## **Introduction to Quantum Mechanics Prof. Manoj Kumar Harbola Department of Physics Indian Institute of Technology, Kanpur**

## **Lecture – 05 Time-dependent Schroedinger equation, the probability current density and the continuity equation for the probability density**

(Refer Slide Time: 00:16)



In the previous lecture we have learned about uncertainty principle. And in terms of x and p what it meant was the delta x, delta px is always going to be greater than or equal to h cross by 2 this was obtained, using the Cauchy Schwartz inequality, along with the quantum condition. And then I gave you arguments about how it appears in quantum mechanics, one was that if I consider a particle as a wave packet. Then the extent of wave packet is the uncertainty in the position of the particle. And this wave packet carries waves of different case so there is momentum also is uncertain and therefore, delta p delta x comes out to be of the order of h.

The other argument I gave you was using the Eigen function for position, which is a delta function. And this contains plane waves of all equal amplitudes so that delta x is although 0 delta p goes to infinity. So, as you make delta x smaller and smaller delta p goes to infinity. Third example I gave you was that of a plane wave, that is if I have a particle with fixed momentum p. Then the corresponding wave is in infinite wave where delta x tends to infinity; however, delta p is 0. So, you have seen the 2 extremes as well as something in between. I want to give you another argument before I start in the new topic today and that is what is known as Heisenberg's microscope.



(Refer Slide Time: 02:56)

This also tells you why I cannot determine delta x and the corresponding momentum with absolutely 100 percent accuracy.

So, consider this suppose I am looking at a particle shown here by a red dot through a microscope is the lens. And the radius of this lens is a and I am shining light on this particle from below. So, that it hits the particle and goes into the microscope if the light hitting the particle goes into microscope it must go within this angle shown by red. So, again let me make it to make it clear it is the microscope it is the particle and the light rays should go into this angle. This being a and we keep the particle at the focal length; that means, this angle theta which I will show here by black color theta is of the order of a over f. Now consider that rays are coming as photons, a photon coming straight go that an angle theta; that means, this moment changes.

So, change in the momentum of photon is going to be p photon times theta, which is p photon times theta is a over f. And the photon therefore, gives a kick to the electron and this implies that the photon therefore, gives a kick to the particle and that implies that the momentum of particle also changes by the same amount p. Photon times a over f that is the change. So, I will change the momentum of this particle. If I measure it later I cannot say what it was before the photon hit it. So, the uncertainty in the momentum of a particle if I observe it is going to be of this order and this momentum changes in the direction x.

Let me show it here this is my direction x, how about the position of the particle? Now resolution of the microscope is of the order of lambda light divided by the aperture size a. And therefore, what we can say is that this particle can be determined within an angle delta theta, this is delta theta within this angle delta theta and therefore, the position delta x is going to be of the order of f times delta theta which is lambda. Light divided by a times f so I cannot determine the position of the particle with much better accuracy than this delta x. And as a consequence there is a momentum change also for the particle and this product delta x times delta p is lambda light divided by a times f times p photon times a over f. This a cancels f cancels and lambda light time's p photon is of the order of h.

So, delta x delta p is of the order of h. So, what you see through this argument is that if I were to observe a particle with an accuracy of delta x, if I want to make delta x better and better I have to use shorter and shorter wavelength. If I use shorter and shorter wavelength the change in the momentum of the particle is more. So, I cannot determine both momentum and the position with a greater accuracy than limited by uncertainty principle. So, this is an argument which is also came inbox. With this completion of uncertainty argument uncertainty principle I am now going to go to the time dependent Schroedinger equation.

(Refer Slide Time: 08:13)

Time-departant Schrödunge Equality Recall that In far we have dealt with STATIONARY-STATE Schrödung equation  $\psi(x)$   $\psi(x,t)$ Time-dependent Schrödunge equation it  $\frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^3} + V(x) \psi(x,t)$ 3 d analyse:  $i^{\frac{1}{2}} \frac{\partial \psi}{\partial t}(\vec{k}t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(\vec{r},t) + V(\vec{r}) \psi(\vec{r},t)$  $\overrightarrow{i} \frac{\partial \psi}{\partial t}$ (Fit) =  $\hat{H} \psi$ (Fit)

What do you mean by time dependent Schroedinger equation recall that so far, we have dealt with stationary state Schroedinger equation. Remember we gave the arguments developing the stationary state to wave equation. Now what we want to understand is how wave function changes with time. So, so far what we have calculated it this gives me psi x, what I also want to know is what is psi x t because once I have a psi it evolves with time and that is governed by time dependent Schroedinger equation. Without really going to the history and how it comes about let me give you the equation it is given as i h cross d psi over dt, I am again restricting myself to one dimension, is equal to minus h cross over 2 m now I am going to use a partial derivative because psi depends on both on x and t. So, partial of psi with respect to x plus v x psi x t.

