vec{j} = 0 \qquad (41)$$

## 4   Analogy with Electrodynamics

This equation is called the equation of continuity. In electrodynamics a similar relation holds between *charge density* ($\rho$) and *current density* ($\vec{j}$) and it represents conservation of total charge. Here, in quantum mechanics, $\rho = |\psi|^2$ represents probability density and therefore $\vec{j}$ is called probability current density. As a consequence of Eq.(41), the total probability $\int_{-\infty}^{\infty}|\psi|^2d\vec{r}$ is independent of time. To see this we integrate (41) over a volume $V$ enclosed by a surface $S$ to get

$$\frac{\partial}{\partial t}\int_V \rho d^3x = -\int_V \vec{\nabla}.\vec{j}\, dV$$
$$= -\int_S (\vec{j}.\hat{n})\, dS \qquad (42)$$

where $\hat{n}$ is the unit vector perpendicular to the surface. If $V$ represents volume of a sphere of radius $R$, $S$ will be the surface of the sphere. The surface area increases as $R^2$ when $R$ becomes very large. If $\vec{j}$ decreases faster than $1/R^2$, as $R \to \infty$, the right hand side of (42) becomes zero when $R \to \infty$. The left side becomes integral over all space and we get

$$\frac{\partial}{\partial t}\iiint_{-\infty}^{\infty} \rho\, d^3x = 0 \qquad (43)$$

Therefore the norm

$$\iiint_{-\infty}^{\infty} \psi^*(x,t)\psi(x,t)\, d^3x = (\psi,\psi) = \|\psi\|^2 \qquad (44)$$

is independent of time and (41) represents conservation of total "norm" and is a consequence of the fact $\hat{H}$ is a hermitian operator. While Eq.(43) representing the conservation of total probability follows from (41), (41) is, in fact, a stronger equation, it represents a local conservation law.

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.\vec{j} = 0$$

| Electrodynamics | Quantum Mechanics |
|---|---|
| $\rho$ = charge density | Probability density |
| $\vec{j}$ = (charge) current density | Probability current density |
| $\int_V \rho d\vec{r}$ = charge in volume $V$ | Probability of finding particle in volume $V$. |
| $\int_S \vec{j}.\hat{n}dS$ current through $S$; charge flowing out of $S$ per unit time | Probability that the particle crosses the surface in unit time. |

## 5  Probability density and current density for plane waves

The physical interpretation of the probability current density can be seen by evaluating it for plane waves

$$\begin{aligned} \psi(\vec{r}) &= N\exp(ipx/\hbar) \\ \rho = |N|^2 \qquad \vec{j} &= |N|^2\vec{p}/m = |\bar{N}|^2\vec{v} = \rho\vec{v} \end{aligned} \qquad (45)$$

The expression (11) for $\vec{j}$ is similar to that for the current density ($\vec{j} = \rho\vec{v}$) in the electromagnetic theory. This expression for $\vec{j}$ can be understood in classical terms if we interpret $\rho$ as number density of particles, then the flux of the beam can be expressed in terms of $\vec{j}$. To see this let us consider a beam of particles incident on a small surface of area $\Delta S$, see Fig.4 below. The number of particles crossing $\Delta S$ in time $\Delta t$ equals the number of particles in a cylinder of height $|\vec{v}|\Delta t$, base $\Delta S$, and having its axis parallel to the velocity $\vec{v}$ of the particles. The volume of the cylinder is given by $\Delta S \cdot \cos\theta(|\vec{v}|\Delta t)$, where $\theta$ is the angle between the velocity $\vec{v}$ and the normal to the surface $\Delta S$. If the number density of the particles is $\rho = |N|^2$, the number of particles in cylinder $= |N|^2\Delta S(\cos\theta)|\vec{v}|\Delta t = \vec{j} \cdot \vec{n}\Delta S\Delta t$. This is the number of particles crossing the surface $\Delta S$ in time $\Delta t$. Thus the flux of particles, defined as the number of particles of the incident crossing a surface per unit area per unit time can be written as $\vec{j} \cdot \vec{n}$

Fig. 4
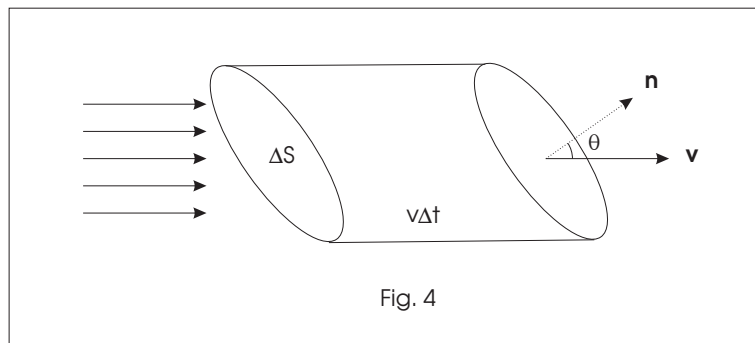
In the above we interpreted $\rho$ as the number density of particles in the beam and concluded that $\vec{j}.\vec{n}$ gives the number of particles crossing a unit area in unit time. For a single particle, $\rho$ has the interpretation of being probability density, and hence $\vec{j}$ will called the probability current density.

# 6   Points to remember

✍ The equation of continuity $\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0$ where

$$\rho(\vec{r}, t) = |\psi(\vec{r}, t)|^2; \qquad \vec{j}(\vec{r}, t) = \frac{\hbar}{2im}\left(\psi^*(\vec{r}, t)\nabla\psi(\vec{r}, t)\right) - \psi(\vec{r}, t)\nabla\psi^*(\vec{r}, t)$$

follows from the time dependent Schrodinger equation.

✍ The equation of continuity implies probability conservation which means that $\iiint_{-\infty}^{\infty} |\psi(\vec{r}, t)|^2$ is independent of time.

✍ We can multiply the wave function by any constant that does not depend on time.

✍ For a beam of particles, for example in scattering experiments, $\rho$ can be interpreted as the number density of particles at position $\vec{r}$. Then $\vec{j}$ has the interpretation of intensity of the beam, *i.e.* the number of particles incident per unit area per unit time.

# §4 Solving Time Dependent Schrodinger Equation

## §1 Recall and Discuss

- The method of separation of variables for partial differential equations.

- If $y_1, y_2, \ldots$ are solutions of a linear partial differential equation, their superposition $c_1 y_1 + c_2 y_2, \ldots$ is also a solution.

## §2 Point particle in a time independent potential

We assume that the Hamiltonian of the particle is independent of time and that it can be written in the form

$$H = \frac{p^2}{2m} + V(\vec{r}) \tag{46}$$

The Schrodinger equation for the particle moving in potential $V(\vec{r})$ can be written as

$$\vec{r} - i\hbar \frac{\partial \psi(t)}{\partial t} = \frac{1}{2M} \nabla^2 \psi(t) + V(\vec{r})\psi(t). \tag{47}$$

The possible states of the particle at a time $t$ will be represented by square integrable wave function wave function $\psi(\vec{r}, t)$.

