Basic Quantum Mechanics

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Module No. # 02

Simple Solutions of the One Dimensional Schrodinger Equation

Lecture No. # 01

The Free Particle

We will be continuing our discussion on the use of the Dirac delta function, and specifically we will consider the solution of the Schrodinger equation for the free particle problem. And we will show that the solution of the Schrodinger equation contains the uncertainty principle.

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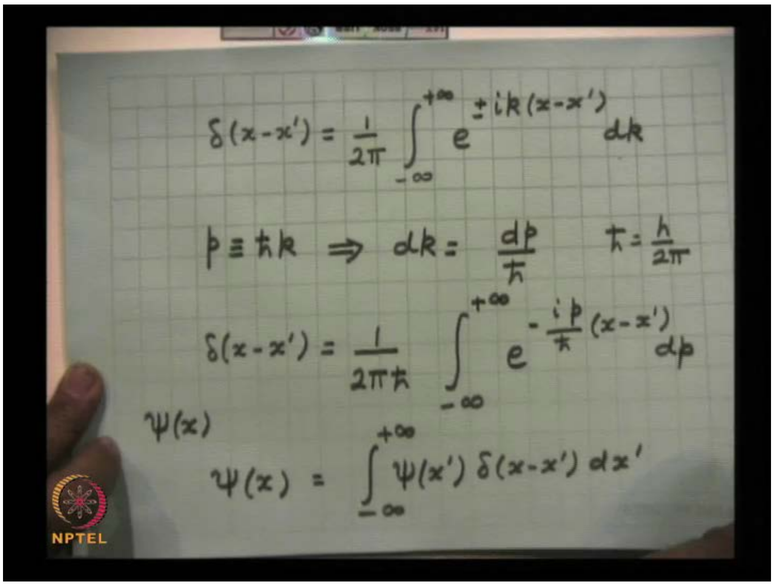

However before we do that, let us recapitulate on what we had done in our previous lecture. We had said that delta of the Dirac delta function the integral representation was given by 1 over 2 pi minus infinity to plus infinity, and there can be both for plus sign as well as minus sign i k into x minus x prime into dk. So, this is known as the integral representation of the Dirac delta function.

Now, let me introduce a variable p which we define as p is equal to h cross k, therefore you will associate this later with momentum, but let us do this right now just as a mathematical variable, then from this equation you will find that dk is equal to dp by h cross, therefore if I substitute it here I will get delta of x minus x prime is equal to dk is equal to dp by d h h cross.

So, this will be 2 pi h cross 2 pi h cross where h cross is the plank's constant h over 2 pi, and this integral we will just choose the minus sign we could have chosen the plus sign also, but we will choose the minus sign here, so this will be e to the power of minus i p by h cross x minus x prime into dp. Now, as we know I consider a function psi of x, so we write down as psi of x is equal to integral psi of x prime into delta of x minus x prime dx prime from minus infinity to plus infinity.

This follows for any well behaved function psi of x, this follows from the definition of the Dirac delta function. What I do next is I substitute for delta of x minus x prime in this equation.

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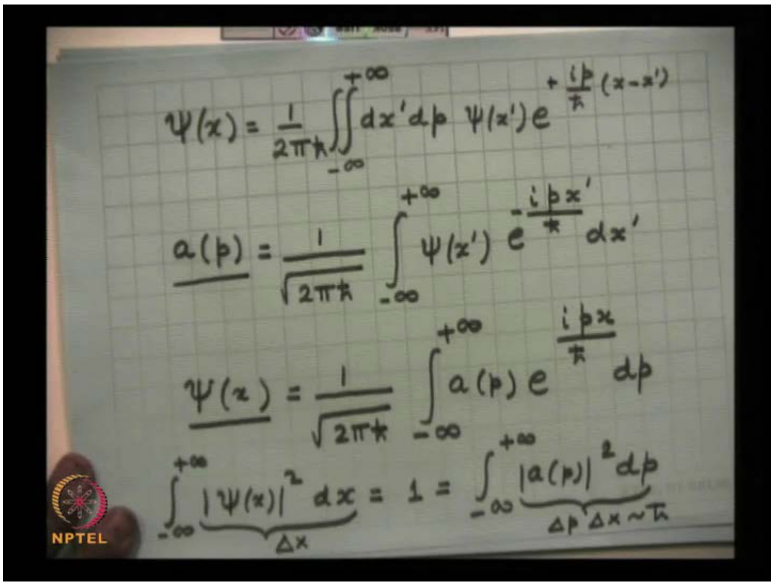

So, what I will get is what I will get is psi of x is equal to 2 pi h cross 1 integral is over x prime, and 1 integral is over d, so psi of x prime e to the power of minus i p by h cross x minus x prime let us say.

So this is what I have done if you recollect that we had these two equations, we have these two equations, so delta of x minus x prime was equal to this, and psi of x was equal to this, so we have substituted for delta of x minus x prime from the top equation in the bottom equation.

Then what we do is the limits there are two integrals minus both limits are from minus infinity to plus infinity, as we had done earlier we write 2 pi h cross we split it into two parts and we define a function a of p, we collect the x prime part outside, and write 1 over under root of 2 pi h cross integral psi of x prime e to the power of i.

P x prime by h prime dx prime, this limit is from minus infinity to plus infinity, and since this is a definite integral, I can remove the prime from here, then I substitute for a of p in this equation, then I will get psi of x psi of x is equal to 1 over under root of 2 pi h cross, a let me let me take a plus sign here, so there is a minus sign here, and a of p e to the power of i p x by h cross dp minus infinity to plus infinity.

We have two parseval's theorem and in which these we can similarly prove here, that the integral minus infinity to plus infinity mod psi x square dx is equal if this is normalized then this equation this a p is also normalized, a of p whole square dp, and as we will show later we will interpret psi of x mod square dx as the probability of finding the particle between x and x plus dx.

We will also interpret that a of p square dp will be the probability of finding the x component of the momentum between p and p plus dp, and we will show from the Fourier transform pair that if the particle is localized within a distance of the order of delta x, then its momentum spread delta p will be such that delta p delta x is of the order of h cross. So, this contains this is contained in the solution of the Schrodinger equation.

So therefore, we will consider an arbitrary function psi of x, its Fourier transform in the momentum space, we will represent by this equation and as I mentioned earlier I can remove the because this is a definite integral, so I can remove the prime from here and then the inverse Fourier transform is given by this. Now, let me write down in the very second lecture we had written down the Schrodinger equation.

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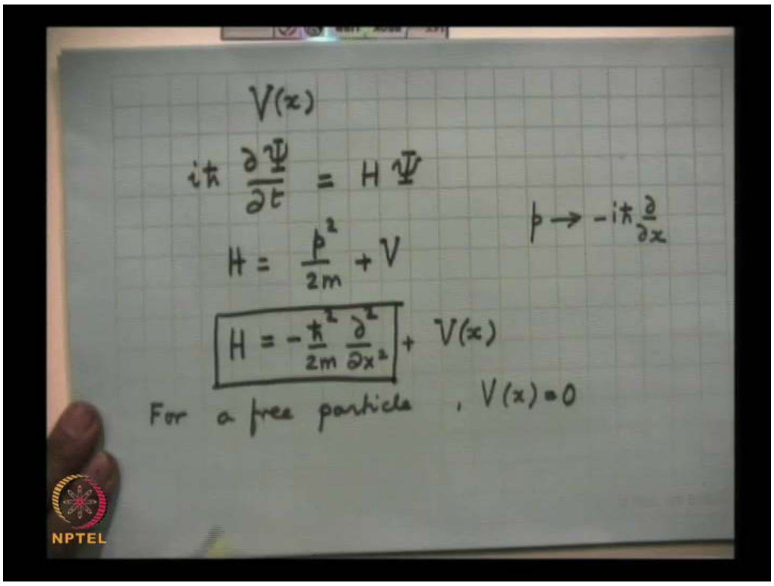

The Schrodinger equation the one dimensional Schrodinger equation for a particle moving in a field given by V of x is given by i h cross delta psi by delta t is equal to H psi, H is the Hamiltonian, and in this case so this is equal to h psi where h is the Hamiltonian which is p square by 2 m plus V and we had in one dimensional case p will be replaced by minus i h cross delta by delta x.