The 3 d analog is going to be i h cross d psi dt r t is going to be equal to minus h cross over 2 m, del square psi r t plus v r psi r t. Now remember that this operator minus h cross square over 2 m d 2 by d x square plus vx is the energy operator or the Hamiltonian. So, most of the time this equation is also written as d psi over dt r t equals H operator psi r t. This is a complete Schroedinger equation which for stationary states goes over to stationary state Schroedinger equation.

(Refer Slide Time: 11:14)

What does TDSE give for stationary-state?  $i \hbar \frac{\partial \psi_n}{\partial t} = \mu \psi_n = E_n \psi_n$ <br>  $i \hbar \frac{\partial \psi_n}{\partial t} = E_n \psi_n$ <br>  $\psi_n(F,t) = \psi_n(F,0) e^{-iE_n t/k}$ <br>  $\psi_n(F,t) = \psi_n(F) e^{-iE_k t/k}$ Robelskty downty =  $|\psi_n(F,t)|^2$  =  $|\psi_n(F)|$ INDEPENDENT

So, let us now see what does time dependent Schroedinger equation; I am going to write as TDSE give for stationary states. So, I have i h cross partial psi over partial t equals H psi, and first stationary state I am going to write H operating on psi n and this gives me E n psi n. For stationary state solutions of the Schroedinger equation, so I have i h cross d psi n over dt equals E n psi n, and immediately you can write the solution that psi n r t is going to be psi n r at 0 or whatever time. So, I can write this as time independent e raise to minus i E n t over h cross. So, this is how wave function or an Eigen function evolves. So, psi n r t is psi n r which is a space part of it e raise to minus i E n t over h cross.

What about the probability density? So, probability density is mod psi n r t square and that is to given as psi n r mod square. Because mod square of e raise to i n t by h cross is one and therefore, this is independent of time. So, for a stationary states the probability density remains independent of time and that is why these are stationary states. In general; however, if I have a wave function which is not an Eigen function, it is going to change with time and this is how it is going to be given.

(Refer Slide Time: 13:45)



So, in general I have i h cross d psi over dt is equal to H psi H operator.

Now, recall that Eigen functions of H form a complete set this is what we did a few lectures ago and therefore, a general psi r t can be written as summation C n psi n r t which is equal to summation C n psi n r which is the stationary state solution minus  $i \nvert E$  n t over h cross. How do we get that? To get this we can write that at time t equal to 0 suppose we prepare a psi r consistent with the boundary condition which is given as summation C n psi n r. This can always be done because psi n form a complete set and this psi r is going to satisfy the equation summation  $C$  n psi psi n r over t i h cross which is summation C n H psi n which is nothing but summation C n en psi n at r.

So, the equation for this is going to be i h cross d psi r t over dt is equal to summation n C n en psi n r t. And this is going to be satisfied by writing psi n as the time dependent psi ns and psi r t is going to be summation C n psi n r t, which is summation n C n psi n r e raise to minus i E n t over h cross.

(Refer Slide Time: 16:13)



And you can immediately see that if I do i h cross d psi r t over dt, this is going to be equal to summation n C n psi n r times i h cross times minus i en over h cross e raise to minus i E n t over h cross which is equal to if I cancel terms i times minus i is 1. So, this is equal to summation n C n psi n r t time's E n. So, this satisfies the same equation as we saw earlier and therefore, this is the solution.

Let me take an example, suppose I have particle in a box problem and the initial state I prepare psi r 0 is given as sin cubed pi x over L the length of the box is L, what is and the question we ask is what is psi r t you may ask I am not attend the normalization constant in front. So, I can write it will remain the same throughout. So, it does not matter all I focus on right. Now is the Eigen function now to find psi r t what I should do is write sin cube pi x by L in terms of the Eigen functions of the problem. And then this is going to be psi n r t or which is same as summation n C n psi n r e raise to minus i E n t over h cross. So, let me find the expansion of sin cube pi x over L in terms of the Eigen functions.