## §3 Solution by separation of variables

When time does not appear in the Hamiltonian of a system, the equation of motion can be solved by the method of separation of variables. Thus by substituting

$$\psi(\vec{r}, t) = u(\vec{r})T(t) \tag{48}$$

in Eq.(47) we get

$$i\hbar \frac{1}{T(t)} \frac{dT(t)}{dt} = \hat{H} u(\vec{r}) \tag{49}$$

Equating each side to a constant, say $E$ we get two equations for $u(\vec{r})$, and for $T(t)$, as follows.

$$i\hbar \frac{d}{dt} T(t) = ET(t) \tag{50}$$

$$\hat{H} u(\vec{r}) = E u(\vec{r}) \tag{51}$$

## §4   Eigenfunctions of energy are required

From (51) we see that we need to solve for eigenvalues and eignefunctions of energy. Let $u_1(\vec{r}), u_2(\vec{r}), ...$ denote the eigenvectors of the Hamiltonian $\hat{H}$ with the eigenvalues $E_1, E_2, ...,$ respectively.

$$\hat{H}u_k(\vec{r}) = E_k u_k(\vec{r}); \qquad k = 1, 2, 3, ... \tag{52}$$

Eq.(50) and Eq.(51) have solutions given by

$$T_k(t) = \text{const} \times \exp(-iE_k t/\hbar), \qquad H u_k(\vec{r}) = E_k u_k(\vec{r}) \tag{53}$$

and (47) has *an infinite number of solutions*, one for each real $k$, given by

$$\phi_k(\vec{r}, t) = u_k(\vec{r}, t) \exp(-iE_k t/\hbar) \tag{54}$$

## §5   Most general solution of TDSE

The most general solution is a linear combination of solutions
$\phi(x) = \sum_n c_n u_n(x)$,
$\phi_k(\vec{r}, t)$ in Eq.(54) and is given by

$$\psi(\vec{r}, t) = \sum_{k=1}^{\infty} c_k u_k(\vec{r}) \exp(-iE_k t)/\hbar. \tag{55}$$

## §6   Solution of initial value problem

If the wave function at time $t_0$, is $\psi(\vec{r}, t_0) \equiv \psi_o(\vec{r})$, the expression (55) evaluated at $t = t_0$ gives

$$\psi_0(\vec{r}) = \sum_{k=1}^{\infty} c_k u_k(\vec{r}) \exp(-iE_k t_0)/\hbar \tag{56}$$

Using the orthogonality of energy eigenfunctions, we can find the coefficients $\alpha_k$ and are given by.

$$(u_k, \psi_0) = c_k \exp(-iE_k t_0)/\hbar \tag{57}$$

and the knowledge of the coefficients $c_k$ allows us to compute the wave function at time $t$ from (55). The final answer for the wave function at time $t$ is given by

$$\psi(\vec{r}, t) = \sum_{k=1}^{\infty} c_k u_k(\vec{r}) \exp(-iE_k t)/\hbar \psi(\vec{r}, t) = \sum_{k=1}^{\infty} (u_k, \psi_0) \exp(-iE_k (t - t_0)/\hbar) \, u_k(\vec{r}) \tag{58}$$

$\psi_0$ is the wave function of the system at time $t_0$.

## §7   Points to remember

✍ If energy eigenvalues and eigenfunctions of the Hamiltonian are $E_n, u_n(x)$:

$$Hu_n(x) = E_n u_n(\vec{r}), \quad n = 1, 2, 3, \ldots$$

then solutions of the time dependent Schrodinger equation are given by

$$\psi_n(\vec{r}, t) = u_n(\vec{r})e^{-iE_n t/\hbar}, n = 1, 2, 3, \ldots$$

and the most general solution of the time dependent Schrodinger equation is a superposition of solutions $\psi_n$ given by

$$\Psi(\vec{r}, t) = \sum_n c_n \psi_n(\vec{r}, t).$$

✍ Suppose the wave function of a system is given at time to be some function$\phi(x)$ and we need to find the wave function at time $t$. Then expand $\phi(\vec{r})$in terms of energy eigenfunctions :

$$\phi(\vec{r}) = \sum_n c_n u_n(\vec{r}),$$

where the expansion coefficients $c_n$ can be found by using the orthogonality property of functions $u_n(\vec{r})$ and we have $c_n = (u_n, \phi) = \int_{-\infty}^{\infty} u_n^*(\vec{r})\phi(\vec{r})d^3r$ Then the wave function at time $t$ is given by

$$\phi(x) = \sum_n c_n u_n(\vec{r})e^{-iE_n t/\hbar}. \tag{59}$$

# §5   Free Particle Energy Eigenfunctions

## §1   Recall and Discuss

The differential equation

$$\frac{d^2y}{dx^2} + \mu y = 0 \tag{60}$$

has two linearly independent solutions.

**Case $\mu > 0$:**   we write $\mu = k^2 > 0$ and we take the solutions as: $\sin kx, \cos kx$. and general solution for a given $k$ is a linear combination

$$y(x) = A \cos kx + B \sin kx.$$

We can also take two linearly independent solutions to be $e^{ikx}, \quad e^{-ikx}$ and write a general solution as

$$y(x) = A e^{ikx} + B e^{-ikx}.$$

**Case $\mu < 0$:**   we write $\mu = -\alpha^2$ and take the solutions as: $e^{\alpha x}, e^{-\alpha x}$. A general solution will be written as $y(x) = A e^{\alpha x} + B e^{-\alpha x}$.

## §2   Free particle in one dimension

The classical Hamiltonian for a free particle in one dimension is

$$H_{\text{cl}} = \frac{p^2}{2m}. \tag{61}$$

The corresponding operator $\hat{H}$ in coordinate representation is given by using $p \to \hat{p} = -i\hbar\frac{d}{dx}$

$$\hat{H} = -\frac{1}{2m}\frac{d^2}{dx^2} \tag{62}$$

and the energy eigenvalue equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x). \tag{63}$$

**No solution exists for $E < 0$.**   We shall now show that the energy eigenvalue problem has no solution for $E < 0$.
For $E < 0$, we define $\alpha^2 = -\frac{2mE}{\hbar^2} = \frac{2m|E|}{\hbar^2}$ and rewrite the differential equation (63) in the form

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi(x) = 0, \tag{64}$$

which has most general solution

$$\psi(x) = Ae^{\alpha x} + Be^{-\alpha x}, \qquad \alpha = \sqrt{\frac{2m|E|}{\hbar^2}} \tag{65}$$

In order that the eigenfunction does not blow up for $x \to \infty$, we must demand $A = 0$. Similarly, demanding that the solution remains finite as $x \to -\infty$ gives $B = 0$. These values together imply that the free particle wave function vanishes everywhere. This does not represent a physical state and is therefore unacceptable. Thus we arrive at the conclusion that $E < 0$ is not possible.

**Solution for $E > 0$:** For $E > 0$, we define $k$ by $k^2 = 2mE/\hbar^2$ and write the eigenvalue equation as

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \tag{66}$$

and its most general solution is given by

$$\psi_k(x) = Ae^{ikx} + Be^{-ikx}, \qquad k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{67}$$

Here $A, B$ are *complex constants*.

**Energy values are doubly degenerate**  There is no restriction on $k$ and hence all positive energies are allowed. For each value of energy there are two solutions

$$\psi_k(x) = e^{ikx}, e^{-ikx} \tag{68}$$

which correspond to momentum eigenvalues $\hbar k, -\hbar k$ and represent the particle moving to the right and left, respectively.

It must be noted that two linearly independent eigenvectors of energy can be written in several ways. A particularly interesting form of solutions is

$$\psi(x) = \sin kx, \cos kx. \tag{69}$$

In contrast with solutions in (68), the above solutions are not eigenfunctions of momentum.

