Basic Quantum Mechanics

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Module No. # 02

Simple Solutions of the 1 Dimensional Schrodinger Equation

Lecture No. # 7.

The Free Particle (Contd.)

We will continue our discussion on the solution of the one dimensional Schrödinger equation for a free particle as we had discussed in our last lecture the electron or the proton or the neutron is described by a function psi such that mod psi square d x represents is proportional to the probability of finding the electron between x and x plus d x.

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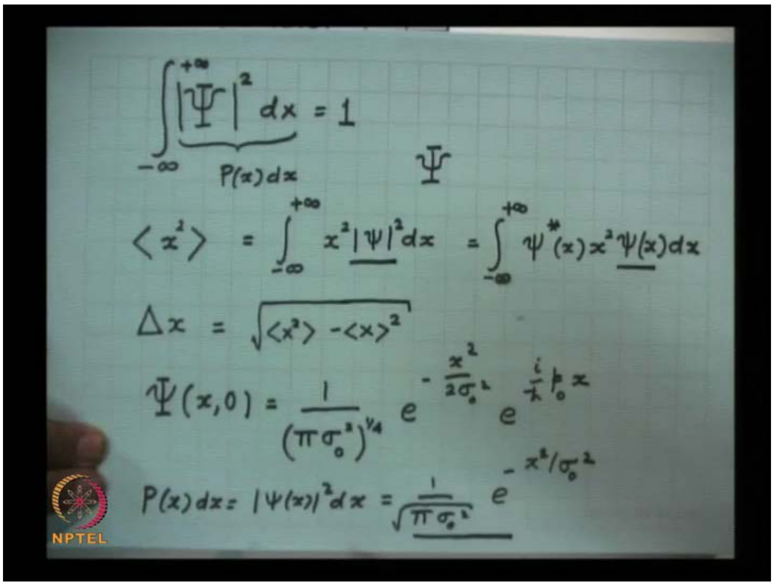

So this is the mod psi square is the probability distribution function and we can always normalize this wave function such that the integral from minus infirmity to plus infinity is equal to one as we had discussed earlier this is known as the normalization condition and when this condition is satisfied this quantity mod psi square d x represents the probability of finding the particle between x and x plus d x this is the max born interpretation interpretation of the wave function. Since this is the probability distribution function p of x d therefore, if the electron or the proton is described by the wave function psi then the expectation value of x and the average value of x will be equal to integral from minus infinity to all limits always all the integral are from minus infinity to plus infinity x mod psi square d x. So this is the expectation value of x and which is usually written like this as we had mention earlier minus infinity to plus infinity psi star x multiplies by x and psi of x d x similarly, the expectation value this is the expectation value of x similarly, one can write down the expectation value of x square. So x will be replace by x square here so this will be psi star x x square d x so if I know the wave function psi of x then in on principle in principle I can evaluate this integral and obtained expectation value of x square and the expectation value of x if we determine this then the uncertainty in x be defined this is equal to under root of the expectation value of x square minus expectation value of x whole square so this is the uncertainty in the in the.

In the measurement of the quantity x now let us suppose that the initial wave function at time t equal to zero. The wave function describing the electron or the proton at time t equal to zero is a Gaussian wave function I have a normalized Gaussian wave function like pi sigma not square rest to the power of one by four e to the power of minus x square by two sigma not square e to the power of I by h cross p naught x. So the probability distribution at t equal to zero is a Gaussian function so p of x d x this is equal to mod psi x square d x and this will be the square of the quantity pi sigma not square under the root because the square of this is under the root and then the modulus square of this is one, so this is e to the power of minus x square by sigma not square. So in order to find the expectation value of x or x square I just have to substitute this quantity in this here and carry out the integration to evaluate x expectation value of x and expectation value of x square.

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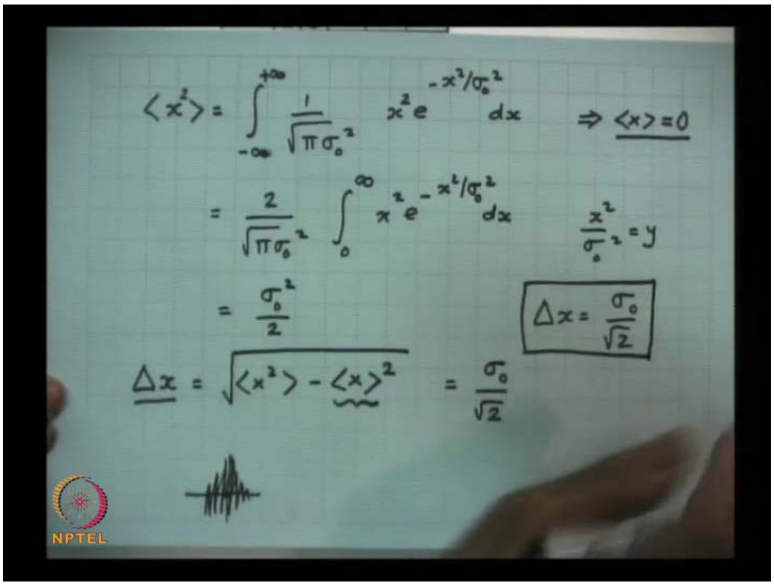

So therefore, we can evaluate if we do that then we obtain that the expectation value of x is equal to from integral minus infinity to plus infinity x times p of x d x so this will be one over under root of pi sigma not square x into e to the power of minus x square by sigma naught square d x and as you can see this is an odd integrant therefore, this implies that x is zero the expectation value of x is zero, so that if you make a large number of observation of the position x coordinate of the position of the particle then and you take the average of these over a large number of measurements you will get the value zero sometimes you will get plus something sometimes you will get minus something but, the average of that will be zero. Now the expectation value of x square will be just if you x square then this integral can be easily worked out in terms of gamma function because this will be equal to two times under root of pi sigma not square integral zero to infinity x square e to the power of minus x square by sigma naught square d x you can now substitute x square by sigma naught square equal to y and the carry out the integration it is a very straight forward integration and the final result will come out to be sigma not square by two. So therefore the delta x this spread in the value of x is equal to x square minus x average whole square under the root this quantity we have shown this to be zero this quantity sigma not square by two so we obtained that for the Gaussian wave packet this becomes zero by root two this is the this is the uncertainty in the measurement of x this is the uncertainty if the the the electron is described a wave packet. So at t equal to zero. It is somewhere located in this region therefore, the average value so this is the origin the average value is zero but, that is a spread in the wave function as I will as I had shown you earlier and this spread in the wave function is described by the uncertainty delta x and that is equal to sigma not by root two. So this result we have obtained delta x is equal to sigma not by root two so this is an important result for a Gaussian wave function we next calculate the expectation value of the momentum operator and the expectation value and the uncertainty in the momentum.

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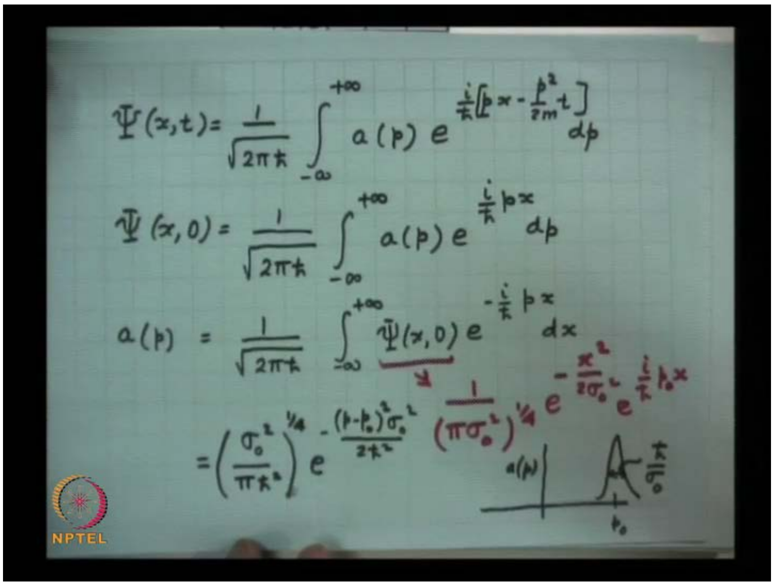

Now as we had discussed earlier that the this general solution of the Schrodinger equation is given by one dimensional Schrodinger equation is actually a wave packet one over under root of two pi h cross minus infinity to plus infinity a of p e to the power of I by h cross p x minus p square by two m t into d p. So at t is equal to zero psi of x comma zero this will be I substitute t equal to zero so I obtain under root of two pi h cross minus infinity to plus infinity a of p e to the power of I by h cross d x d p thus this psi of x not is Fourier transform of a of p and conversely the Fourier transform of a f p inverse Fourier transform will be given by as we had discussed earlier this is the inverse Fourier transform one over two pi h cross psi of x not x comma zero and now it will have a minus sign minus I by h cross p x d x. So if I know psi of x comma zero the recipe is this as we had discussed earlier the recipe is this if I know psi of x comma zero, I can calculate a of p once I calculate a of p I substitute it this equation carryout this integration and obtain psi of x of t that will describe the evolution of the wave packet with time. So we have we have assumed that that psi of x comma zero we had psid that this quantity we assume to be this equal to 1 over under root pi sigma zero square raise to the power of one by four e to the power of minus x square by two sigma not square e to the power I by h cross p naught x.