So, we had shown that this was equal to therefore minus h cross square by 2 m delta 2 by delta x square plus V of x. For a free particle for a free particle the potential energy is 0, V of x is equal to 0 here, so H is given by just this quantity, therefore the one dimensional Schrodinger equation for a free particle

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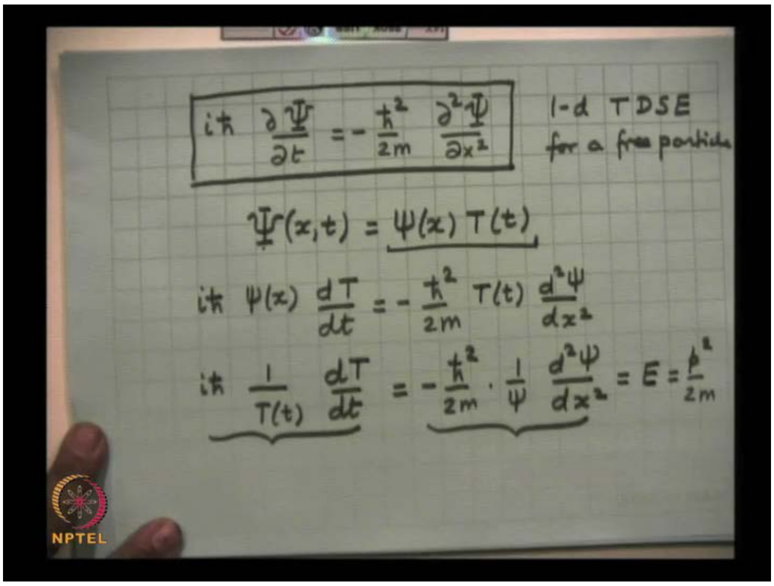

so i h cross delta psi by delta t is equal to minus h cross square by 2 m delta 2 psi by delta x square. This equation is known as the 1 dimensional time dependent Schrodinger equation for a free particle. for a free particle. We will solve this equation we will solve this equation we will obtain a rigorously correct solution of this equation, this is a partial differential equation so we will try to solve this equation with the help of the method of separation of variables.

So, we will assume that psi of x comma t is a function of x and t, is a function of x and a function of time, so I substitute it here, so I will get i h cross, now when I substitute it here I will get dT by dt, and psi can be taken because this is partial differentiation with respect to t I, therefore I will get psi of x dT by dt, this is equal to minus h cross square by 2 m this becomes T of t d 2 psi by dx square.

The variables have still not separated because the left hand side consists of a function of x and time, the right hand side also consists of a function of x and time, the trick is we divide the entire equation by capital psi, that is we divide this equation by psi times T of t, if we do that, i h cross 1 over T of t dT over dt becomes equal to minus h cross square by 2 m 1 over psi d 2 psi by dx square. You must realize that in this equation we have partial differentials because capital psi is a function of x and time.

Whereas in this equation I am considering the differential of a time dependent function, so the partial differential is represented by a total differential, now this on the left hand side is a function of time, and right hand side is a function of x, so function of time cannot be equal to a function of x, unless both of them are equal to a constant e. So, we say that the method of separation of variables has worked, and so therefore we can set the left hand side equal to a constant and a right hand side also equal to constant.

This e on the right hand side is a number and I write this e, I can write this as just p square by 2 m, where p is now a number, and I will tell you why I have written that, so I solve each part.

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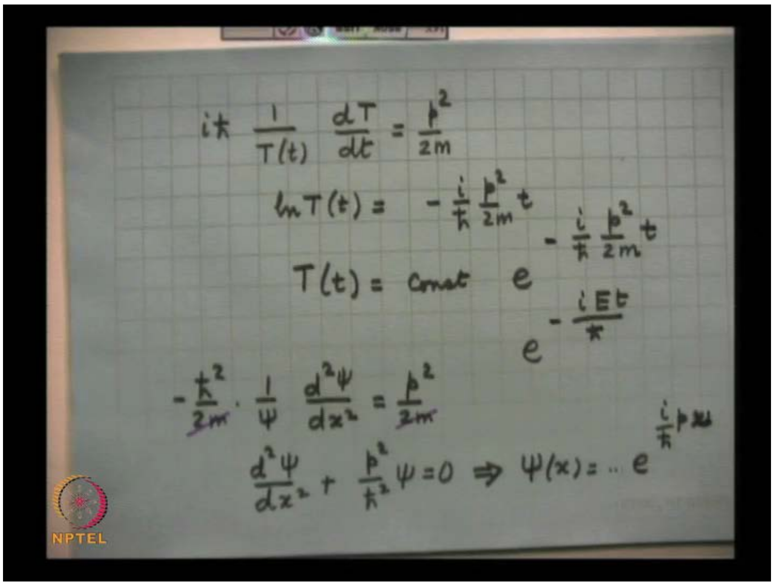

So, let me first solve the time dependent part time dependent part is i h cross, 1 over T of t dT over dt is equal to p square by 2 m, so if you integrate this out so you get log of T log of t is equal to some constant plus into minus i by h cross p square by 2 m into t.

So, T of t is constant, times e to the power of minus i by h cross p square by 2 m into t. This quantity is also sometimes written as e, so therefore I can write this down as minus i e t by h cross. Where e here and p here is a number, m is of course the mass of the particle. Let me solve the other side of the equation other part of the equation namely minus h cross square by 2 m, the x part 1 over psi d 2 psi by dx square is equal to p square by 2 m.

So, 2 m 2 m cancels out, so I can cancel this and this, I take h Cross Square on this side, so I get d 2 psi by dx square plus p square by h cross square psi is equal to 0. And the solution of this equation is trivial is very simple psi of x is some constant, times e to the power of I by p i by h cross times p psi i p by sorry x.

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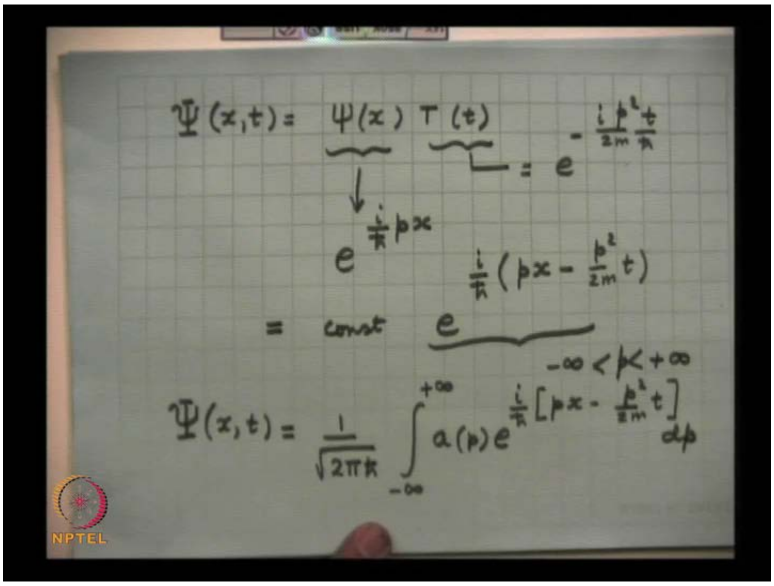

So, the complete solution the complete, so we have found out that the that we wrote first that the we assume psi of x comma t, as equal to psi of x into T of t, and then we said that we found that T of t was equal to constant, e to the power of minus I, p square by 2 m t by h cross i e t by h cross, and psi of x was equal to e to the power of i by h cross p x. So, the total solution will be some constant times e to the power of i by h cross p x minus e t that is p square by 2 m into t.