**Normalisation**  For $E > 0$ the eigenfunctions are not square integrable and hence cannot be normalized. For solutions of eigenvalue problem for continuous eigenvalue one generally uses delta function normalization which for the present case reads

$$\int_{-\infty}^{\infty} \psi_{E_1}^*(x)\psi_{E_2}(x)\, dx = \delta(E_1 - E_2), \tag{70}$$

## §3   Free particle in three dimensions

It can again be shown that there are no solutions for $E < 0$. The free particle solution in three dimensions corresponding to energy eigenvalue $E > 0$ are given by

$$u_E(x, y) = N \exp(ik_1 x + ik_2 y + ik_3 z) \tag{71}$$

where

$$E = \frac{\hbar^2 k^2}{2m}, \qquad k^2 = k_i^2 + k_2^2 + k_3^2 \tag{72}$$

and $k_1, k_2, k_3$ are otherwise arbitrary. If we write $\vec{k} = k\,\hat{n}$, where $\hat{n} = (\vec{k}/k)$ is a unit vector, the solution $u_E(x, y, z)$ can be written as

$$u_E(x, y, z) = N \exp(i\vec{k} \cdot \vec{r}) = N \exp(ik\,\hat{n} \cdot \vec{r}). \tag{73}$$

Here $\hat{n}$ denotes the direction of $\vec{k}$.

## §4   Energies have infinite degeneracy in higher dimension

The energy eigenfunctions in (73) are also eigenfunctions of momentum operator with eigenvalue $\vec{p} = \hbar\vec{k}$.

For a fixed energy there are infinite number of energy eigenfunctions. Fixing energy fixes only absolute value, $k = |\vec{k}|$, of vector $\vec{k}$. There is one solution corresponding to each direction of momentum.

One can impose a delta function normalisation or periodic boundary conditions with box normalisation on the free particle eigenfunctions. Similar results hold for a free particle in two dimensions.

## §5   Points to remember

✐ There are no solutions for $E < 0$. There are two linearly independent solutions in one dimensions for all $E > 0$.

✐ The energy eigenfunctions can be written in several forms. In one dimension we van write, for example

   (a) $\sin kx, \quad \cos kx, \quad k > 0$;      (b) $e^{ikx}, e^{-ikx}, \quad k > 0$.

A useful way to describe all free particle solutions is $e^{ikx}, -\infty < k < \infty$. These are eigenfunctions of momentum ( eigenvalue=$\hbar k$). With similar expressions in two and three dimensions. So for example in 3 dimensions

$$u_{\mathbf{k}}(x) = e^{i\vec{k}\cdots\vec{r}},$$

Here $\vec{k} = (k_1, k_2, k_3)$ can take all possible values.

# §6  Particle in a Box

## §1  Recall and Discuss

Solution of differential equation $\frac{d^2y}{dx^2} + k^2 y = 0$ can be written as $\sin kx$ and $\cos kx$ and general solution is a linear combinations

$$y(x) = A \cos kx + B \sin(kx).$$

## §2  Box in one dimension

The energy levels of a particle in one dimensional infinite well

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ \infty & \text{outside} \end{cases} \tag{74}$$

can be found by solving the Schrödinger equation for $0 \leq x \leq L$, where the particle is like a free particle and the solution is given by

$$u(x) = A \sin kx + B \cos kx, \qquad k^2 = \frac{2mE}{\hbar^2}. \tag{75}$$

Out side the box, the potential is infinity and the solution vanishes:

$$u(x) = 0, \qquad \text{if } x < 0, \text{ or } x > L. \tag{76}$$

**Impose boundary conditions**   The boundary conditions to be imposed on the solution are

$$u(0) = u(L) = 0, \tag{77}$$

and no restriction on the derivatives at the boundary points $x = 0, x = L$. This gives

$$u(0) = 0 \quad \Rightarrow \quad B = 0, \tag{78}$$
$$u(L) = 0 \quad \Rightarrow \quad \sin kL = 0. \tag{79}$$

The solutions of this equation are $k_n = n\pi/L, n = 1, 2, \ldots$. The energy levels are given by

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{80}$$

and the corresponding wave functions are

$$u_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \leq x \leq L \\ 0 & x < 0 \text{ or } x > L. \end{cases} \tag{81}$$

*It should be noted that for $k = 0$ the solution vanishes identically and therefore $n = 0$ is unacceptable. The solutions for negative integral values of $n$ coincide, up to an overall constant, with those for positive $n$. Therefore (81) with $n$ equal to positive integral values gives all independent solutions.*

## §3   Particle in cubical box

A potential representing three cubical dimensional box of side $L$ can be written as

$$V(x, y, z) = \begin{cases} 0 & \text{inside the box} \\ \infty & \text{outside the box} \end{cases} \tag{82}$$

For simplicity we choose one corner of the box at the origin and take the coordinates of the diagonally opposite corner at $(L, L, L)$.

The wave function will be zero outside the box. Inside the box, for positive energies, the Schrodinger equation

$$-\frac{\hbar^2}{2m}\nabla^2 u(x, y, z) = Eu(x, y, z) \tag{83}$$

can be solved by writing

$$u(x, y, z) = f(x)g(y)h(z). \tag{84}$$

and separating the variables in Cartesian coordinates. This give three equations of the same type as particle in one dimensional box.

$$\frac{d^2 f(x)}{dx^2} + E_1 f(x) = 0; \quad \frac{d^2 g(y)}{dy^2} + E_2 g(y) = 0 \quad \frac{d^2 f(z)}{dz^2} + E_3 f(z) = 0 \tag{85}$$

The answers can be written down following the solution for the one dimensional rigid box problem. There is no solution for negative $E_1, E_2, E_3$. For positive $E_1, E_2, E_3$ the solutions vanishing at the boundaries are given by

$$f(x) = \sin(n_1\pi x/L); \quad g(y) = \sin(n_2\pi y/L); \quad h(z) = \sin(n_3\pi z/L); \tag{86}$$

The total energy eigenvalues are given by

$$E = E_1 + E_2 + E_3 = \frac{(n_1^2 + n_2^2 + n_3^2)\hbar^2}{2mL^2} \tag{87}$$

and the normalized energy eigenfunctions are given by

$$u_{n_1,n_2,n_3}(x, y, z) = \sqrt{\frac{8}{L^3}} \sin(n_1\pi x/L) \sin(n_2\pi y/L) \sin(n_3\pi z/L) \tag{88}$$

Here $n_1, n_2, n_3$ are positive integers. It is easy to see that the many ground state corresponding to $n_1 = n_2 = n_3 = 1$ is non-degenerate. The excited states are all degenerate. For example, the first excited state has energy $E_1 = \frac{6\hbar^2}{2mL^2}$ and has three linearly independent wave functions corresponding to combinations corresponding to the following values of $n_1, n_2, n_3$

(i) $n_1 = 2, n_2 = 1, n_3 = 1$;(ii) $n_1 = 2, n_2 = 1, n_3 = 1$;(iii)$n_1 = 2, n_2 = 1, n_3 = 1$;

✍ The energy eigenfunctions in one dimensional $(0, L)$ box are

$$E_n = \frac{n^2 h^2}{8ml^2}, u_n(x) = \sin(n\pi x/L), n = 1, 2, 3, \ldots$$

✍ For any box in one dimension of length $L$, such as $(-L/2, L/2)$, or $(L, 2L)$, the energy eigenvalues will be the same as above; however the eigenfunctions will be a linear combinations of $\sin(n\pi x/L)$ and $\cos(n\pi x/L)$.