So if I substitute this expression for psi of x comma zero I can carry out the integration using that integral e to the power minus alpha x square plus beta x is very straight forward integration and if you do that we will obtain the following expression for a f p and you will obtain a of p is equal to sigma 0 square plus pi please work this out pi h cross square raise to the power of one by four and the Fourier transform of Gaussian is Gaussian minus p minus p naught whole square sigma naught square divided by 2 h cross square. So this function the wave function is is is Gaussian its Fourier transform is also Gaussian and if you plot this you will find that the Fourier transform that the a of p function a of p function is peaked around p equal to around p naught and with the spread which is of the order of h cross by sigma naught then so this is the Fourier transform function so then if I want to measure the x component of the momentum or just we say that the p and the average value of momentum we had discussed this.

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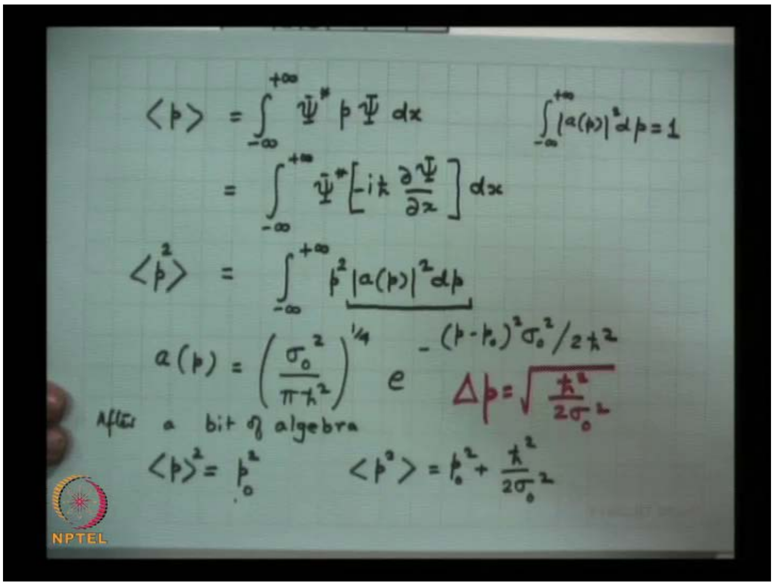

So the average value of momentum will be equal to minus infinity to plus infinity psi star p psi d x so p psi will be equal to we have to replace this by its operator we had discussed this in detail so minus infinity to plus infinity psi star minus I h cross I can put a bracket here delta psi by delta x d and if you carry out if you substitute for psi this particular expression this particular expression and you carry out this integration then you will find that this will come out to be minus infinity to plus infinity p of mod a p square d p. Therefore we can interpret that a of p mod square d p is the probability of finding the momentum between p and p plus d p and for from parcel able theorem if psi square is normalized then this is also normalized that is minus infinity to plus infinity a of p square one p square d p is equal to one if the wave function is normalized then its Fourier transform is also normalized. So this is the expectation value of p similarly, you can calculate the expectation value of p square for p square this will be a p square here and so this will be minus h cross square delta two by delta x square and if you did the algebra once again as we had done earlier so this will come to the p square a of p one square d p.

We do have the expression for a of p so a of p as we had derived it a few minutes back sigma not square by pi h cross square raise to the power of one by four e to the power of minus p minus p naught whole square sigma naught square by two h cross square. So all that I have to do is therefore, I have the expression for a of p and analytical expression I substatute a of p square will be square of that I substitute it here multiply by p square and carry out the integration that will give me p square and for p I just have to multiply by p and carry out the integration the the algebra is slightly involve but, it involve simple evaluation of the integral. So one fine with a little bit of algebra I would request all of you to carry out with algebra so after a bit of algebra which is just evaluation of the integrals we will obtain that the expectation value of p that the average value the x component of the momentum is p not and the expectation value of p square will come out to be p not square plus h cross square by two sigma not square I would request all of you to work this out it is a very straight forward algebra but, 1 must do that. So therefore, delta p is p square average minus p average square so p average square will be p naught square if you subtract this from this the p naught square p naught square cancel out so delta t will come out to be if you find out delta p that will be equal to delta p will be equal to under root of p square minus p average square so this will be h cross square by two sigma naught square so.

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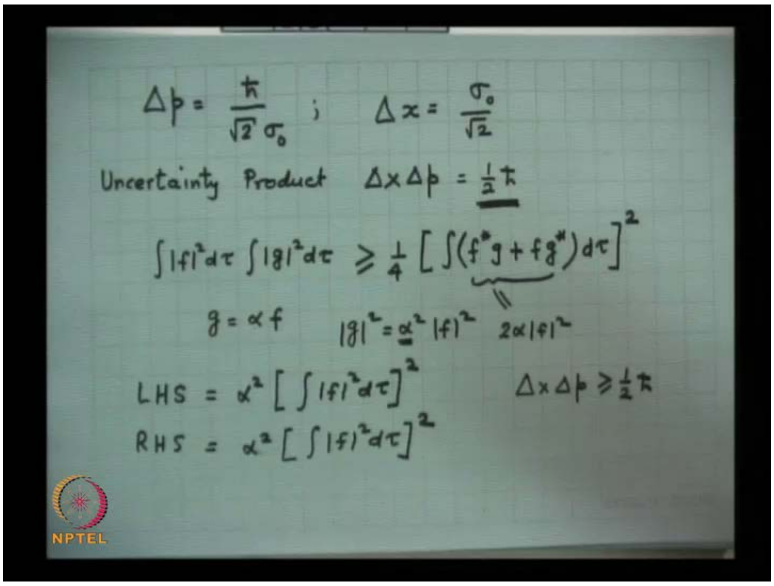

So we obtained finally, the following expressions for delta p and delta x delta p we have just found out that this will be equal to h cross by root two sigma naught delta x we had found out to be equal to sigma naught by root two. So therefore, the uncertainty product this is known as the uncertainty product delta x delta p the sigma not sigma not cancel out this will become out to be and this is typical of a Gaussian wave packet the Gaussian wave packet corresponds to the minimum uncertainty product so we obtained this.

Now this is actually the uncertainty product is minimum and 1 can show this analytically because you may recall that when we derive when we had derive the uncertainty principle we had first proved sources in equality and the inequality was mod f square d tau times mod g square d tau this was greater than nor equal to quarter of integral f star g plus f g star d tau and whole square. Now I can easily show that if g is a multiple of f that is let us suppose g g can be complex but, let us suppose it is a multiple of f therefore, the time being we can assume that alpha is a real number let us suppose so this becomes f square and this g square so g g star so mod g square becomes alpha square mod f square where alpha is a constant and I am assuming this to be a real constant so alpha square so the left hand side left hand side becomes alpha square and this also becomes f square d tau this also becomes f square d tau. So you will have integral mod f square d tau whole square on the other hand this quantity f star g will be equal to this will be equal to alpha mod f square this will be also alpha mod f square so the sum of the two will be two alpha mod f square and if I square this it will be 4 alpha square mod f square d tau whole square the four will cancel out with four. So the right hand side will also be equal to alpha square mod f square d tau whole square what I have done is the following. I had proved earlier that this inequality is always valid I had just now shown that if g is a multiple of f and let this multiplicative constant be real then the left hand side and the right hand side become equal so that this inequality becomes an equality. So therefore, using this inequality we had proved that delta x delta p x is greater than equal to half h cross and we had assumed that we had assumed that f was equal to f was equal to p psi which is equal to minus I h cross say d psi by d x and we assume that g was equal to I x psi.

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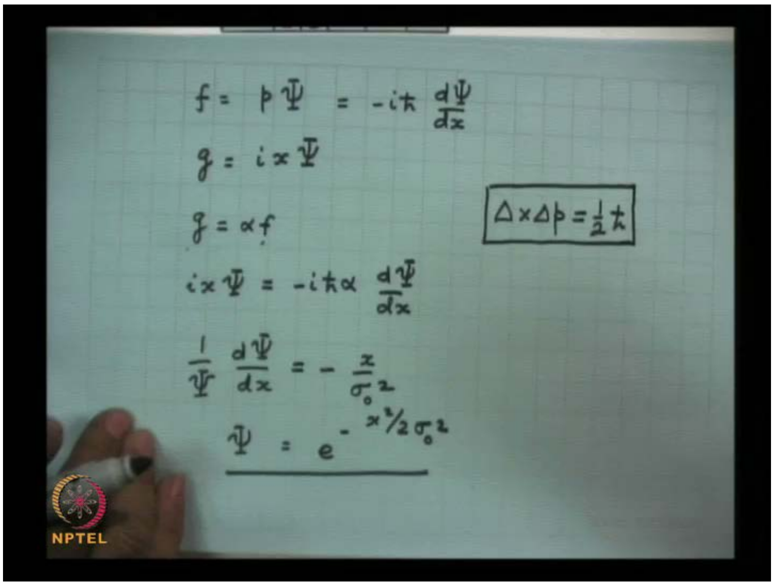

So if if g is a multiple of f then you have this if I assume that g is a multiple of f or f is a multiple of g does not matter either way so then this tells us that I x psi will be equal to minus I h cross alpha d psi by d x so the I on both sides cancel out and if I take psi in the denominator then I will obtain one over psi d psi by d x is equal to minus minus h cross alpha and let me put it as x by sigma naught square just the sigma naught square is just h cross alpha. So if I integrate this out so this becomes log psi so psi becomes equal to e to the power of minus x square by two sigma not square so the when the wave function is Gaussian g is g is a multiple of f and therefore, the inequality becomes an equality so that for a Gaussian and wave function delta x delta p becomes equal to half h cross finally, now we had shown so this is the uncertainty product so finally, we.