Now, what is p; p is a number and p can take any value from plus infinity to minus infinity, minus infinity to plus infinity.

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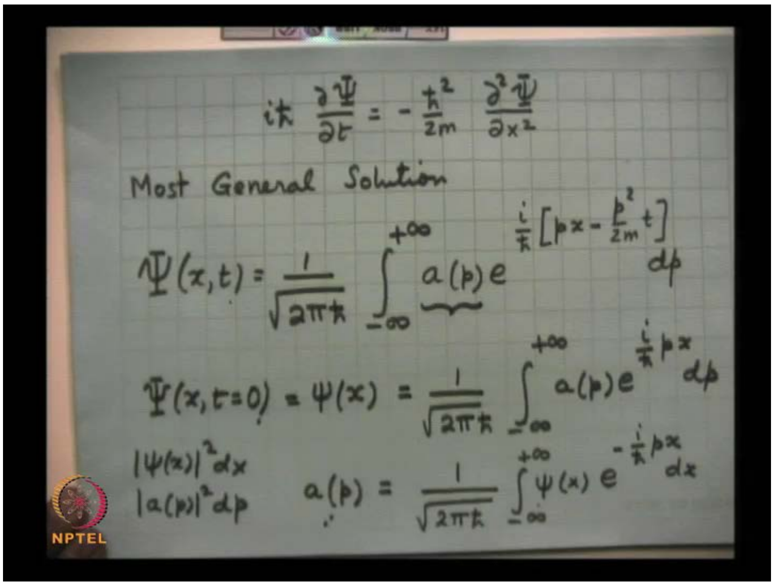

So, therefore the most general solution of the one dimensional Schrodinger equation is psi x comma t is a superposition of this solution, so I write this as 1 over i use this as a constant 1 over 2 pi h cross integral minus infinity to plus infinity a of p a to the power of i by h cross times p x minus p square by 2 m t dp.

So, what I have done is here p goes from minus infinity to plus infinity, so the most general solution will be a superposition of all the solutions, and that is what is known as a wave packet, so therefore the most general solution of the one dimensional Schrodinger equation i h cross delta psi by delta t is equal to minus h cross square by 2 m delta 2 psi by delta x square, the most general solution.

Most general solution of the above equation is given by psi of x comma t, is equal to 1 over under root of 2 pi h cross integral minus infinity to plus infinity a of p e to the power of I by h cross p x minus p square by 2 m into t into dp. Now, I still do not know what is a of p, so that is determined by the initial form of the wave function.

So, let at time t equal to 0 psi of x comma t equal to 0 at t equal to 0, let it be psi of x, you know if I put c psi t equal to 0, then it becomes 1 over under root of 2 pi h cross integral minus infinity to plus infinity a of p e to the power of 1 by I by h cross p x dp. this is just a Fourier transform.

So, therefore a of p as we have been discussing in the earlier lecture this would be inverse Fourier transform of this function, so this will be 1 over 2 pi h cross, psi of x, if this is a plus sign here, and this will be a minus sign here, dx. So, the recipe is the following I want to know the initial, I already know the initial wave function, psi of x, if I know the initial wave function psi of x, then from the knowledge of psi of x i can calculate a of p, once I know a of p, i will substitute in this equation, and carry out the integration to find out what is psi of x comma t.

So, that is the complete solution of the problem, if psi of x i will interpret, mod psi x square, as the probability of finding the particle, between x and x plus dx, and then we will interpret mod of a p square dp as the probability of finding the particles momentum between p and p plus tp.

So, if the function is localized within a distance of the order of delta x, then its momentum will be localized with a distance of the order if h cross pi sigma. Now, let me give you an example.

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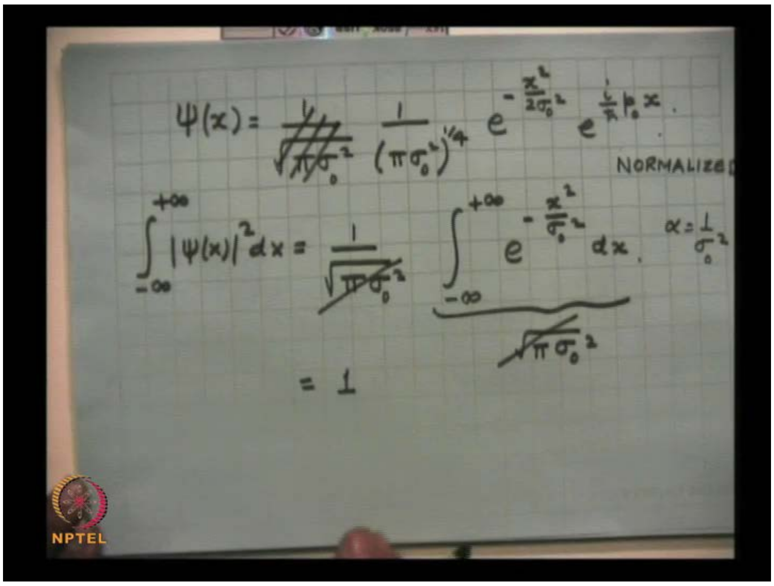

Let us calculate let us assume that psi of x with wave function at t ninety equal to 0, is given by under root of pi sigma 0 square raise to the power of 1 by 4, so that is square root of square root. So, let me delete this.

So, I am sorry so this will be 1 by pi sigma 0 square raise to the power of 1 by 4, and then it is given by e to the power of minus x square by 2 sigma 0 square, and e to the power of let us suppose that the particle is at time t equal to 0, is described by this wave function. I can tell you that if you integrate this square of this minus infinity to plus infinity mod psi x whole square dx then this will be this is one fourth power.

So, this will be one over under root of pi sigma 0 square mod psi square will be minus infinity to plus infinity, e to the power of minus x square by sigma naught square dx, because mod of this quantity is unity. And if you integrate this you get e to the power of minus alpha x square alpha is 1 over sigma naught square, so this will be this integral will be under root of pi divided by alpha alpha is so much so sigma naught square.

So, this factor will cancel out with this factor, so this quantity is one. And we say that this function is normalized Eigen function.