✍ The bound states for one dimensional box are non-degenerate.

✍ For a cubical box with diagonally opposite corners at the origin and at $(L, L, L)$ the energy eigenvalues and eigenfunctions can be given by

$$
\begin{aligned}
E_n &= \frac{\hbar^2 k^2}{2m}, & k^2 = k_1^2 + k_2^2 + k_3^2 = \hbar^2 k^2(n_1^2 + n_2^2 + n_3^2), & \quad (89) \\
u_E(x, y) &= N \sin(n_1\pi x/L) \sin(n_2\pi y/L) \sin(n_3\pi z/L); & & \quad (90)
\end{aligned}
$$

The excited states are, in general degenerate.

# §7   Motion of Wave Packets

## §1   Goals

1. In this lesson you will learn an example of finding wave function at time $t$ when the wave function at time $t = 0$ is given. We are doing as an illustrate the case when the energy eigenvalues are nondegenerate.

2. The energy eigenfunctions describe a plane wave extending all over space. The probability density is same everywhere *it is independent of position.* This does not correspond to particle with a well defined position.

3. The classical equations (free particle) of motion hold for averages $\langle x(t) \rangle, \langle p(t) \rangle$; see Eqs. (105) and (106). These equations are examples of Ehernest theorem [3].

4. You will also learn that uncertainty in position increase with time.

## §2   Recall and Discuss

Solving time dependent Schrodinger equation requires

- solving for energy eigenfunctions,

- writing most general solution as a superposition of states with definite energy. This introduces some unknown coefficients or functions used to form superposition.

- using the given wave function at time $t = 0$, we can fix the expansion coefficients using orthogonality properties of the energy eigenfunctions.

  To form a wave function that represents a localized particle, we need to form a superposition of states different position values. We start one such wave function and find its time evolution and compare answers for average position with classical position as function of time.

## §3   Motion of a Wave Packet

**Problem 1:** Find the wave function of a particle at time $t$ if its initial wave function at time $t = 0$ is given to be

$$\psi(x,t)|_{t=0} = (2\pi\Delta^2)^{-\frac{1}{4}} \exp\left( -(x - x_0)^2/4\Delta^2 + ip_0 x/\hbar \right). \tag{91}$$

---

[3]To be discussed in a later lecture

**Solution**    To find the wave function at time $t$, we need to solve the time dependent Schrodinger equation

$$i\hbar\frac{\partial \psi(x,t)}{\partial t} = H\psi(x,t). \tag{92}$$

subject to initial wave function at time $t = 0$ given by (91) and where $H$ is the free particle Hamiltonian,

$$H = \frac{p^2}{2m} \rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}. \tag{93}$$

To find the wave function at time $t$ we proceed as follow.

1. The Hamiltonian for a free particle is time independent, and (92) can be solved by separation of variables. Substituting

$$\psi(x,t) = T(t)u(x)$$

   gives equations

$$i\hbar\frac{dT(t)}{dt} = ET(t), \qquad Hu(x) = Eu(x). \tag{94}$$

2. Next we note that the eigenfunctions of the Hamiltonian, and for a free particle these are given by plane waves

$$u_k(x) = e^{ikx}, \qquad -\infty < k < \infty. \tag{95}$$

   and have energy $E_k = \frac{\hbar^2 k^2}{2m}$.

3. This gives us the following solutions of time dependent Schrodinger equation

$$\psi_k(x,t) = u_k(x,t)e^{-iE_k t/\hbar}, \quad \text{where} \quad E_k = \frac{\hbar^2 k^2}{2m} \tag{96}$$

   Here $k$ takes all real values. The most general solution of the time dependent Schrodinger equation is then given by a superposition of solutions $\psi_k(x,t)$

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k)\psi_k(x)\,dk = \int_{-\infty}^{\infty} \phi(k)u_k(x,t)e^{-iE_k t/\hbar}\,dk \tag{97}$$

4. Here in (97) the superposition 'coefficients', $\phi(k)$, can be fixed by using the given form of the wave function at time $t = 0$

$$\Psi(x,0) = \int_{-\infty}^{\infty} \phi(k)e^{ikx}\,dk. \tag{98}$$

   Therefore the superposition coefficients $\phi(k)$ are computed by taking the inverse Fourier transform and are given by

$$\phi(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x,0)e^{-ikx}\, dx \tag{99}$$

$$= (2\pi\Delta^2)^{-\frac{1}{4}} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \exp\left(-(x-x_0)^2/4\Delta^2 + ip_0x/\hbar\right). dx \tag{100}$$

5. The wave function $\Psi(x,t)$, at time $t$, is obtained by supplying a factor $\exp(-iEt/\hbar)$ with the plane wave inside the integral in Eq.(100).

$$\Psi(x,t) = \int_{-\infty}^{\infty} \phi(k)e^{ikx}e^{-iE_kt/\hbar}\, dk. \tag{101}$$

6. Computing $\phi(k)$ from Eq.(100) and substituting in Eq.(101) and doing the $k$ integral gives the wave function at time $t$.

   In the present case of free particle, $E_k = \frac{\hbar^2 k^2}{2m}$, all the integrals are Gaussian and are easy to do. We shall skip the details and write the final answer

**Remarks on Solution**  The position probability density at time $t$ is given by

$$|\Psi(x,t)|^2 = (2\pi\Delta^2)^{-1/4}\left(1 + \frac{i\hbar^2 t^2}{2\Delta^2 m}\right)\exp\left[-\frac{x^2}{4\Delta^2(1 + \frac{\hbar^2 t^2}{(1+4m^2\Delta^2)})}\right]. \tag{102}$$

$$\Psi(x,t) = (2\pi\Delta^2)^{-1/4}\left(1 + \frac{i\hbar t}{2\Delta^2 m}\right) \times$$
$$\exp\left[-\frac{1}{1 + i\hbar t/2\Delta^2 m}\left\{-\frac{x^2}{4\Delta^2} + \frac{ip_0 x}{\hbar} - \frac{ip_0^2 t}{2m\hbar}\right\}\right]. \tag{103}$$

The average position at time $t$, and the uncertainty in position at time $t$ are given by

$$\langle x \rangle_t = \int_{-\infty}^{\infty} \Psi^*(x,t)x\Psi(x,t)dx, \tag{104}$$

$$= x_0 + \frac{p_0 t}{m} = x_0 + vt \tag{105}$$

$$\langle x \rangle_t = p_0 \tag{106}$$

$$(\Delta x)_t = (\Delta x)_0\left(1 + \frac{\hbar^2 t^2}{4\Delta^2 m^2}\right)^{1/2}. \tag{107}$$

The average position changes with time as expected according to the classical free particle motion. Also remembering that the spread in position at time $t$ is $(\Delta x)_t$, we see that the uncertainty in position increases with time. Thus there is a spreading of of the wave packet with time. The spreading takes place because the wave packet is a superposition of plane waves and different waves have different velocities.