(Refer Slide Time: 18:40)



So, I can write sin cubed pi x over L as sin pi x over L times sin square pi x over L, which is same as sin pi x over L times 1 over 2 1 minus cosine 2 pi x over L, which is I can write as sin pi x over L 1 half minus 1 half sin pi x over L cosine of 2 pi x over L. Which I can write as 1 half sin pi x over L minus 1 half sin pi x over L cosine 2 pi x over L I can write as sin of 2 pi x over L plus pi x over L minus sin of 2 pi x over L minus pi x over L times 1 half. So, this comes out to be 1 over 2 sin of pi x over L minus a quarter sin 3 pi x over L minus minus plus a quarter sin pi x over L, which is same as 3 over 4 sin pi x over L minus 1 over 4 sin 3 pi x over L. So, I have written now sin cube pi x over L in terms of 2 Eigen functions. With the corresponding energies E 1 and E 3 these are known from a our previous lectures E 1 is for n equals 1 and this is h cross square pi square over 2, m L square E 3 is for n equals 3 and therefore, this is 9 h cross square pi square over 2 m L square.

(Refer Slide Time: 21:10)



And therefore, this wave function is going to evolve as, So psi x t is going to be given as summation n C n psi n x e raise to minus i E n t over h cross. And in this case this is going to be equal to C n which is a normalization constant 3 over 4 sin pi x over L e raise to minus i E 1 t over h cross minus 1 4th sin 3 pi x over L e raise to minus i E 3 t over h cross. So, this is how wave functions evolve in time. So, time dependent Schroedinger equation, i h cross d psi over dt equals H psi tells you how wave functions evolve in time. The probability density for Eigen functions of Hamilton Hamiltonian energy Eigen functions do not change with time on the other hand, you can see from this example that the probability density for a general wave function is going to change with time.

Now, let me derive a relationship, using time dependent Schroedinger equation between the current density and the probability density. So, current density and probability density in time dependent theory. Why should there be a current density in time dependent theory? That is very easy to say because as I just said that probability density let me write this as rho and again restrict myself to one d which is psi x t mod square is time dependent. Therefore, d rho dt is not equal to 0.

And if the probability is to be conserved which should be because total probability always remains 1, then the continuity equation will be satisfied. And you should have d rho dt plus del dot j and in one d it will be d rho dt plus dj in x direction dt is equal to 0. And therefore, there should be a current that makes the whole probability conserve, and let us now derive that expression for the current.

(Refer Slide Time: 24:02)

 $\sqrt{x}$   $x$   $\left( + \frac{t \hbar}{\partial t} \frac{\partial \psi}{\partial t} = - \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi \right)$ <br>  $\frac{t \hbar}{\partial t} + \frac{\partial^2 \psi}{\partial t} = - \frac{\hbar^2}{2m} \psi^2 \frac{\partial^2 \psi}{\partial x^2} + V(x) \psi^2 \psi$  - 0 - ik +  $\frac{\partial \psi^*}{\partial t} = -\frac{\pi^2}{2m} \psi \frac{\partial^2 \psi^*}{\partial x^2} + V^{(n)} \psi^* \psi = 0$ <br>Subtract (i) from (i) + set<br>ik  $(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t}) = \frac{\pi^2}{2m} (\psi \frac{\partial^2 \psi^*}{\partial x^2} - \psi^* \frac{\partial^2 \psi}{\partial x^2})$ it  $\frac{3}{2k}(\psi^*\psi) = \frac{\pi^2}{2m} \frac{3}{2k} (\psi \frac{3\psi^*}{2k} - \psi \frac{3\psi}{2k})$ 

So, let me write the equation minus plus i h cross d psi over dt is equal to minus h cross square over 2 m d 2 psi over dx square plus v x, psi and multiplied by psi star. So, I am going to multiply this by psi star and get i h cross psi star d psi over dt is equal to minus h cross square over 2 m, psi star d 2 psi over d x square plus v x psi star psi that is my equation 1.