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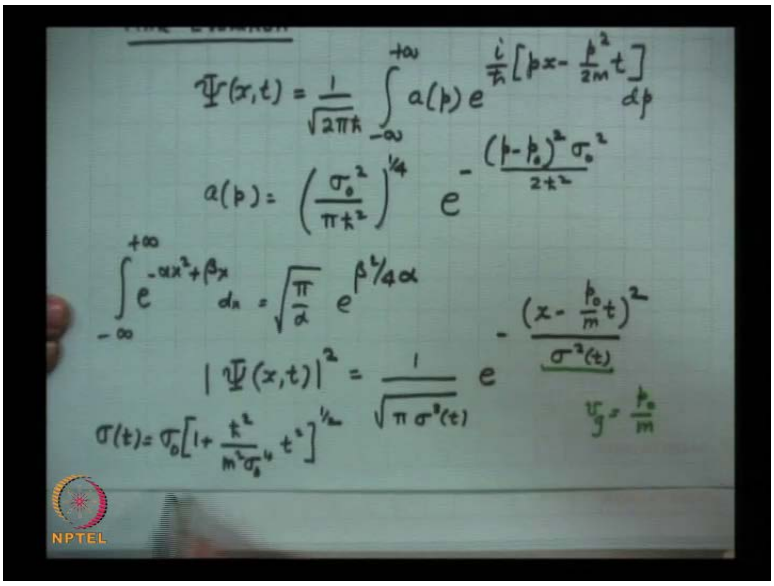

We have that the wave function I want to study the time evolution that how I had shown you a diagram but, maybe we will show this again today time evolution of the wave function so that is given by psi of x t is equal to under root of two pi h cross integral the limits are from minus infinity to plus infinity e to the power of I by h cross p x minus p square by two m t d p minus infinity. So if I know psi of x comma zero I know a of p and in fact for the Gaussian wave packet we have shown that a of p is equal to sigma not square by pi h cross square raise to the power of one by four it was a Gaussian momentum distribution minus p minus p naught whole square sigma naught square by two h cross square so I know the function a of p I substitute it here and carry out the integration of p over p once again it is a slightly cumbersome integral but, you just have to repeatedly use you just have to again use the integral that we had first written on the first day alpha x square plus bets x d x from minus infinity to plus infinity this is equal to square root of pi by alpha e to the power of beta square by four alpha. If you do that you obtain an analytical expression for psi of x comma t and if you take the modulus of that then you will get psi of x comma t mod square this is equal to under root of pi sigma square as the function of time e to the power of minus x minus p naught over m into t whole square divided by sigma square of t where sigma of t after carrying out the integration you can show comes out to be sigma naught one plus h cross square by m square sigma not four sigma not four into t square raise to the power of half. So there are two very important points in this formula the first point is that the centre of the wave packet is moving with the velocity p not by m this is the group velocity of the wave packet the whole wave packet moves with a certain velocity the average velocity the group velocity and that group velocity of the wave packet is given by p not by m and the second important point is that the width of the packet is increasing with time so that initially the packet was the real part of the wave function was something like this.

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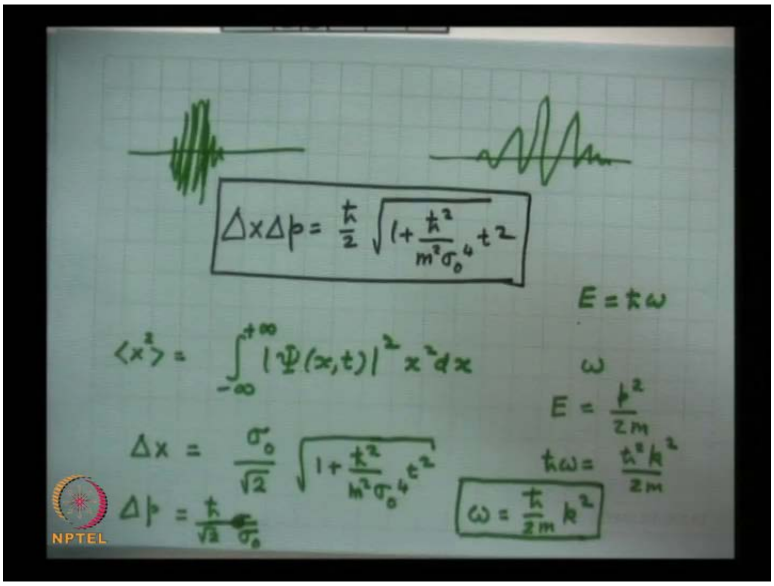

At a later time it would have expanded and it as I will show you this whole thing expands the delta x increases in fact if you use this wave function and evaluate x which is equal to is equal to mod psi x comma t whole square into x d x from minus infinity to plus infinity. If you first evaluate mod x expectation value of x and when you evaluate mod x’s square then you will find that that the uncertainty in x will come out to be equal to sigma naught by under root of two into under root of one plus h cross square by m square sigma naught four t square that is the packet expands and the packet expands because of the dispersion relation that omega that you see you have here e is equal to h cross omega and you have also e is equal to p square by two m so h cross omega is equal to p square by two that is h cross square k square by two m so your omega is equal to h cross by two m times k square. So you have a non-linear relationship if omega is proportional to k as it is indeed true for electromagnetic waves in free space there is no broadening of the pulse but, if there is dispersion what is dispersion when omega and k has a non-linear relationship then there is a broadening of the pulse so the broadening of the pulse is because is a manifestation of the fact that we have a dispersive media in which omega k relationship is not linear. So delta x is so much the delta p remains the same the delta p is equal to h cross by under root of 2 that does not change with time h cross by under root 2 what was the expression for h cross by under root 2 into sigma naught divided by sigma naught this does not change with time so that the uncertainty product the uncertainty product will change with time and you will have delta x delta p will be equal to h cross by 2 h cross by 2 1 plus h cross square by m square sigma naught 4 into t square. So this is the uncertainty product for a propagating Gaussian beam the beam expands along the x direction along the direction of propagation of the wave so we have done all the algebra let me just quickly go through the the my slides which will tell you the same thing so we continue with our discussion with the free particle this is the as you may be called this is the 1 dimensional Schrodinger equation for a free particle we had discussed the general solution of that.

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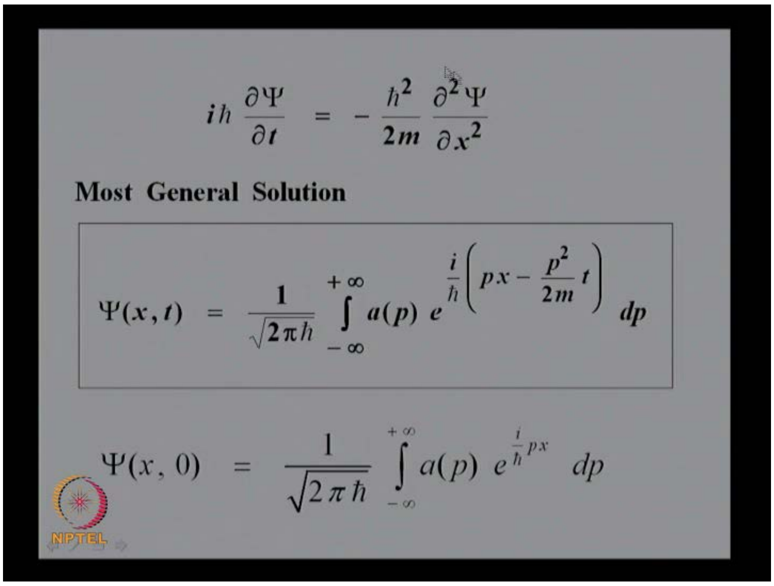

So the general solution of this equation is given by this equation this equation describes the propagation of a wave packet so how do we study the evolution of the wave packet so I put t equal to zero, so in this term becomes zero so this becomes a p e to the power of I pi h cross p x.