## §4   Discussion

- The expansion coefficients $\phi(k)$ have the following interpretation. The absolute square $|\phi(k)|^2 \Delta k$ gives the probability that wave vector will be in the range $k$ and $k + \Delta k$. The total probability will be equal to

$$\text{Total Prob} = \int_{-\infty}^{\infty} |\phi(k)|^2 \, dk \qquad (108)$$

  This expression is also equal to $\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx$ and hence the total probability will add up correctly to one if then wave function is normalized.

- The function $\phi(k)$ is called *momentum space wave function.*

- To find wave function at any time we need to expand it in terms of eigenfunctions of energy. So we should ask
  Question 1:*when is it possible that any wave function in terms of eigenfunctions of energy?*

- We are fixing the expansion coefficients by using orthogonality. So we are lead to ask
  Question 2:*when do we have energy eigenfunctions obeying orthogonality?*

- The absolute squares of expansion coefficients give probability of energy having different values. Therefore we need to know
  Question 3:*What is the guarantee that all probabilities will add up to one?*

**A sufficient condition, that ensures that all the three requirements are met, is that the Hamiltonian operator should be hermitian. This explains why operators associated with dynamical variables are hermitian.**

## §5   Points to remember

- ✐ The plane solutions of free particle Schrodinger equation do not correspond to the intuitive picture of a localized particle. For such a state $\Delta p = 0, \Delta x = \infty$.

- ✐ A localized particle is described by a wave packet formed by superposition of several states of a range of momenta. If $(\Delta p)$ is the range of momenta superposed, then the wave function will correspond to a particle having a well defined position within a range $\Delta x$ as given by the uncertainty principle.

- ✐ In general the uncertainty $\Delta x$ increases with time.

# §8   Constants of Motion; Stationary States

## §1   Recall and Discuss

- Time dependent Schrodinger equation;

- Solutions with definite energy are of the form

$$\psi(x,t) = N u_n(x) e^{-iE_n t/\hbar}$$

- The classical Hamiltonian equations of motion can written in Poisson bracket form as

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \big[F, H\big]_{\text{P.B.}} \tag{109}$$

- If $\hat{H}$ is a hermitian operator, then

$$(H\phi, \psi) = (\phi, H\psi) \tag{110}$$

  where $(\phi, \psi)$ denotes the scalar product of two wave function $\phi(x), \psi(x)$.

- The scalar product $(\phi, \psi)$ has properties

$$(\lambda\phi, \psi) = \lambda^*(\phi, \psi), \qquad (\phi, \lambda\psi) = \lambda(\phi, \psi) \tag{111}$$
$$(\phi, X\psi_1) + (\phi, Y\psi) = (\phi, (X+Y)\psi) \tag{112}$$

  where $X,$ and $Y$ are linear operators.

## §2   Stationary states

If a particle has a definite value of energy $E_m$, if its state at time $t = 0$ is written as $\psi(x, 0) = u_m(x)$, the wave function at time $t$ will be given by

$$\psi(x,t) = u_m(x) e^{-iE_m t/\hbar} \tag{113}$$

The wave function at any time is the wave function at time $t = 0$ times a complex number $(= e^{-iE_m t/\hbar})$. Therefore the state at any time $t$ is same as the state at time $t = 0$ (First Postulate). The energy eigenstates are therefore called *stationary states*.

It is easy to see that any quantity that can be measured such as position probability density does not change with time. As another example, when a measurements of a dynamical quantity is made, the probability of different possible outcomes of measurements does not change with time.

## §3 Time evolution of averages

The average of a dynamical variable $F$ will be denoted by $\langle F \rangle_\psi$ in a state $\psi(x)$ is given by

$$\langle F \rangle_\psi = \int_\infty^\infty \psi^*(x,t) \widehat{F} \psi(x)\, dx \tag{114}$$

For a dynamical variable $\widehat{F}$ which may or may not depend explicitly on time, we will derive an equation for time evolution of the average values.
Consider

$$
\begin{aligned}
\frac{d}{dt}\langle \widehat{F} \rangle_\psi &= \frac{d}{dt}(\psi, \widehat{F}\psi) \\
&= \left(\frac{\partial \psi}{\partial t}, \widehat{F}\psi\right) + \left(\psi, \frac{\partial \widehat{F}}{\partial t}\psi\right) + \left(\psi, \widehat{F}\frac{\partial \psi}{\partial t}\right) \\
&= \left(\frac{1}{i\hbar}\widehat{H}\psi, \widehat{F}\psi\right) + \left(\psi, \frac{\partial \widehat{F}}{\partial t}\psi\right) + \left(\psi, \frac{1}{i\hbar}\widehat{F}\widehat{H}\psi\right) \\
&= -\frac{1}{i\hbar}\left(\widehat{H}\psi, \widehat{F}\psi\right) + \left(\psi, \frac{\partial \widehat{F}}{\partial t}\psi\right) + \frac{1}{i\hbar}\left(\psi, \widehat{F}\widehat{H}\psi\right) \\
&= \left(\psi, \frac{\partial \widehat{F}}{\partial t}\psi\right) + \frac{1}{i\hbar}\left(\psi, \widehat{F}\widehat{H}\psi\right) - \frac{1}{i\hbar}\left(\psi, \widehat{H}\widehat{F}\psi\right) \\
&= \left(\psi, \frac{\partial \widehat{F}}{\partial t}\psi\right) + \frac{1}{i\hbar}\left(\psi, (\widehat{F}\widehat{H} - \widehat{H}\widehat{F})\psi\right)
\end{aligned}
\tag{115}
$$

We write the above result in the form

$$\frac{d}{dt}\langle \widehat{F} \rangle_\psi = \left\langle \frac{\partial \widehat{F}}{\partial t} \right\rangle_\psi + \frac{1}{i\hbar}\left\langle [\widehat{F}, \widehat{H}] \right\rangle_\psi \tag{116}$$

Comparing the above equation with the classical equation in the Poisson bracket notation

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \{F, H\}_{\text{P.B.}} \tag{117}$$

we see that the time development of averages is similar to the classical equation and $\frac{1}{i\hbar}\times$ commutator of operators $\widehat{A}, \widehat{B}$ corresponds to the Poisson bracket of $A, B$ in classical mechanics. In fact it can be proved that this correspondence is exact in the limit $\hbar \to 0$.

For a point particle in potential $V(\vec{r})$, one can easily see that (117) implies that

$$\left\langle \frac{d\widehat{\vec{r}}}{dt} \right\rangle = \left\langle \frac{\widehat{\vec{p}}}{m} \right\rangle \tag{118}$$

$$\left\langle \frac{d\widehat{\vec{p}}}{dt} \right\rangle = -\langle \nabla V(\vec{r}) \rangle \tag{119}$$

These equation for averages coincide with the classical equations of motion. This result is known as Ehrenfest theorem.

## §4 Constants of motion

Suppose a dynamical variable $F$ not having explicit $t$ dependence commutes with Hamiltonian. From Eq.(117) we see that

$$\frac{d}{dt}\langle \widehat{F}\rangle_\psi = \left\langle \frac{\partial \widehat{F}}{\partial t}\right\rangle_\psi + \frac{1}{i\hbar}\left\langle [\widehat{F},\widehat{H}]\right\rangle_\psi = 0. \qquad (120)$$

Therefore the average value of $F$ remains constant and we say that say that $F$ *is a constant of motion.*

## §5 Points to remember

✍ The stationary states are defined to be states with definite energy.