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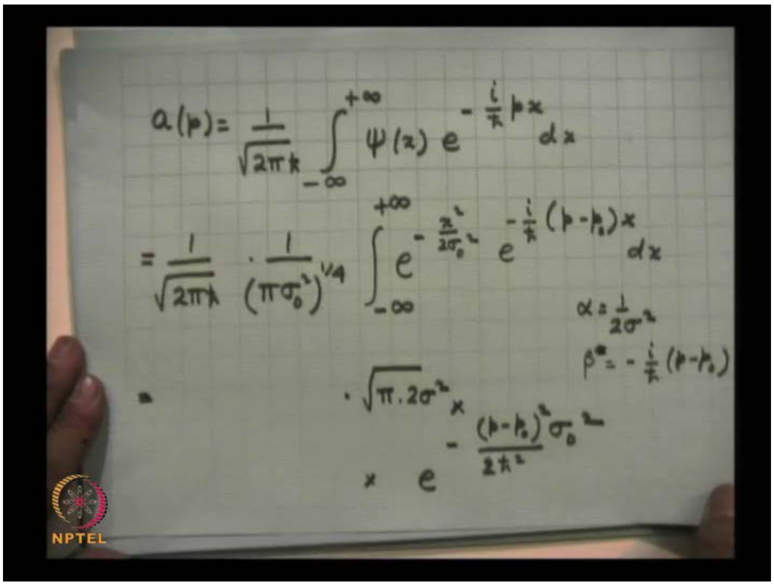

Now, we calculate with this function the corresponding a of p, so a of p is equal to 1 over under root of 2 pi h cross, minus infinity to plus infinity, psi of x, e to the power of minus i by h cross p x dx. And then what I do is I substitute for psi of x which is which is given which is by this expression.

So, I just substituted it there, so I will obtain I will obtain 1 over under root of 2 pi h cross 1 over pi by sigma 0 square raise to the power of 1 by 4, and then you will have psi of x is e to the power of x square by 2 sigma 0 square, into e to the power of I by h cross, the p will come from here, p minus p naught into x dx, the limits are again from minus infinity to plus infinity.

So, here alpha is equal to 1 over 2 sigma square, and beta as you can see is equal to beta x, that will be minus i by h cross p minus p naught, so if you substitute this you will get you will get these 2 factors will come in, e to the power under root of pi 2 sigma square and this is beta sorry, so exponential multiplied by exponential beta square, so therefore this will be beta square will be minus p minus p naught whole square by h cross square by 4 into 2 0, so 2 into sigma 0 square, because alpha is 1 over 2 sigma 0 square.

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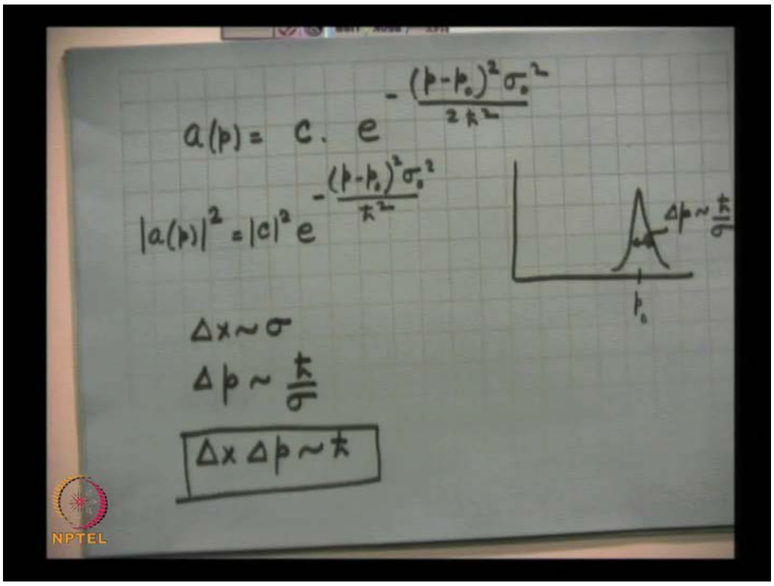

So, if you work it out and then use then you will get the following, so you will have the following relation that a of, i will leave aside the sum constant, so let us suppose this constant, this will come out to be e to the power of minus p naught whole square sigma naught square by 2 h cross square, and if you plot a of p mod square, so it will be Gaussian.

It will be Gaussian with shift with its peak at p naught, this is p naught and the delta p will be of the order of h cross by sigma. So, this is known as the mod a p square is known as the momentum distribution function, so this will be mod c square, into e to the power of minus p minus p naught whole square sigma naught square by h cross square.

So, if the particle is initially located in a distance which is of the order of sigma, then its momentum spread is located within a distance of the order of h cross by sigma, so that delta x, delta p is of the order of h cross. So, the uncertainty principle is contained in the solution of Schrodinger equation. So, let me illustrate this with the I will just go through what I have tried to say.

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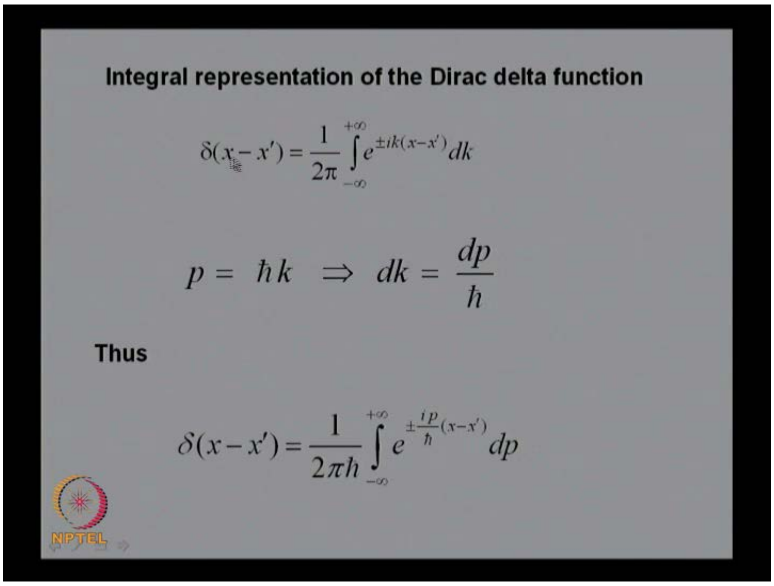

So, first of all I have the I had mentioned the integral representation of the delta function, so first I replaced k by the variable p, so p i define as h cross k h cross is equal to h by 2 pi, so dk is equal to dp by h cross. So, I have here plus minus i p by h cross, x minus x prime, dp

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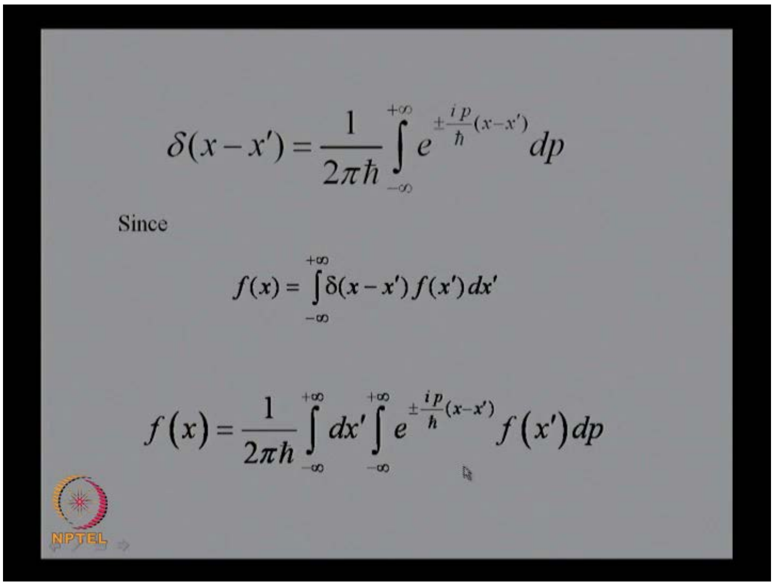

So, this is the this is again the integral representation of the delta function, and because of the delta function f of x is equal to so much. So, because f of x is equal to integral delta of x minus x prime f of x prime so I substitute it here and I will get this as f of x.