Let me also now write the equation for the complex conjugate of psi and this becomes minus i h cross d psi star over dt is equal to minus h cross square over 2 m, d 2 psi star over dx square plus vx psi star. Let me multiply this by psi and write my second equation as minus i h cross psi del psi star over del t is equal to minus h cross square over 2 m psi del 2 psi star over del x square plus vx psi star psi that is my equation number 2.

Subtract 2 from 1 to get i h cross psi star d psi by dt plus psi d psi star over dt is equal to h cross square over 2 m psi d 2 psi star over dx square minus psi star d 2 psi over dx square. That is why I am left with. The hand side now can be written as i h cross d by dt of psi star psi which is equal to h cross square over 2 m d by dx of psi d psi star dx minus psi star d psi over dx.

(Refer Slide Time: 26:56)

 $i\overrightarrow{\lambda} \frac{\partial}{\partial t} (\psi^* \psi) = \frac{\overrightarrow{\lambda^2} \frac{\partial}{\partial t} \left( \psi \frac{\partial \psi^*}{\partial x} - \psi^* \frac{\partial \psi}{\partial x} \right)}{2m^2}$  $rac{\partial}{\partial t}$   $\left(\frac{\gamma^k \gamma}{\gamma} \right)$  =  $\frac{\hbar}{2m\varsigma}$   $\frac{\partial}{\partial x}$   $\left(\frac{\gamma}{2} \frac{\partial \gamma^k}{\partial x} - \gamma^* \frac{\partial \gamma}{\partial x} \right)$  $\frac{2}{3k}$   $f(x,t)$  +  $\frac{2}{3k}$   $\oint x = 0$ <br>  $\qquad \qquad \left( \oint x = \frac{\frac{1}{2}}{2k} \left( 4 + \frac{3\sqrt{1}}{3k} - 4 \frac{9\sqrt{1}}{3k} \right) \right)$ Example: plan were  $k \rightarrow 2$  parties moonly will

So, what we have is i h cross d by dt of psi star psi is equal to h cross square over 2 m psi d psi star over dx minus psi star d psi over dx hence derivative. I can cancel h cross one of the h crosses from both sides, and I get d by dt of psi star psi is equal to h cross over 2 m i d by dx of psi del psi s by del x minus psi star del psi over del x. This is nothing but the probability density rho r t or x t in this case. So, I get d by dt of rho x t plus d by dx of let me write this jx is equal to 0 where jx from the expression above can be written as h cross over 2 m i psi star d psi over dx minus psi d psi star over dx. This is nothing but the current density.

If you look at it carefully it is very easy to understand, you see h cross over I d psi by dx is the momentum operator. So, it operates on psi in the first term gives you the momentum. Time psi starts gives you the momentum density divided by m gives you the velocity. So, jx is like velocity times psi star psi which is the current which you know from classical physics. So, d psi by dx this is like momentum times psi. So, p psi star psi over m gives you velocity time's probability density which is nothing but the current density.

Why we do minus psi d psi star by dx, is to make the whole thing real let me give you an example. Take the plane waves which represent a particle moving with momentum p.

(Refer Slide Time: 29:42)



So, I have plane wave psi equals e raise to i k x and let me put a normalization constant c. Psi star psi is nothing but mod c square which is the density. And the current density j is going to be equal to H over 2 m i psi star which is c star e raise to minus i k x d by dx of e raise to i k x, minus c this going to be c here. Minus c e raise to i k x d by dx of c star e raise to minus i k x which comes out to be h cross over 2 m i times 2 mod c square k, which is nothing but h cross k over m times mod c square which is nothing but the velocity which is p over m time's rho. So, it makes perfect sense to define current density like this. In 3 d we are going to have rho which is given as psi star psi and j is now going to be written as h cross over 2 m i psi star gradient of psi minus psi gradient of psi star.

(Refer Slide Time: 31:27)



So, I used to conclude now to this lecture by writing the main features of this lecture one, we gave the microscope example to demonstrate delta p delta x is of the order of H. Then we considered time dependent Schroedinger equation, which is i h cross d psi over dt is equal to H psi. And just as the foot note for Eigen functions of H psi r t is given as this is space part times e raise to minus i E n t over h cross. And then we defined the current or to we more precise probability current density using time dependent Schroedinger equation. And showed that it satisfies d rho dt plus del dot j is equal to 0.

So, with this I conclude this lecture on time dependent Schroedinger equation.