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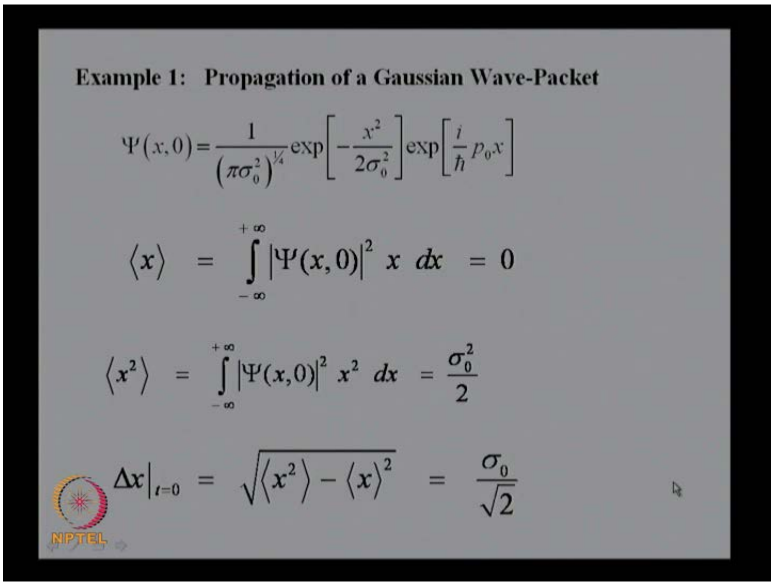

So the recipe is that I find out a of p by taking the inverse Fourier transform and if I take the f p by taking the inverse Fourier transform and I substitute it in this equation and I will get psi of x comma t so in a in a Gaussian wave packet this is the form of the wave function that is given to us so my problem is that if I know the wave function at t equal to zero what is the wave function at at a later time t in order to do that first we first showed that the expectation value of x is zero then we showed that the expectation value of x's square is sigma zero square by two therefore, this is zero. So the expectation value of x at time t equal to zero at time t equal to zero is sigma zero by root two.

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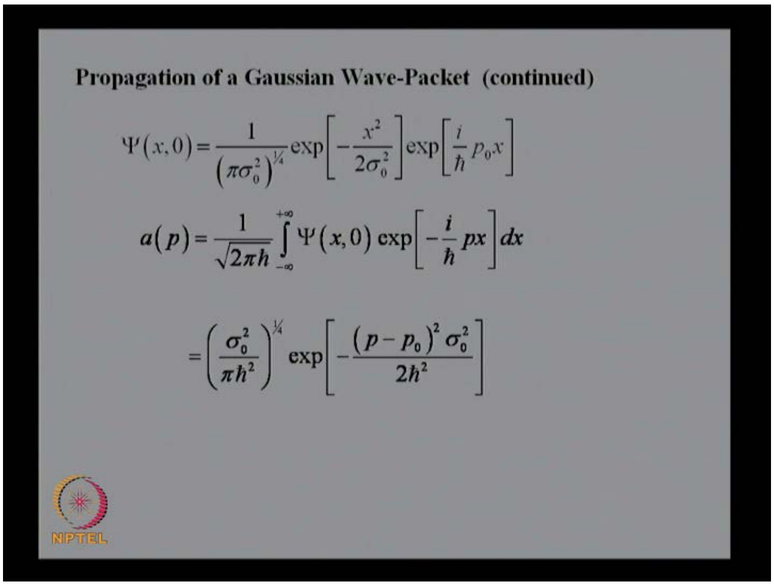

Then in order to study the evolution of the wave packet we calculated the a of p the momentum distribution function so that is the inverse Fourier transform of psi of x comma zero. If I substitute this here and carry out the straight forward integration I will obtain this equation which is also a Gaussian but, peaked around p equal to p zero.

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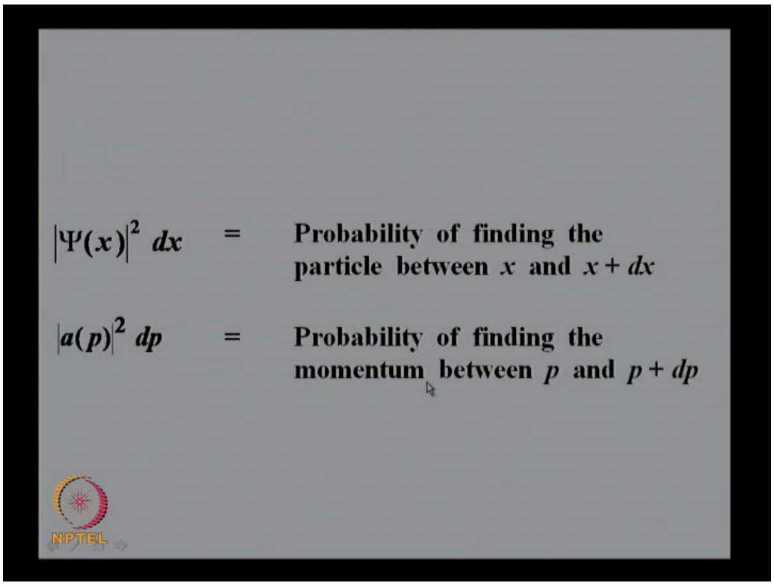

And therefore, we can interpret mod psi of x d square d x as the probability of finding the particle between x and x plus d x and a of p mod square d p is the probability of finding the x component of the momentum of course, we are considering the one dimensional case the x component of the momentum between p and p plus d p

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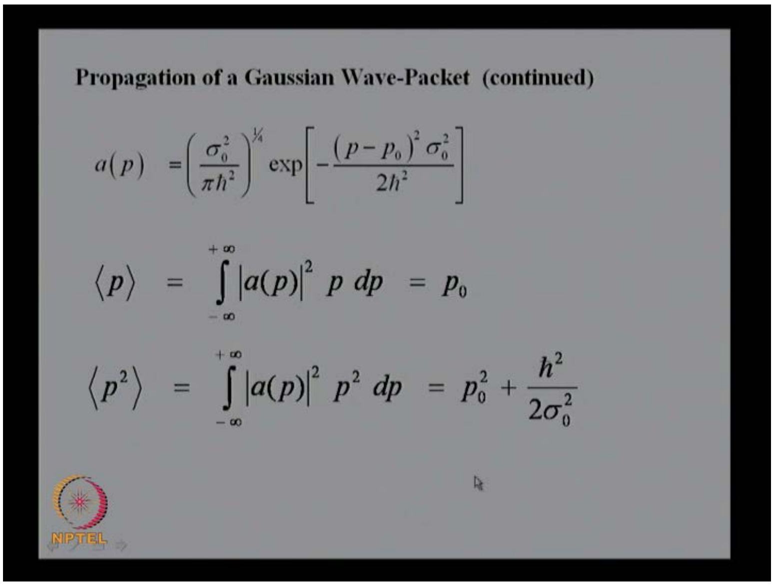

So since a of p is given by this I can then calculate the expectation value of p if I if I i would request all of you to carry out this integration and if I multiply the square of this function with p and carry out this straight forward integration this is the average momentum this is the average momentum with which the wave packet moves and similarly, you can calculate p square so you do this and you obtain this.

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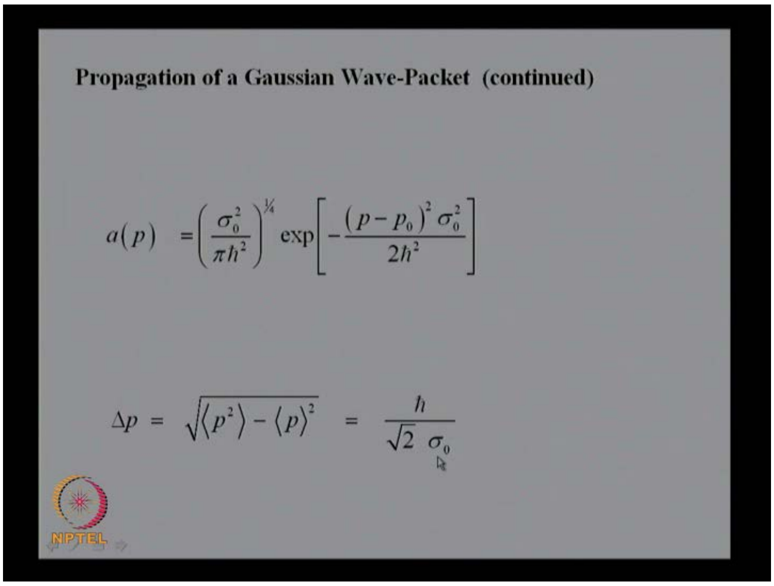

So delta p which does not change with time which does not change with time becomes h cross by root two sigma naught a so at time t equal to zero delta p is so much delta x is so much so delta x delta p is the minimum uncertainty product and that we had discussed earlier.