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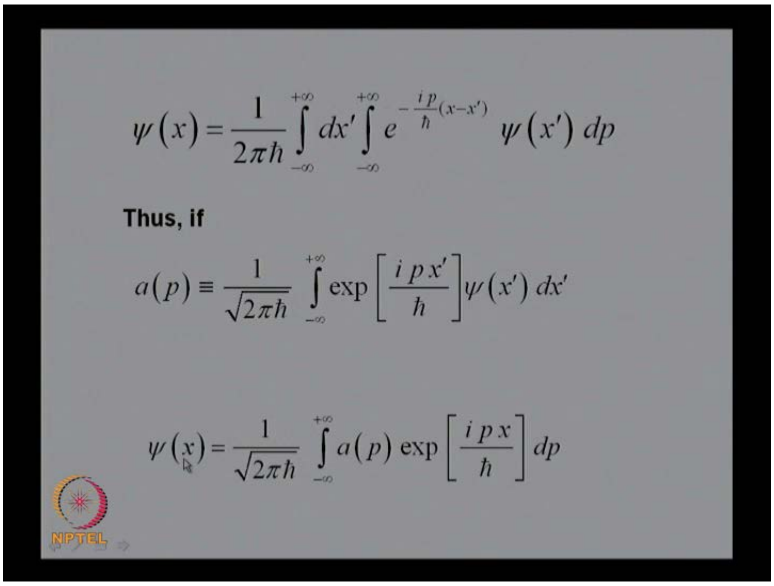

So, thus if thus psi of x is equal to so much, so you will have if a of p, i define as the Fourier transform of psi of x, and when I quietly remove the prime from here, then psi of x is equal to a of p into the power of i p x by h cross into dp.

So, psi of x and a f p form a what is known as the Fourier transform pair, and if this function is located within a distance of delta x, and if this function in the p space is located within a momentum spread of delta p, then delta x, delta p is of the order of h cross.

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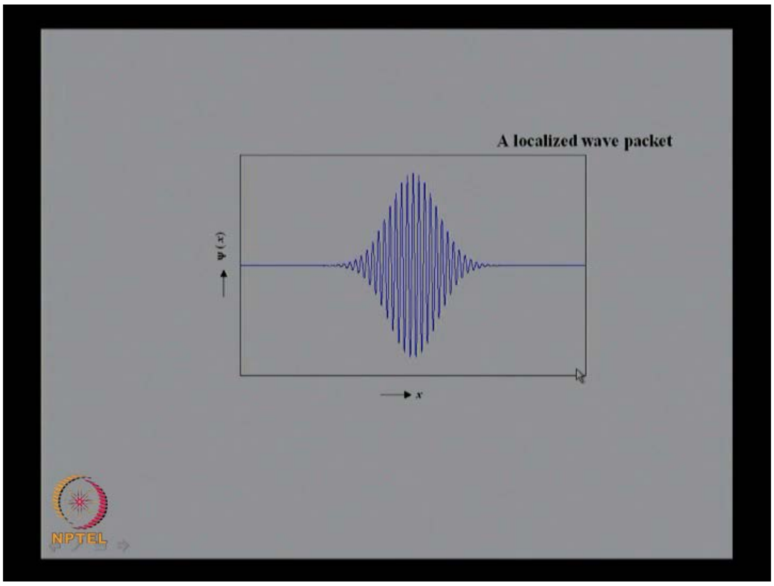

So, if I have a localized wave packet psi of x which is of the order of delta x,

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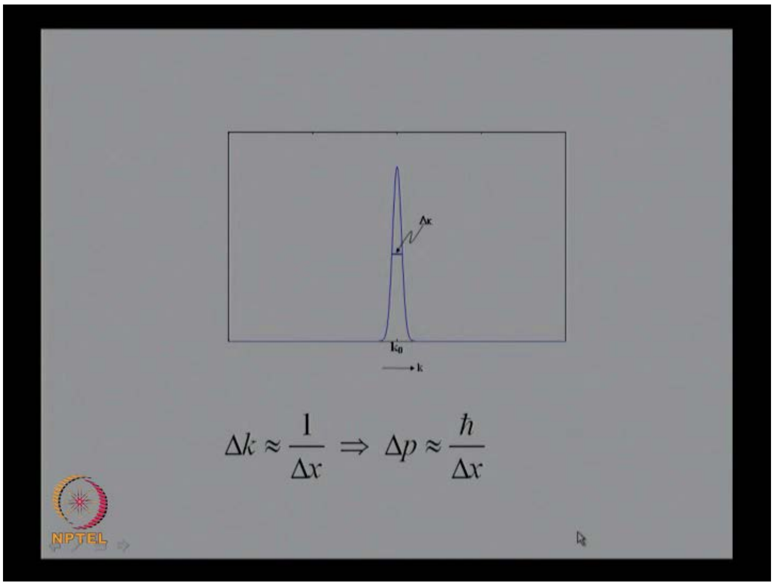

Then its corresponding momentum spread will be of the order of h cross by delta x. So, that the uncertainty principle is contained in the solution of the wave wave equation.

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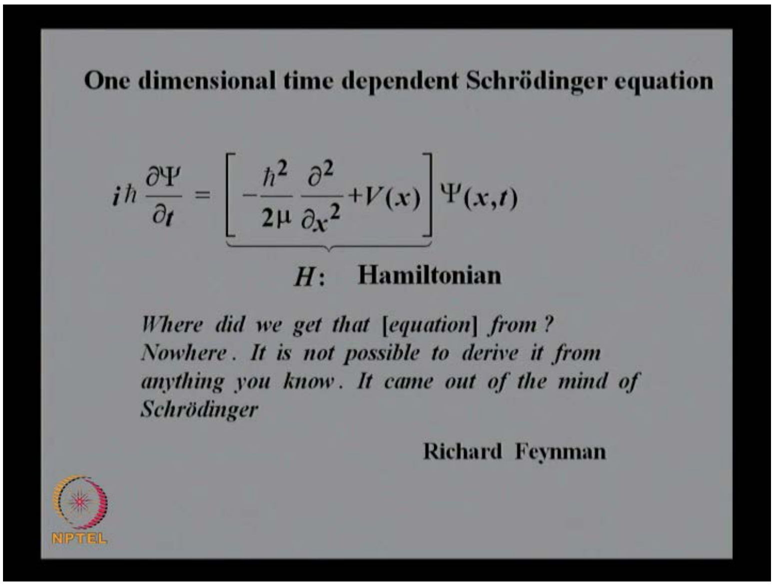

As I we had discussed last time 2, 3 times back the 1 dimensional time dependent Schrodinger equation, so we had i h cross by delta psi by delta t minus h Cross Square by 2 mu delta 2 by delta x square plus V of x this quantity is known as the Hamiltonian times psi of x t, so as Feynman has written where did we get that equation from nowhere it is not possible to derive it from anything you know.

It came out of the mind of Schrodinger actually we did give a heuristic derivation of the Schrodinger equation, and but that was that did not that lacked rigor, so we say that the Schrodinger equation came from the mind of Schrodinger.