✍ If $X$ commutes with Hamiltonian and does not depend on time explicitly, $X$ is a constants of motion.

✍ In a stationary state the average values of all variables, whether is commutes with the Hamiltonian or not, is independent of time.

✍ The average value of a constant of motion in every state, stationary or not, is independent of time.

✍ The equation for a charged particle is obtained from free Schrodinger equation by making the replacements

$$H \to H' = H + q\phi; \text{ and } \nabla \to \nabla + iq\vec{A}$$

✍ Under a gauge transformation

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla\Lambda(\vec{r},t), \qquad \phi \to \phi' - \frac{\partial\Lambda}{\partial t},$$

the wave function transforms as

$$\psi(\vec{r},t) \to \psi'(\vec{r},t) = e^{-iq\Lambda(\vec{r},t)/\hbar}\psi(\vec{r},t).$$

# §9 Charged Particle, Time Reversal

## §1 Schrodinger equation for a charged particle

The Lagrangian for a particle, having charge $q$, and moving in electric and magnetic field described by vector potential $\vec{A}(\vec{r}, t)$ and scalar potential $\phi(\vec{r}, t)$ is given by

$$L = \frac{1}{2} m \vec{v}^2 + \frac{q}{c} \vec{v} \cdot \vec{A}(\vec{r}, t) - q\phi(\vec{r}, t), \tag{121}$$

where $\vec{v} = \frac{d\vec{r}}{dt}$ is the velocity of the particle. You must verify that this is the correct Lagrangian by showing that it gives correct equations of motion. The classical Hamiltonian for a charged particle in electromagnetic field is easily obtained by first computing the canonical momentum $\vec{p}$ defined by

$$\vec{p} = \frac{dL}{d\vec{v}} \ = \ m\vec{v} + \frac{q}{c} \vec{A}(\vec{r}, t), \tag{122}$$

$$\therefore \quad \vec{v} \ = \ \frac{1}{m} \left[ \vec{p} - \frac{q}{c} \vec{A}(\vec{r}, t) \right]. \tag{123}$$

The Hamiltonian is seen to be

$$H_{\text{cl}} \ = \ \vec{p} \cdot \frac{d\vec{r}}{dt} - L \tag{124}$$

$$= \ \frac{1}{2m} \left( \vec{p} - \frac{q}{c} \vec{A}(\vec{r}, t) \right)^2 + q\phi(\vec{r}, t) \tag{125}$$

Comparing this with the free particle Hamiltonian $\frac{\vec{p}^2}{2m}$, we see that the Hamiltonian in presence of electromagnetic field is obtained from the free particle Hamiltonian by making replacements

$$\vec{p} \to \vec{p} - \frac{q}{c} \vec{A}, \qquad H \to H + q\phi. \tag{126}$$

The Hamiltonian operator is obtained from (126) using the quantisation rule $\vec{p} \to -i\hbar\nabla$. This gives the time dependent Schrödinger equation

$$i\hbar \frac{d\psi}{dt} = \frac{1}{2m} \left( -i\hbar\nabla - \frac{q}{c} \vec{A} \right)^2 \psi + q\phi(\vec{r}, t)\psi. \tag{127}$$

## Gauge invariance

The electric and magnetic fields remain unchanged under gauge transformation of the potentials

$$\vec{A} \to \vec{A}' \ = \ \vec{A} - \nabla\Lambda(\vec{r}, t), \tag{128}$$

$$\phi \to \phi' \ = \ \phi - \frac{1}{c} \frac{\partial\Lambda(\vec{r}, t)}{\partial t}. \tag{129}$$

Under a gauge transformation the change in Lagrangian (121) is a total time derivative and hence the equations of motion remain unchanged. In quantum mechanics the Schrödinger equation does not remain invariant under a gauge transformation. The observable quantities remain unchanged if the wave function transforms as

$$\psi(\vec{r}, t) \rightarrow \psi'(\vec{r}, t) = \exp\left(\frac{iq}{c}\Lambda(\vec{r}, t)\right)\psi(\vec{r}, t). \tag{130}$$

It should be noted that the wave function, and the vector and scalar potentials are not physical quantities and are not measurable. The measurable quaties are average values of gauage invariant dynamical variables. The averages of gauge invariant quantities computed using the potentials $\vec{A}, \phi$ and the wave function $\psi$ will be the same as those computed using the transformed potentials $\vec{A}', \phi'$ and transformed wave function $\psi'$.

## §2    Time reversal symmetry

Consider classical motion of a particle under influence of a force field. If at some instant $t_0$ the direction of velocity is reversed, the particle will retrace its path. For a charged particle in magnetic field, the path will be retraced if the magnetic field is also reversed.

To see the time reversal symmetry of the classical equations in another way consider a thought experiment of motion of a particle thrown up in a gravitational field. Let the motion of the particle be captured on a film while going up and on a second film while going down. Now let one of the films be run backwards, what you see cannot be distinguished from what you see in the second film running forward. Assuming that the effect of air friction to be negligible, no measurement on the motions seen in the two films, one running backwards and the other film running forward, will be able to distinguish between them.

We say that the classical Newton's laws retain their form under time reversal $t \rightarrow t' = -t$. This means that one cannot distinguish the motion of a particle in a force field with time reversed motion. What about quantum mechanics? In quantum mechanics the time evolution is described by the Schrödinger equation.

$$i\hbar\frac{d\psi(\vec{r}, t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}, t) + V(\vec{r})\psi(\vec{r}, t). \tag{131}$$

It is easy to see that the form of the Schrödinger equation does not change if we take take complex conjugate of the Schrodinger equation and then make a

replacement $t \to -t \equiv t'$, we would successively get

$$-i\hbar\frac{d\psi^*(\vec{r},t)}{dt} = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\vec{r},t) + V(\vec{r})\psi^*(\vec{r},t), \tag{132}$$

$$i\hbar\frac{d\psi^*(\vec{r},t')}{dt'} = -\frac{\hbar^2}{2m}\nabla^2\psi^*(\vec{r},t') + V(\vec{r})\psi^*(\vec{r},t'). \tag{133}$$

The wave function $\psi^*(\vec{r},t')$ describes the time reversed motion. The Schrodinger equation for a charged particle in presence of magnetic field has time reversal symmetry, if the sign of the magnetic field is also reversed. As a simple example, $\exp(ikx)$ represents a (free) particle moving to the right on $x$ axis, and the complex conjugate wave function, $\exp(-ikx)$, represents a particle moving to the left.

# §3 Points to remember

✍ The equation for a charged particle is obtained from free Schrodinger equation by making the replacements

$$H \to H' = H + q\phi; \text{ and } \nabla \to \nabla + iq\vec{A}$$

✍ Under a gauge transformation

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla\Lambda(\vec{r},t), \qquad \phi \to \phi' - \frac{\partial\Lambda}{\partial t},$$

the wave function transforms as

$$\psi(\vec{r},t) \to \psi'(\vec{r},t) = e^{-iq\Lambda(\vec{r},t)/\hbar}\psi(\vec{r},t).$$

- The Schrodinger equation has time reversal symmetry in the following sense. If $\psi(x,t)$ is a solution of time dependent Schrodinger equation, $\psi^*(x,-t)$ is a solution of the time reversed Schrodinger equation obtained by replacing $(t \to t' = -t)$...