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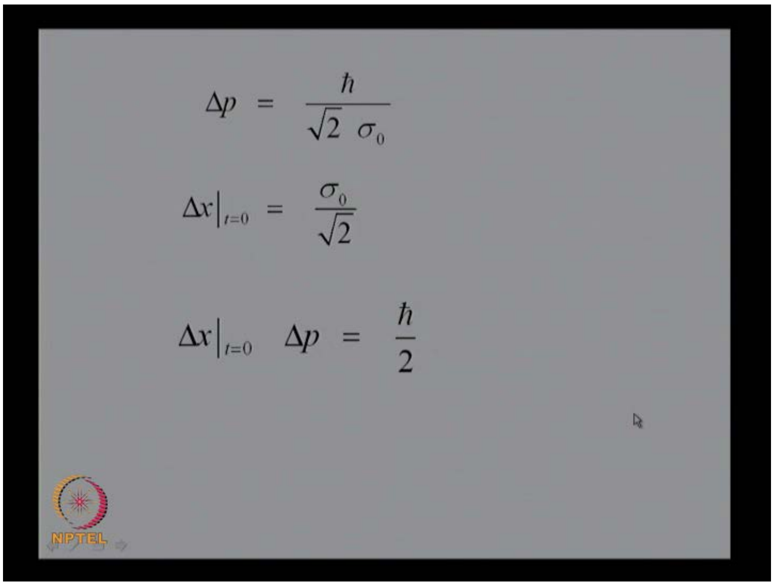

So how do we find the evolution of the wave packet as I said earlier that the psi of x t is given by this and if psi of x comma zero is known.

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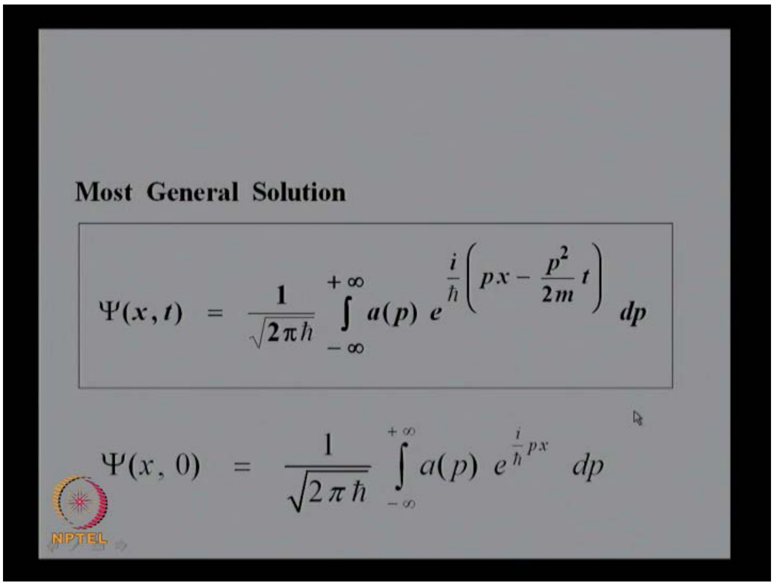

Then I can find out a of p by taking the inverse Fourier transform so I will able to find the a of p I substitute it here and carry out the integration and once again the integration is not very straight forward is is little cumbersome.

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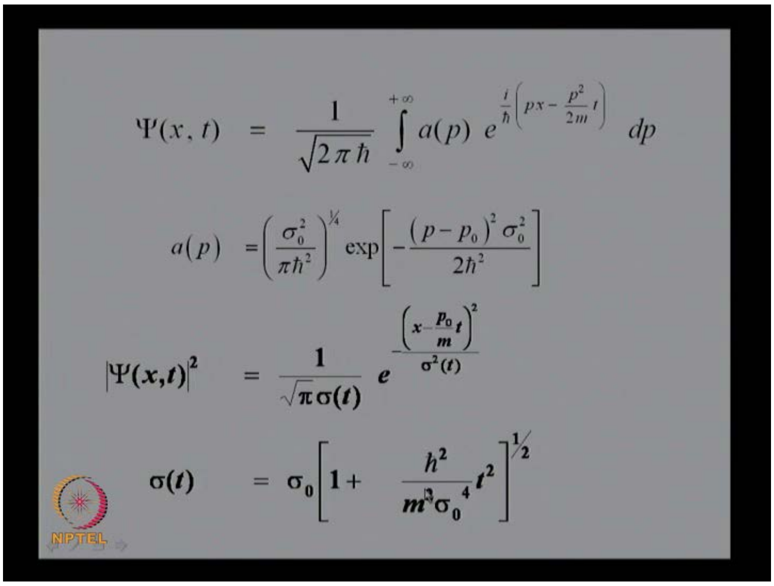

But, it is very straight forward if you do that you will find that mod psi of x t square is equal to one over root two pi mod root pi sigma of t and the wave packet itself moves with the center of the wave packet moves with the velocity p zero by n. This is the group velocity of the wave packet and the width of the Gaussian pulse increases with time increases with time.

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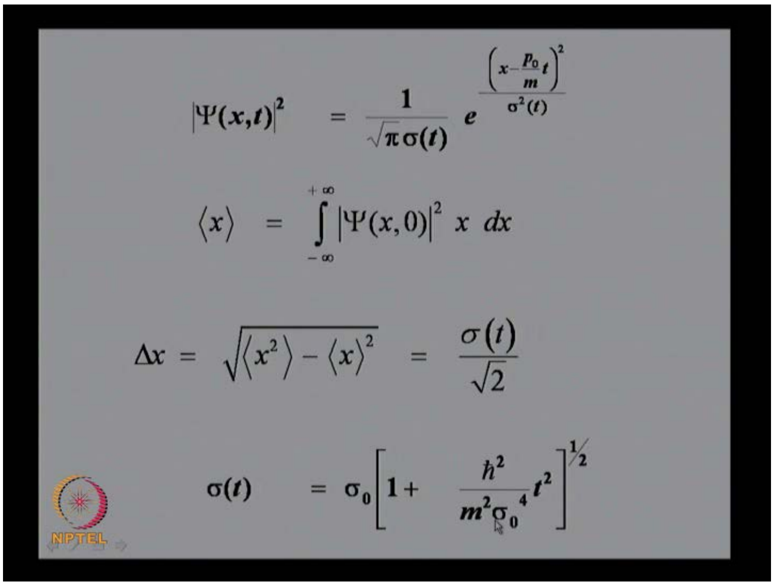

So you will have this wave functions so x is so much so delta x actually increases with time because the sigma of t increases with time.

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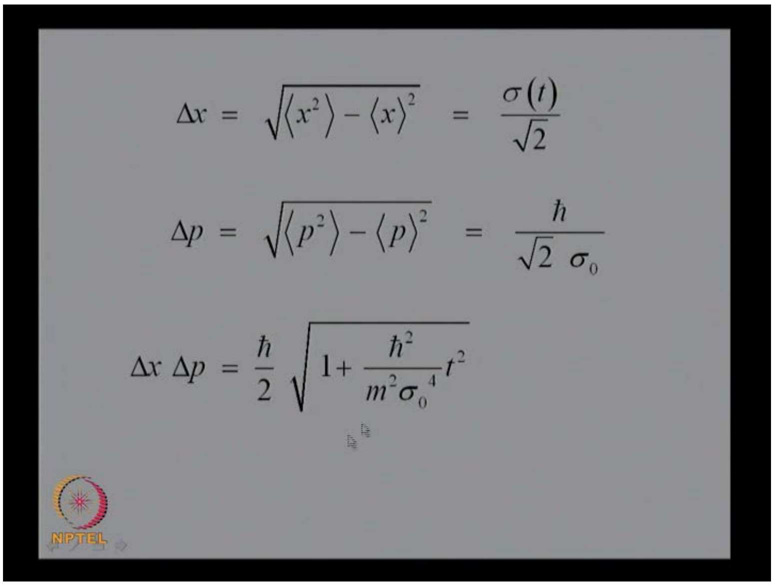

Therefore, the uncertainty product increases with time at t equal to 0 it is the minimum so this is my localized wave packet the electron is described by this wave packet.

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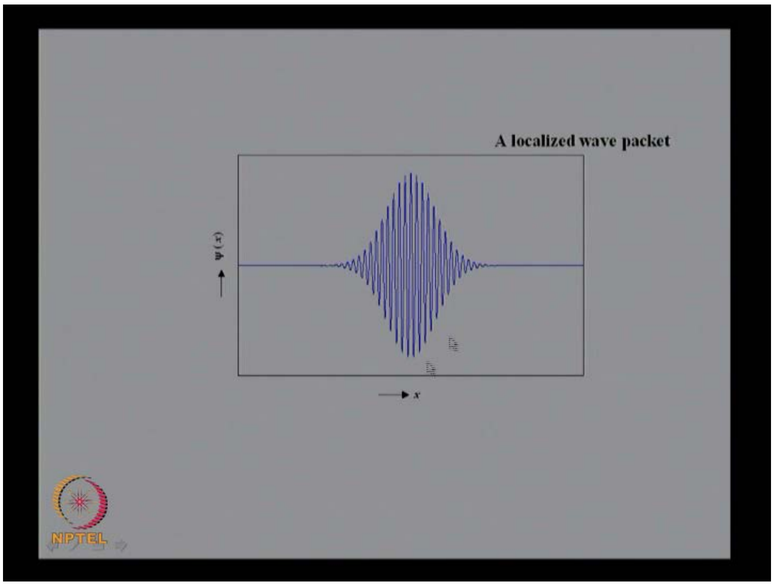

This localized somewhere here somewhere between the here the localization is within the distance of the order of sigma naught and the corresponding momentum distribution is of the order of h cross by delta x so that the 1 certainty product is satisfied.