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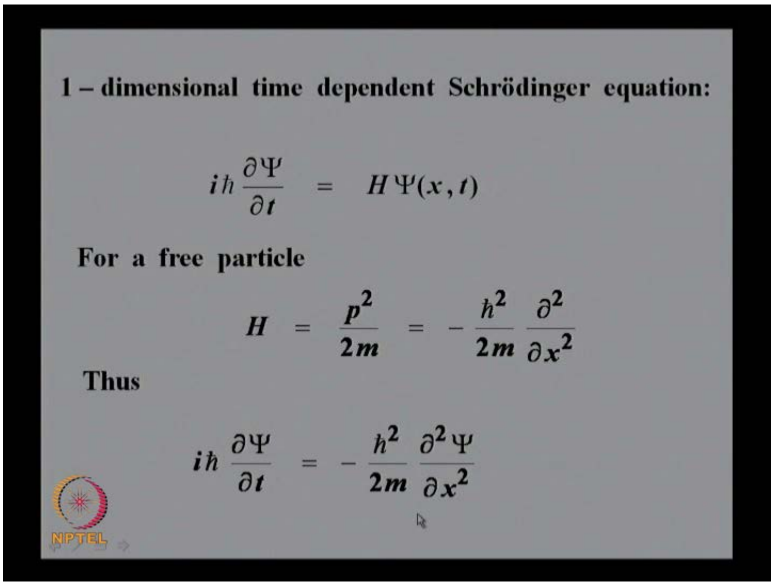

So, this is my Schrodinger equation and for a free particle V of x is 0, so my Hamiltonian is p square by 2 m, which is equal to minus h cross square by 2 m delta 2 by delta x square.

So, this equation is the 1 dimensional time dependent Schrodinger equation for a free particle, once again this equation is the one dimensional time dependent Schrodinger equation for a free particle and you would like to solve this equation.

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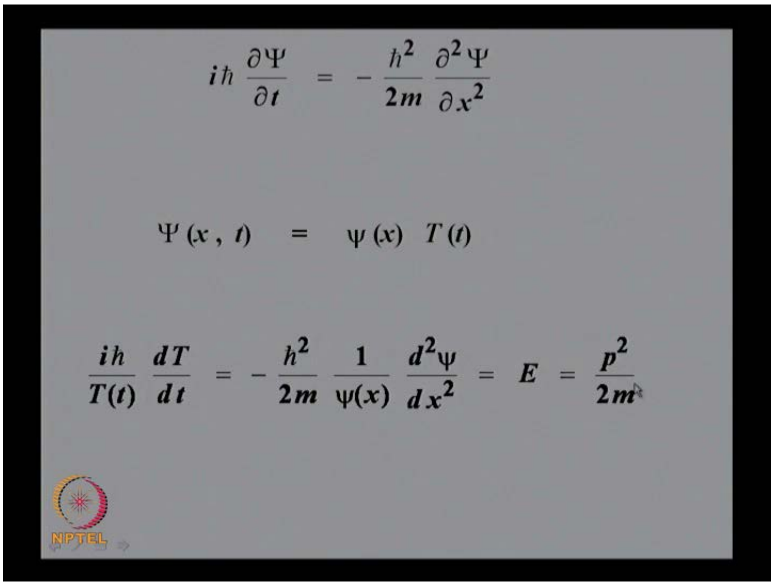

We would like to have this solution the most general solution of this equation for a free particle. So, as I had mentioned earlier we solve this equation by using the method of separation of variables, if I use the method and substitute this solution in this equation then I will get and divide by psi of x t mod psi of x T capital psi of x t, then I will get i h cross by T by t of d dT by dt minus i h cross h cross by 2 m psi of x d.

So, we say that the method of separation of variables has worked because of the because left hand side you have the function of time, and on the right hand side you have a function of x, both cannot be equal to each other unless each one of them is equal to a constant, this is the method of separation of variables, so we write this constant as e or equal to p square by 2 m.

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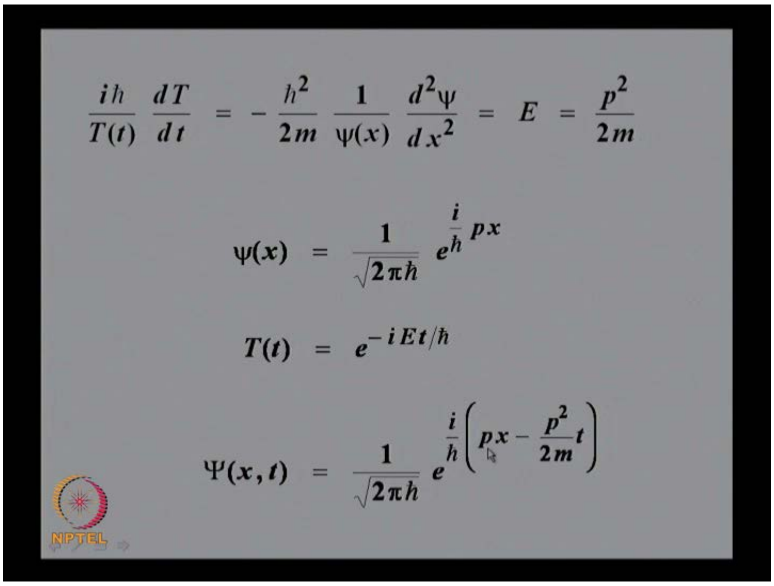

So, these 2 are numbers therefore we have as we have discussed earlier we said this equal to a constant which I write as p square by 2 m, here m is the mass of the particle, so the solution of the space dependent part if you write this then 2 m, 2 m cancels out this becomes plus p square by h cross square, so this space dependent part is psi of x is equal to so much.

And the time dependent part is e to the power of minus I, e, t, by h cross, but e is equal to p square by 2 m, so this is a solution of the 1 dimensional time dependent Schrodinger equation for a free particle, what is the value of p, p take can take any value from minus infinity to plus infinity.

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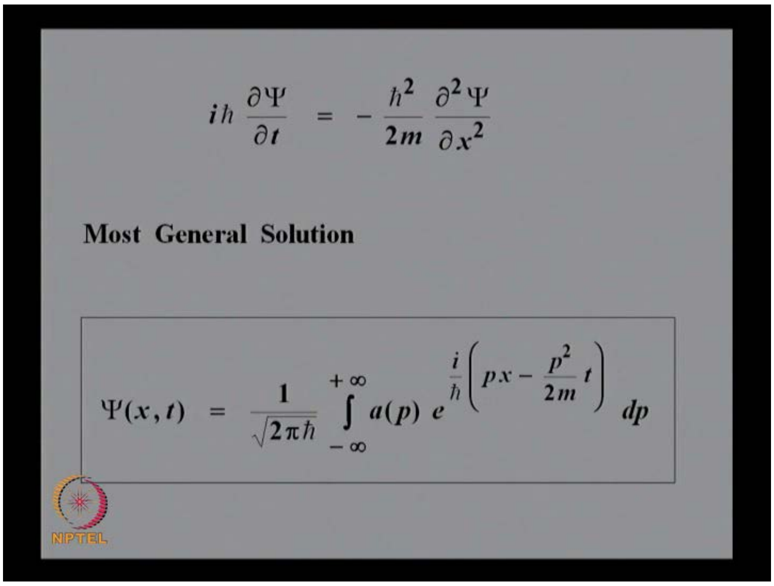

So, therefore the most general solution of this equation is an integral like this, so if I look at the back previous slide this equation I still do not what is the value of p; p can take any value from minus infinity to plus infinity, and therefore since this is a linear differential equation so the most general solution of this equation is this, so this is the most general solution and it is said that it is it describes what is known as a 1 dimensional wave packet.