- If state of a point particle is described by wave function $\psi(x,t)$, the time reversed state is descries by $\psi^*(x,-t)$

# §10  Wave Mechanics of a Particle with Spin

## §1  Introduction

Today I am going to describe how you do wave mechanics of particle with spin half. I have decided to pull this topic early in the course for several reasons. Normally in a regular course and in most text books this topic comes. I wish to introduce it as early as possible.

There are several reasons for this. For one thing it is an important topic. When we want to compute some predictions of quantum mechanics and compare it with experimental data, we have to bring in spin at some stage.So let me ask what is spin?

Secondly, to describe, as we will see, spin is very easy.

The third reason is that the way I have organised this course is to emphasize how postulates are applied to solve problems. I wish to illustrate how postulates are applied to solving problems. The postulates give you starting point to solve the problem. For most problems you want to solve you will need to go back to the postulates.

Time dependent Schrodinger equation (TDSE) has been my starting for free particle and rigid box problems, If we know the wave function at initial time, solving TDSE gives you wave function at any time. This can be used to compute any measurable quantity and compare with experiments. How do you do computations is contained in the third postulate (Measurement postulate).

What all we wish to compute? Average values, probabilities, wave fucntion at a later time etc.

We have seen how all this is computed for free particle and for particle in a box. I am going to repeat story for a particle with spin. So that you can understand postulates. You will that calculation part, *i.e.* the algebra, is very simple as compared to other situations.

What all we need to start? You will need to recall the postulates. I have finished typing postulates for you and print copies and give you a copy each. Once you have a it copy, you must bring this print out in every lecture.

So let us start. The questions that we need to answer are :

- **Q1: What is spin?**

- **Q2: How do we describe a particle with spin in quantum mechanics?**

- **Q3: How do we compute various properties and observables quantities?**

## §2   What is spin?

You have already learned how to do wave mechanics of a particle without spin. We have to start with it wave function. What is wave function of a spin one particle? for spin one particle? and so on.

Before we take up question number two, let me ask you what do you understand by spin. An earlier lecture "Rise of Wave Mechanics" has a brief description of why spin was needed? when it was introduced? and by whom?

Spin is a new concept, whenever you come across a new concept like this do not accept until you have understood very precisely.

*So let me ask what is spin?*

> Ans 3:     Spin is a measurable quantity.

Priyanka's answer is very good answer and will be starting point for my discussion.

We understand what is position, momentum, acceleration etc. from our school days. This answer does not give me any understanding of spin. But answer does not give me any understanding in the same sense. The above statement does not tell me what is spin all about?

> So give me some more answers.
>
> Ans: Spin is a angular momentum of a point particle at
>      rest.
>      quantity.
>
> Que: *So if it is angular momentum of the particle at rest, how is it different from $\vec{r} \times \vec{p}$?*
>
> Ans: For a point particle the angular momentum $\vec{r} \times \vec{p}$? is
>      zero.
>
> Que: *Why is it zero?*
>
> Ans: Because the particle is at rest.

I will explain Chetan's answer. Suppose we have a point particle.In classical theory its state is described by position and momentum. For a particle at rest the momentum is zero. Therefore $\vec{L} = \vec{r} \times \vec{p}$ is zero. When we say that electron has spin half, it means it has angular momentum $\frac{\hbar}{2}$ in addition to orbital angular momentum that particle $\vec{L} = \vec{r} \times \vec{p}$.

Note that a **point particle** cannot have angular momentum other than $\vec{L}$; a

rigid body can. So for example a ball or this duster can rotate and have angular momentum even if its center of mass is at rest.

Thus spin of a point particle is an extra angular momentum on top of $\vec{L}$. This is an new thing that is coming from experiments. You have to keep asking questions. Why does one need it? and so on. You have to keep asking questions like lawyers will ask twenty questions in a court?

So let us recall where spin it came from. Why was it introduced? It was first introduced for electron. Remember that an electron is a charged particle, angular momentum for a charged particle comes with magnetic moment. So does spin angular momentum for an electron. Thus an electron has magnetic moment associated with orbital angular momentum and and an extra magnetic moment associated with spin angular momentum.

The extra magnetic moment is sometimes called intrinsic magnetic moment. This gives rise to observable effects in Zeeman effect and spectral lines. A 'part' of Zeeman effect, *normal Zeeman effect* could be explained as coming from orbital motion. A 'part' could not be explained that way and required introduction of spin and associated magnetic moment.

You know that the sodium yellow line has a fine structure and actually consists of two line of wave lengths 5890 A and 5896 A. All atomic spectra exhibit a fine structure. This is now explained in terms of intrinsic magnetic moment.

> Q: **If a particle is moving in a straight line, it has angular momentum?**
>
> Ans: *Yes it has angular momentum. If a particle is moving in a circle it has angular momentum. In general use $\vec{r} \times \vec{p}$.*
>
> Q: **Then, what will be its total angular momentum?**
>
> Ans: *The total angular momentum will be a sum of orbital and spin angular momenta. In QM addition of angular momenta is different and has to be taken up separately.*

If I have a new particle discovered today, how will the spin be measured? One can, for example, do a Stern Gerlach kind of experiment? This will work for a particle which has sufficiently long life time. Electron is stable and does not decay so one can use Stern Gerlach experiment. How do you fix spin of a particle having short life time, for example $10^{-24}s$? There are other indirect methods that can be used. For example one could use conservation of law of angular momentum to determine spin experimentally.

This is about all I want to say in answer to Q1 posed in the beginning.We now

move on to the second question:

**Q2: How do we describe a particle with spin in quantum mechanics?**

## §3   Quantum mechanics of a particle with spin

So we have a particle with some extra angular momentum. This extra angular momentum is on top of angular momentum $\vec{L} = \vec{r} \times \vec{p}$. The angular momentum $\vec{L}$ will be called *orbital angular momentum*, and the extra angular momentum will be called *spin angular momentum* or spin.

Now we want to do quantum mechanics of particle with spin. We want to do quantum mechanics because electrons protons cannot be described by classical theory and also because spin is a quantum effect.

How do we describe a a particle with spin in quantum mechanics? e get back to postulates. This where the answer (Ans 3) becomes important. Spin is a measurable quantity, it is a dynamical variable. The postulates of quantum mechanics tell us that the spin is represented by hermitian operator(s).

> Spin will be represented by some hermitian Operator(s)

But this statement "...some operator(s).." is very vague and we cannot hope to do any calculations making use of this statement. This gives us only a starting point and it does not point to you any scheme of calculations.

Now we have said that spin is angular momentum at rest. So spin should have all the properties of angular momentum.Let us see how far we can go. Angular momentum is a vector quantity so we should have *three hermitian operators $S_x, S_y, S_z$*, one operator will not do.

We have made some progress. But still we cannot do any calculations. We have only said that there should be three operators for spin. It is like saying that position and momentum become operators in quantum mechanics;just saying this does not give any scheme of calculation. We need commutators. Remember what I said about canonical quantization. For position and momentum operators the canonical quantization postulate gives commutators and that's a powerful tool for doing calculations. In fact it contains all quantum mechanics.

So we need to make a guess for commutators of spin operators. Can we guess what should assume for commutators of spin operator.