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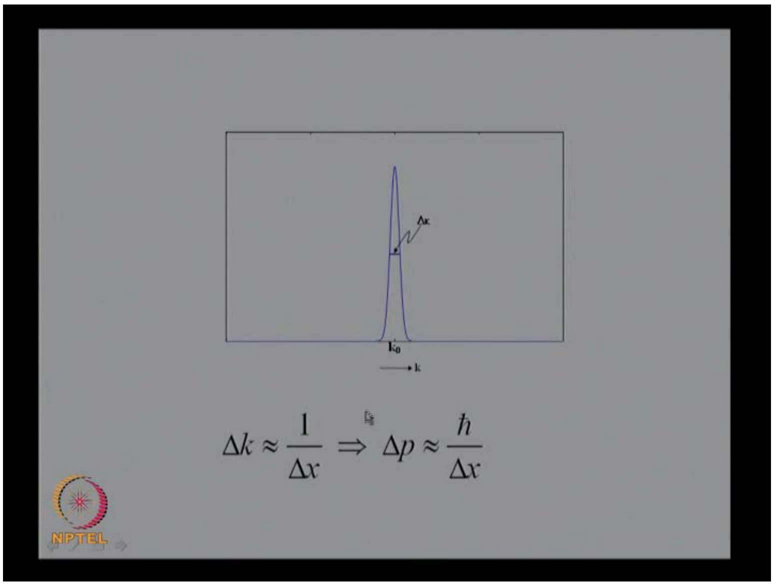

Now this is what I have showed earlier also, this is the evolution of the wave packet and let me do it very carefully so the wave packet.

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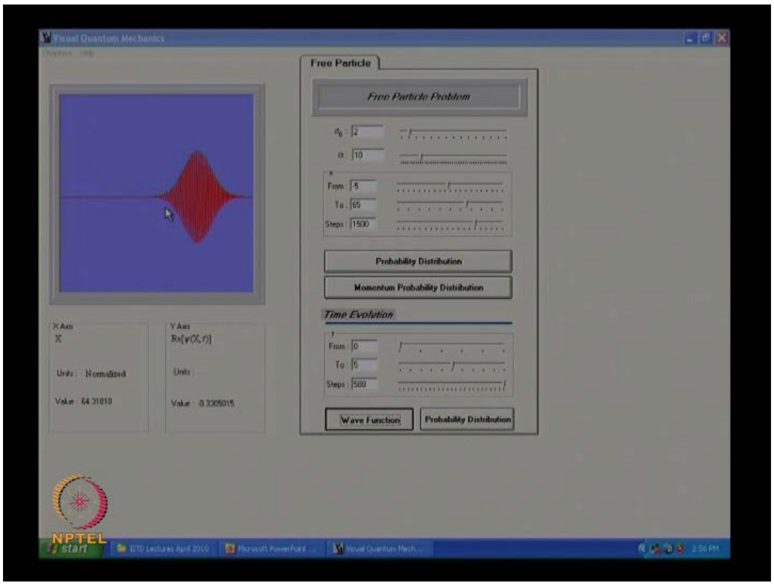

The electron is let me do it more slowly so let us suppose we put it five hundred here and so the electron is described by this wave function so if you ask me the question is the electron a particle or a wave the answer is it is neither it is describe by a wave function so it is somewhere localized where the wave function is finite you can tell you can predict a probability distribution of finding the electron as it evolves with time and therefore, there is an uncertainty in the measurement of x there is an uncertainly in the measurement of p and that is contained in my uncertainty in in in the solution of the Schrodinger equation. So therefore, Schrodinger equation itself contains uncertainty principle so you see I have here the electron is described by this wave function actually it is the real part of the wave function so it is somewhere localized here and the packet itself broadens with time and that is because of dispersion. So therefore, to summarize an electron or a proton or a neutron is neither a particle nor a wave it is describe by the wave function a free particle let us suppose the propagation is only in the x direction and I neglect the y and z variation this described by a wave packet so when I when the electron leaves the filament it is described by the localized wave packet which moves with a velocity equal to p zero by m. So the packet itself moves forward it is localized somewhere there and the localization is consistent with the uncertainty principle so that is what my quantum mechanics tells me that the electron or the proton or the neutron is neither a particle nor a wave it is described by the wave function by the wave function by a wave function psi which is a solution of the Schrodinger equation.

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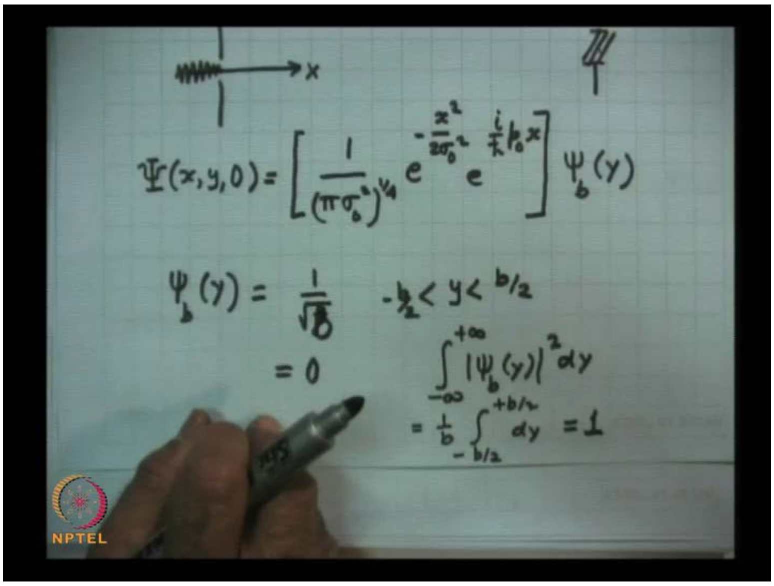

Now let me consider a slightly more difficult problem not difficult little more involved problem but, I have a Gaussian wave packet which is propagating in the x direction this is my x direction and then it has a slit of width d in the y direction so I am just I am neglecting z, so the packet is moving in the x direction. But constructed in the y direction. So so the wave packet here is a Gaussian wave packet so I have here therefore, a wave function psi of x comma y comma zero at time t equal to zero first the x part at time t equal to zero is a pi sigma zero square raise to the power of one by four e to the power of minus x's square by two sigma naught square e to the power of I by h cross p naught x so this the way Gaussian wave packet. Just similar to one that we had considered localized within a distance of sigma naught and propagating in the x direction but, I now multiply by a function y function of y which is such that psi b of y is equal to one over under root of y sorry one over under root of b I am sorry for y less than b by two and minus b by two and zero everywhere else. So I allow this the wave function to be finite only in this region and 0zeroeverywhere else this is my y axis so it is the a Gaussian wave packet encounters a slit of width b now this wave function is normalized that is minus infinity to plus infinity mod psi b of y mod square d y this is equal to one over b from minus b by two to plus b by two this is psi b y square is one over root b so that the square of that is one over b multiplied by d y so this is b by two minus minus b by two that is b by b, so this is one so it is normalized in the x direction and also in the y direction so I want to study the evolution of this wave packet so then what I do is instead of taking a one dimensional Fourier transform I take a two dimensional Fourier transform.

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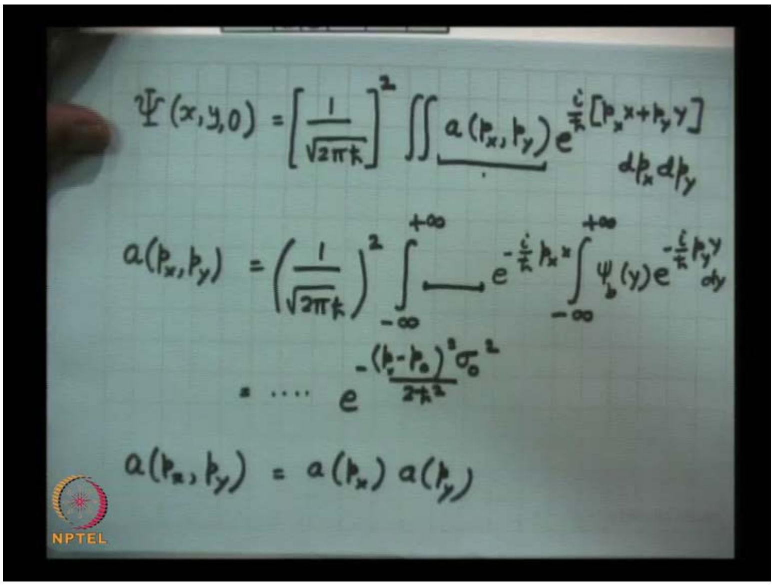

So we will have we write this down as that psi of x comma y comma zero is equal to one over root two pi h cross whole square then integral integral a of p x comma p y e to the power of I by h cross p x x plus p y y d p x d p y. So therefore, in order to determine a p x y I take the two dimensional Fourier transform of psi of x y so I get a p x comma p y is equal to one over under root of two pi h cross whole square and then the integral first integral over x multiplied by e to the power of minus I by h cross p x x and then there is a second integral that is psi b of y e to the power of minus I by h cross p y y d y this is the this is the Gaussian wave packet that we had written down that this this quantity we will substitute here and this quantity is one over root two b so this is also from minus infinity to plus infinity and this is also minus infinity to plus infinity the x part integral will come out to be the same thing so, me factors into e to the power of p minus p naught whole square sigma naught square by two h cross square so that is the integral that just similar to one that we had found out earlier. So actually I can write down a p of x comma p y so this is a product to product function a p x and a p y actually this should be a p x and a p y will be the integral of that.