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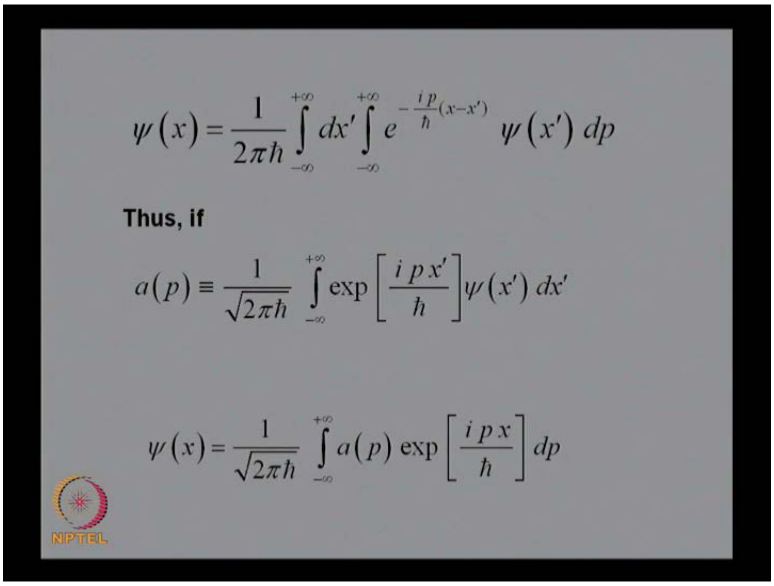

So, this we had discussed earlier if a of p is given by this, then Fourier's transform is given by this, so localized wave packet its Fourier transform is h cross by there.

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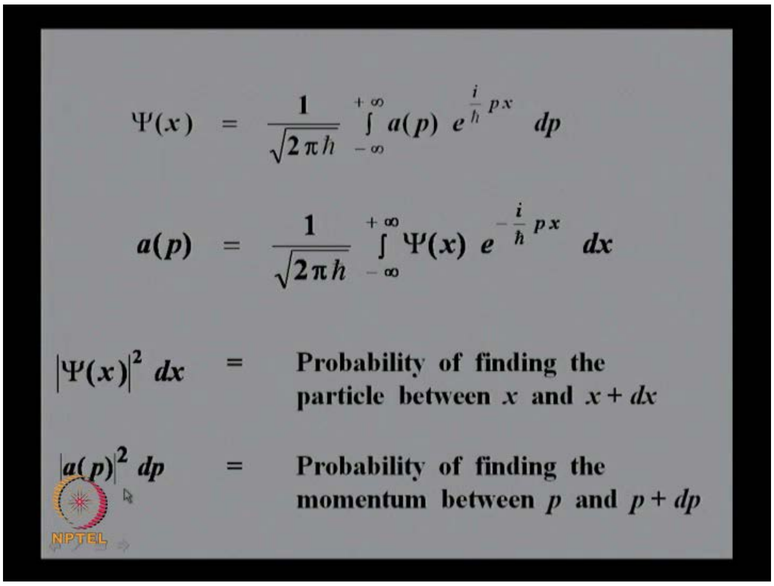

So, we have the wave function psi of x i write it as a of p, e to the power of I by h cross p f x, in the inverse Fourier transform is given by this, and because of parseval's theorem as I said this integral if this is 1 then this integral is equal to 1.

We will discuss this little later may be in a turn of two that we will interpret this is the max burn's interpretation for the probability density function, and he describes that this is the probability of finding the particle between x and x plus dx, and this will represent the probability of finding the momentum between p and p plus dp.

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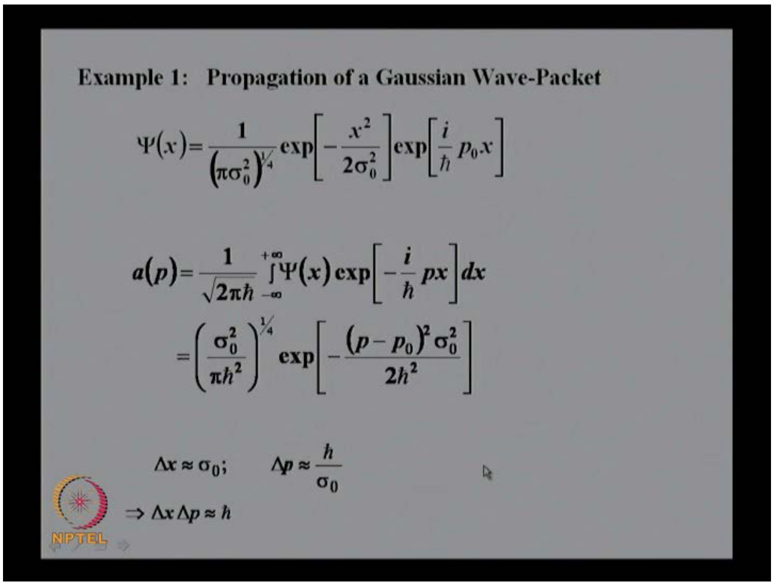

Then we consider a simple Gaussian wave packet, so at t equal to 0 psi of x is given by this, this is normalized this factor is such that mod psi x square dx is 1, if you write down the corresponding Fourier transform then you will find that it is given by this, so psi of x is normalized then a of p is also normalized, in the sense mod a p square dp is equal.

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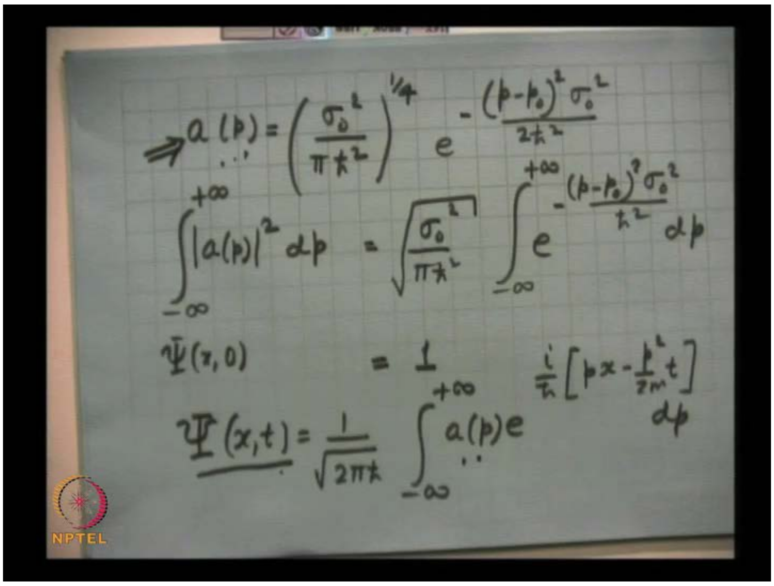

So, let me write this down so we have actually we have the numbers now that a of p is equal to sigma 0 square by pi h cross square, raise to the power of 1 by 4 e to the power of minus p minus p 0 whole square sigma square sigma naught square by h cross square so mod a p square mod a p square let me leave a little space this will be sigma 0 square by pi h cross square under root because 1 by 4 time plus 1 by and this will become e to the power of minus p minus p naught whole square sigma naught square by h cross square.

And if I integrate this from minus infinity to plus infinity and if I integrate this from minus infinity to plus infinity, I leave this is an exercise using the same formula this will come out to be equal to 1, so a particle is represented by a Gaussian wave packet, once I have a of p then I can substitute you remember that the most general solution of the Schrodinger equation was psi of x t is equal to 1 over under root of 2 by h cross a of p, e to the power of I by h cross p x minus p square by 2 m into t.

Now, minus infinity to plus infinity so you see if I know a of p, i can substitute it here, carry out the integration and I will get an analytical expression for psi of x t, so I solved the problem that by knowing psi of x comma 0, at time t equal to 0, I found out what I a of p, once I find out what is a of p, i can substitute it here and carry out the integration to calculate psi of x comma t.

So, this is so if the particle is localized within a distance of sigma naught, then this momentum spread is of the order of h cross of sigma naught, so my uncertainty principle is contained in the solutions of this equations.