Que: *What is your guess?*

Ans: `Spin operators commute with themselves.`

Rem: *Why? Do the angular momentum operators commute? NO!*

So we should assume the spin commutators to be same as that for angular momentum. So my nest statement is that we know the commutation relations for angular momentum. So we write the same thing for spin. Thus we assume

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y. \tag{134}$$

With these equations, the quantum mechanics of spin is over. We do not need any more information. What we ever want to know, or we want to compute, will come out of the commutation relations.

You might want to know what kind of wave function an electron will have or a spin one particle will have. All this can be inferred from the commutation relations. Heisenberg did not have wave functions. All quantum could be done using commutators. Pauli could derive Hydrogen atom energy levels using commutation relations. Heisenberg did not have wave function; wave function came later.

Wave functions are useful, All the information about wave functions will come out of commutators. Only thing that is required is that you must know your mathematics well and you must know how to use postulates.

So we add some more information that for a point particle, each spin operator commutes with position and momentum operators. The basis for assuming this is that there is no evidence that there is uncertainty relation between spin and position (or momentum). So we will

Q: If a particle is moving in a straight line, it has angular momentum?

Ans: *Yes it has angular momentum. If a particle is moving in a circle it has angular momentum. In general use $\vec{r} \times \vec{p}$.*

Q: Then, what will be its total angular momentum?

Ans: *The total angular momentum will be a sum of orbital and spin angular momenta. In QM addition of angular momenta is different and has to be taken up separately.*

$$[\vec{S}, x_k] = 0, \qquad [\vec{S}, p_k] = 0. \qquad k = 1, 2, 3. \tag{135}$$

Another justification for assuming the above commutators is that whatever we predict, using the above commutation rules, this agrees with experiments. There is no contradiction with experiments. So these assumptions are fine.

Now next question is what can we do with the spin operators using commutation relations. You have already done one course. You have seen ladder operators. You have seen how eigenvalues of $J^2, J_z$ can be computed using commutation rules only. All those results were obtained using commutation rules only and the commutators for spin are assumed to be the same. Therefore we can adopt all the results from theory of angular momentum. Thus we have the following results:

- $\vec{S}^2$, commutes with $S_x, S_y, S_z$.

- $Sr$ has eigenvalues $s(s+1)\hbar^2$, where $s = 0, 1/2, 1, 3/2, \ldots$.

- For a given value $s$ of spin, the $z$ component will have a value $m\hbar$ can be one of the $(2s+1)$ values $m = -s, -s+1, \ldots, s$.

- $S^2$ and $S_z$ commute so they will have simultaneous eigenvectors. Let us denote the simultaneous eigenvectors by $|s, m\rangle$. Then we have

$$S^2|s,m\rangle = s(s+1)\hbar^2|s,m\rangle, \qquad S_z|s,m\rangle = m\hbar|s,m\rangle \qquad (136)$$

- If we define $S_\pm = S_x \pm S_y$, then $S_\pm$ act like ladder operators for $S_z$. Thus we write

$$S_\pm|s,m\rangle = \sqrt{s(s+1) - m(m \pm 1)}\,\hbar\,|s, m \pm 1\rangle \qquad (137)$$

Thus if we measure total spin, $S^2$, the answer will be $s(s+1)\hbar^2$ and a measurement of $S_z$ will give one of the values between $-s\hbar$ to $+s\hbar$. Remember, the total spin is like mass and charge of a particle. Just as mass and charge do not change and remain the same, the spin, value of $s$ remains the same for particle of a particular species. A spin two particle will always remain spin two particle. But its $S_z$ can change and have any one of the values(-2,-1,0,1,2).

For an electron spin $s$ is always half, only $S_z$ can change from time to time taking values $\pm 1/2$.

Let us assume that we are interested only in spin properties of a particle and we are not interested in its position and momentum. Take for example a nucleus bound inside a lattice. It motion may be neglected in certain situations. Consider a particle going through a magnetic field as in a Stern Gerlach experiment. Here we only want to know. "what pattern we see on the screen? in how many parts the beam splits?" In situations we can ignore the orbital motion and concentrate only on spin degrees of freedom.

The wave function has the information about probability amplitudes for different outcomes of a measurement.

What else do you want to know about quantum mechanics of a particle with spin? We want to know more about its wave function and how they act on wave function. . For sometime our discussion of spin wave function etc. will be carried out for electrons only.

We must list all possible values of a **commuting set** of hermitian operators. A commuting set means that operators in the set commute pair wise; each operator in the set commutes with every other operators from the same set.

We note that $S^2, S_z$ is a commuting set. We cannot add any other spin operator, such as $S_x 0r S_y$, because that operator will not commute with $S_z$.

To understand what is the wave function of a system we must ask what all can be measured simultaneously and list all possible combination of eigenvalues.

Let us list possible values for a complete set commuting set of operators, $S^2, S_z$, for an electron. These are just combination of eigenvalues of $S^2, S_z$ as listed below.

<div align="center">

Possible values of commuting observables

| $S^2$ | $S_z$ |
|---|---|
| $\frac{3}{4}\hbar^2$ | $1/2$ |
| $\frac{3}{4}\hbar^2$ | $-1/2$ |

</div>

The wave function should tell us the probability amplitudes for all possible combinations of simultaneously measurable quantities. In our case about probability amplitudes for all combinations of $S^2, S_z$ for a particle. Now $S^2$ for a particle, like mass and charge has a fixed, value. Thus wave function should give me one probability amplitude value of $S_z$ and nothing less or nothing more.

The wave function is just the complete information about all such probability amplitudes. So,ignoring position and momentum, and restricting our attention to spin only the complete information about all possible probability amplitudes requires only two complex numbers $\alpha, \beta$ giving probability amplitudes for the two outcomes listed in the above table. The wave function – spin part – is just these two numbers. Thus an electron wave function can be written as a two component column vector:

$$\chi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{138}$$

Actually this is not the full wave function we have ignored the coordinates and momenta. So we will call $\chi$ as spin wave function. Thus spin wave function of a spin half particle is a two component column of complex numbers.

Any question about spin can now be answered if we know the spin wave function. For example, we can compute average value of any component of spin; we can compute the ratio of probabilities of $S_y$ having values $\pm 1/2$, and so on.

I will summarize the situation for a spin half particle. The spin wave function of a spin half particle is a column vector of two complex numbers as in $\chi$ of (139). Then $|\alpha|^2$ gives the probability of spin being up and $|\beta|^2$ gives the probability of spin being down (along $z$- axis). For an electron there is nothing more to be done. All questions regarding spin alone can be answered in terms of spin wave function and spin operators. You will learn more about spin operators in the next lecture.

I am not going stop at spin 1/2 particle. Most people and text books will stop at spin half particle. I will giving you problems on spin one, spin 3/2 and spin 2.

So for example, we may want to know how does spin wave function for look for a spin one particle. The spin operators obey the same commutation rules. We can only measure $S^2 and S_z$ simultaneously. The value of $S^2$ for a particle is in any case is a single value $s(s+1)\hbar^2$. The possible $S_z$ values are 1,0,-1. So list all possible out comes of simultaneous measurement of $S^2$ and $S_z$ in a table similar to spin half given previously.

Possible values of commuting observables

| $S^2$ | $S_z$ |
|---|---|
| $2\hbar^2$ | 1 |
| $2\hbar^2$ | 0 |
| $2\hbar^2$ | -1 |

The wave function should tell us all three probability amplitudes for the above three possibilities. If we write complex numbers for each of these outcomes, we get three component wave function.

$$\chi = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \tag{139}$$