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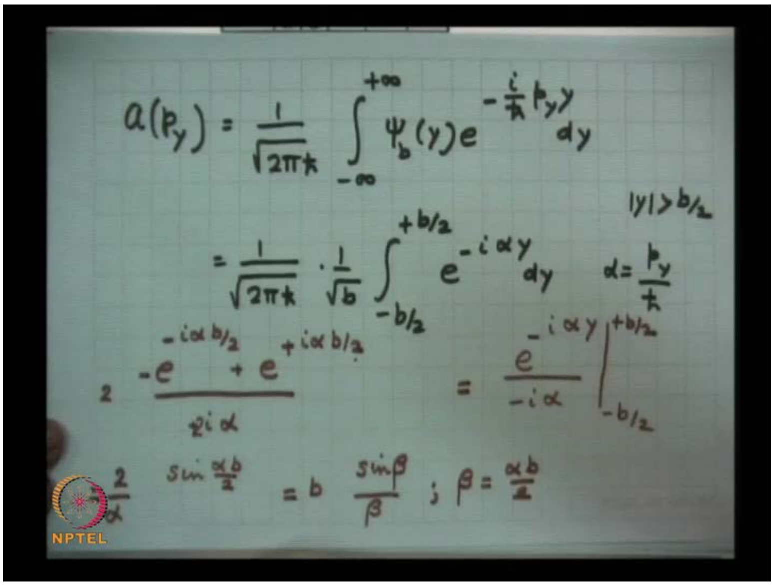

So let me evaluate this so a p y is equal to 1 factor I will take here two pi h cross please see this this is very it will give me a very important result psi b of y p y y d y but, this is 0 for y greater than mod b by two. So therefore, this comes out to be 1 over under root of two pi h cross one over under root of b and then from minus b by two to plus b by two let me put this as e to the power of minus alpha y where alpha is equal to p y by h cross the integration of this is very straight forward that is the integration will be you just have to integrate this and you will find e to the power of minus I alpha y divided by minus I alpha from minus b by two to plus b by two. So this will become if I do it like this so this will become e to the power of minus I alpha b by two minus e to the power of plus I alpha b by two divided by minus I alpha so there is a minus sign sitting in the denominator I put it plus sign here plus sign here and minus sign here multiplied by two here and multiplied by two here so this becomes two by two alpha two by alpha this becomes two by alpha and this will be e to the power of I alpha b by two minus e to the power of minus i alpha b by two divided by alpha divided by alpha divided by two I so that will be sin of alpha b by two. So this is equal to this this is equal to this so I can write this down as I can put a b factor here sin beta by beta where beta is equal to alpha b by two where beta is equal to alpha b by two.

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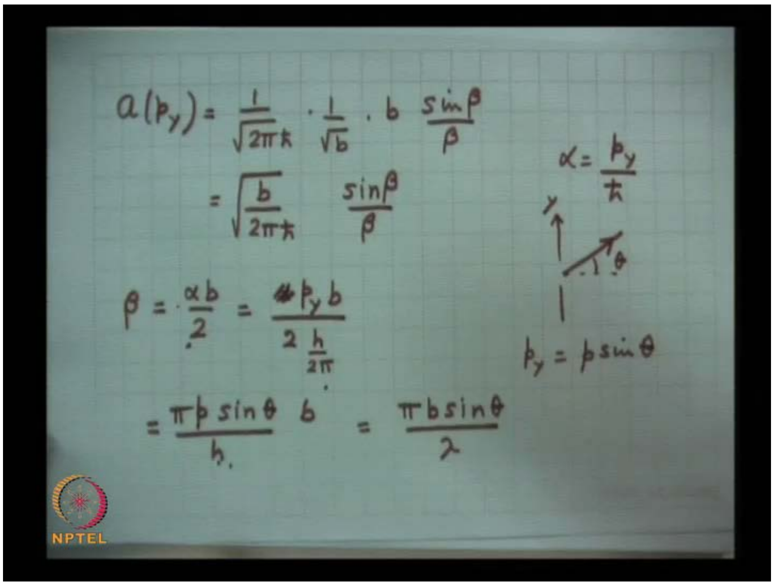

And let me write down what is so we obtain we obtain a of p y a of p y as one over under root of two pi h cross one over under root of b times b sin beta by beta. So this becomes equal to some constant in front b by two pi h cross sin beta by beta and what is beta beta is equal to alpha b by two if you may recall that alpha was equal to p y by h cross so this becomes alpha p y b by two h cross h cross is h over two pi so, that is alpha sorry alpha is equal to p y by h cross so alpha is equal to p y by h cross is a factor two here so the two two cancel out and what is p y. If you see this if the electron gets moving in this direction and if this angle which is the angle of diffraction is theta and this is the y direction then p y is equal to p sin theta, so you will have p y is equal to p sin theta pi will come above and then h multiplied by b h by p is lambda so you obtain pi b sin theta by lambda pi b sin theta by lambda.

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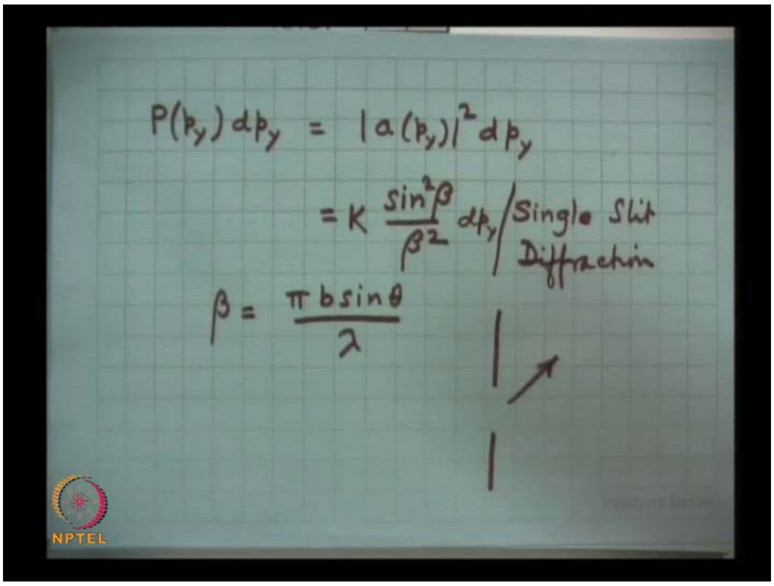

So the probability distribution function will be proportional to that is probability of the momentum lying between p y and d p y will be equal to mod a p y square d p y and that will be proportional to sin square some constant sin square beta by beta square where beta is equal to pi b sin theta by lambda.

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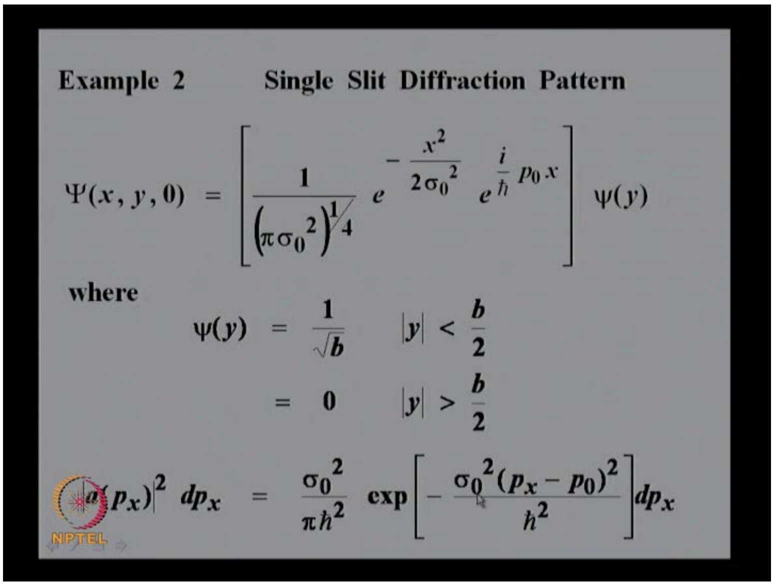

And this is my single slit diffraction pattern this is the single slit diffraction pattern so how do I explain the diffraction phenomenon as soon as I constrict the electron so this slit itself imparts a momentum in the y direction and the probability of the momentum being lying between p y and p y plus d p y will be proportional to sin square beta by beta square and that is the single slit diffraction experiment. So if I show you to conclude this lecture so I have the I have the single slit diffraction experiment in which you have a Gaussian wave packet in the x direction and in the y direction you have a single slit therefore, the probability of the momentum x component of the momentum lying between p x and p x plus d p x is given by a Gaussian function.