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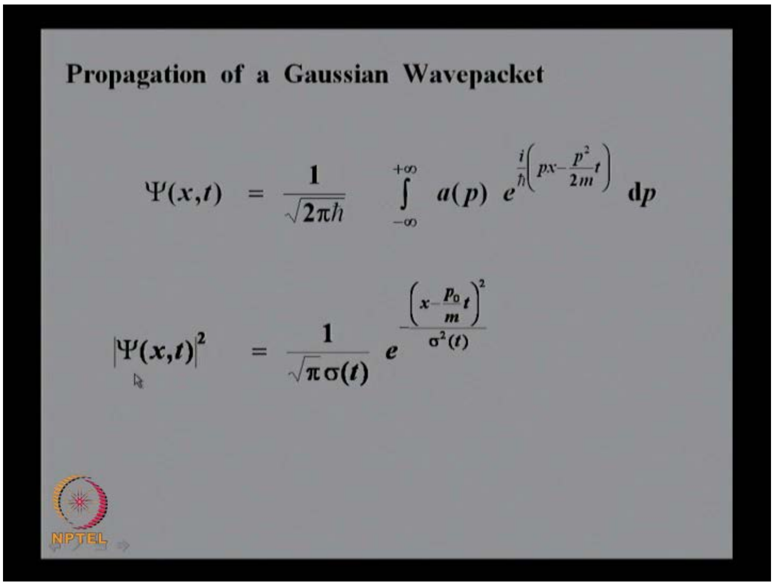

So, if I substitute the expression then I will find that the evolution of the wave function is something like this, now let me show you a software to conclude this lecture by showing you a software we have developed.

And we assume a certain width and we consider the time evolution of the wave function, so this is the real part of the wave function let us do it in 150 steps, so that you can see this slowly so this is the particle is described by this kind of let me do even more slowly, so the particle this is the real part of the wave function, and this is how it evolves with time please see this.

So, as the if I know the initial wave function then the particle is somewhere localized here, I do not know exactly I can only tell you a probability distribution and in fact as this Gaussian wave packet evolves, it spreads it spreads and this is the uncertainty in the localization of the particle, so we described the we described the electron or the proton or the neutron by a localized function.

The corresponding probability distribution at t equal to 0 is somewhere here, the corresponding momentum probability distribution is also a Gaussian, so you have how will it evolve with time if a particle is localized within a distance this, at time t is equal to 0, as the time progresses as the time progresses the wave function evolves with time like this.

And at all times you will have the probability distribution describing the motion of the particle and the momentum distribution function satisfying the uncertainty relation, so this is how the wave packet follows with time.

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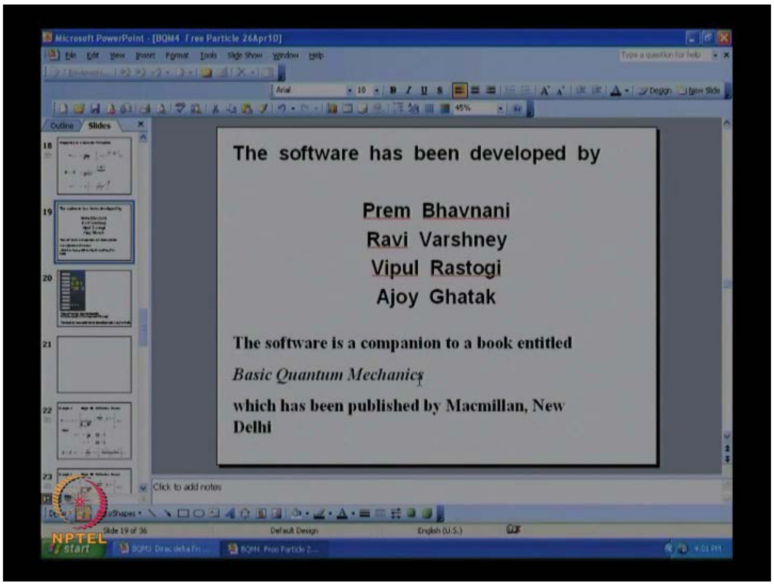

So, I thought I will show this to you that and the software that I have just now shown we will be discussing other examples has been developed by my colleagues Prem Bhavnani, Dr. Ravi Varshney and Dr. Vipul Rastogi.

And Dr. Vipul Rastogi is right now in IIT rookie, and it is in the software is a companion to a book which entitled basic quantum mechanics which I had referred to earlier, and we will show you other examples from this book at later cources.

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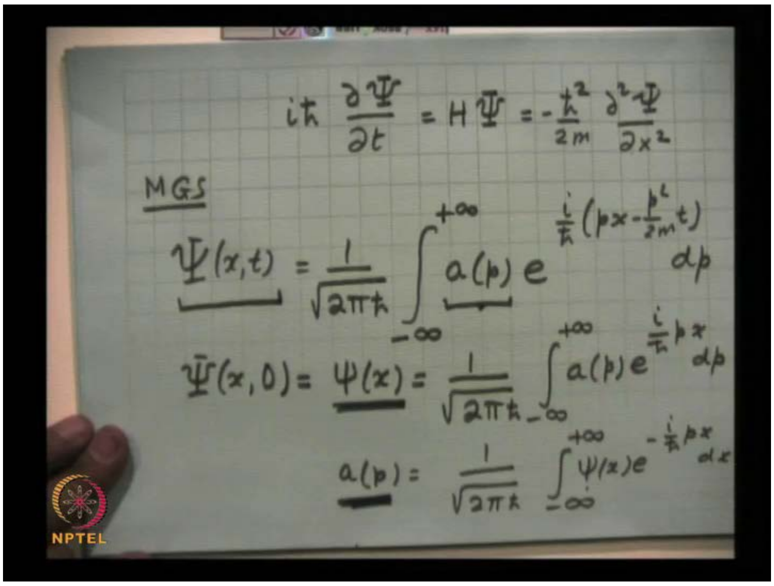

So, let me summarize what I have done, first of all we wrote down that the Schrodinger equation cannot be derived, and that is given by i h cross delta psi by delta t is equal to h psi, now for a free particle.

For a free particle one dimensional free particle this is equal to minus h cross square by 2 m, delta 2 psi by delta x square. So, what is the most general solution of this equation the most general solution the most general solution of this equation is psi of x comma t, is equal to I write down a factor 2 pi h cross for the sake of convenience, and I integrate the functions like this e to the power of I by h cross p x minus p square by 2 m t dp.

So, this is the most general solution, now the only unknown part what my objective is to determine what is psi of x comma t, the only unknown part is a of p, so this is from minus infinity to plus infinity, so what I say is this you tell me the form of wave function at t equal to 0, so let us suppose psi of x comma x at time t equal to 0, I know that.

Let us suppose I know that so that is equal to psi of x, then this is equal to 1 over 2 pi h cross a of p e to the power of i by h cross, p x into dp. So, this is now a Fourier transform relation this limit is from minus infinity to plus infinity, so then a of p is given by 1 over under root of 2 pi h cross, this we have derived and we have psi of x e to the power of minus i by h cross p x dx, minus infinity to plus infinity.

So, you tell me the wave function at time t equal to 0, then using that I will find out a of p, once I have found out a of p i will substitute it here and calculate psi of x of t, this is how, so what is psi of x comma t, it describes the electron, or the proton, or the neutron it describes how it evolves with time, and then we showed that a particle is described by a localized Gaussian wave packet, and it propagates with a certain velocity which is known as the group velocity of the wave packet.

It propagates as such and in the process there is also a broadening of the wave packet, so we have given you a complete solution of the Schrodinger equation for the free particle. What we will do next time is consider the more solutions of the Schrodinger equation and proceed from there. Thank you.