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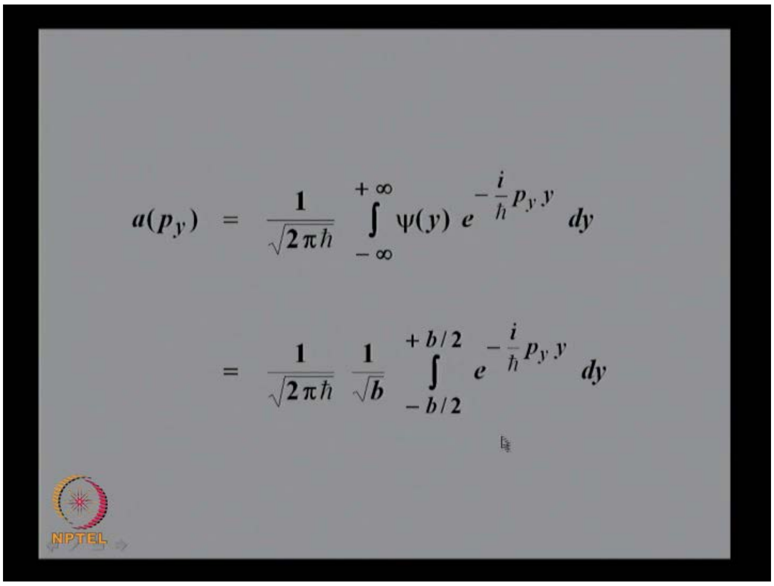

On the other hand if I want to find out the probability distribution function for p y then I integrate this.

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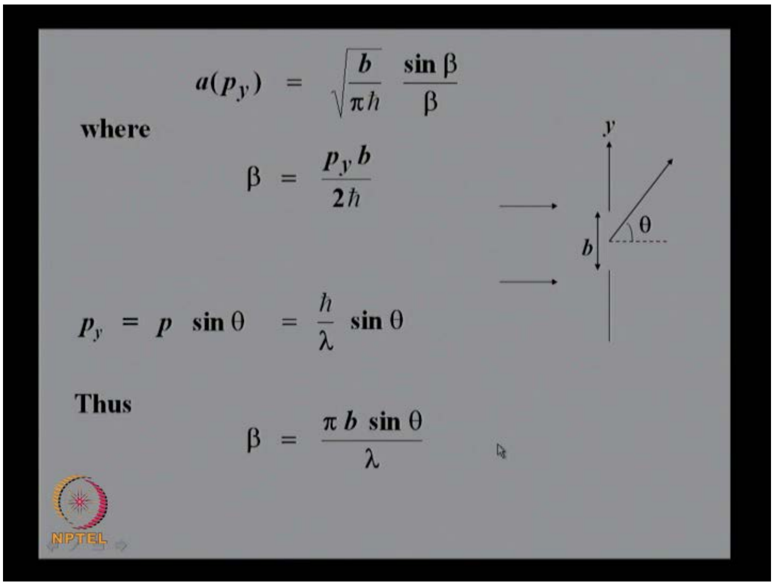

And I obtain sin beta by beta so that the probability of the y component of the momentum lying between p y and p y plus d p y will be proportional to the sin square beta by beta square into d p y.

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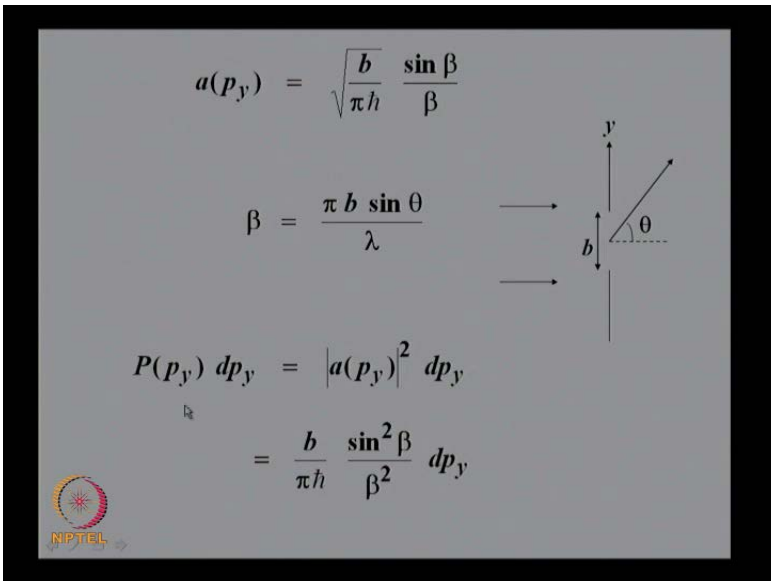

So that as soon as you constrict the particle to pass through the slit the slit itself imparts a momentum and you obtain the single slit diffraction experiment.

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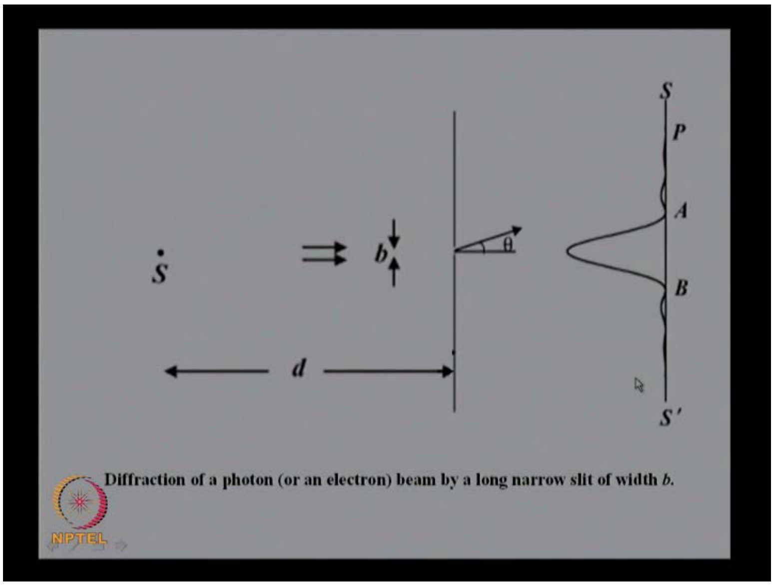

Where an individual electron will lie I cannot I can only predict a probability distribution function so that if the experiment was carried out with a large number of electrons the single slit diffraction pattern will be observed therefore, I have a source of electrons protons neutrons alpha particles or anything that you can think of it is the I describe this as a Gaussian wave packet propagating in the x direction and then I constrict it within a distance of the order of b to obtain the single slit diffraction pattern.

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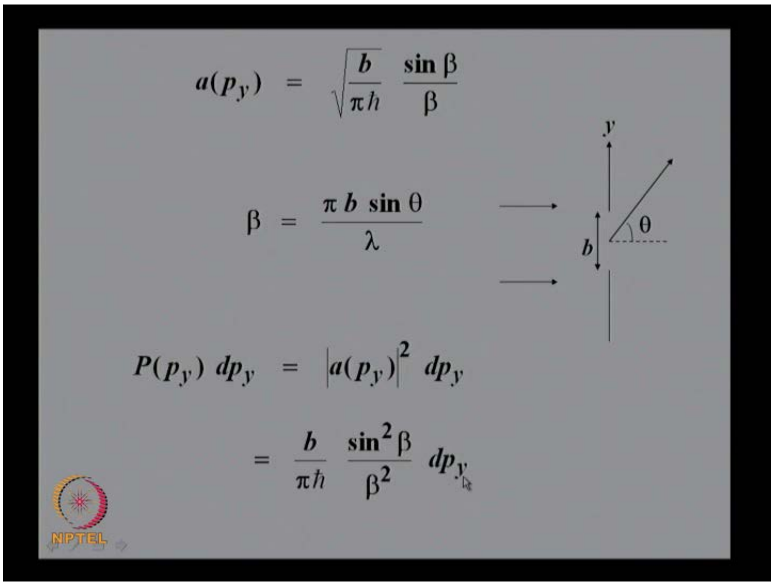

Where an individual electron or the proton will land up no 1 can predict 1 can only predict a probability distribution and therefore, and that probability distribution is the same as the as the single slit diffraction pattern as you must have read in your under graduate optics course.We will continue from this point onwards in my next lecture thank you.