Basics Quantum Mechanics

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Module No # 02

Simple Solutions of the 1 Dimensional Schrodinger Equation.

Lecture No # 06

Expectation Values and the Uncertainty Principle

In the last lecture we had obtained a physical interpretation of the wave function. The Schrodinger equation has written in the terms of wave function psi and we had said we had derived an equation of continuity from which we could interpret mod psi square d tau as the probability of finding the particle between in the volume element d tau.

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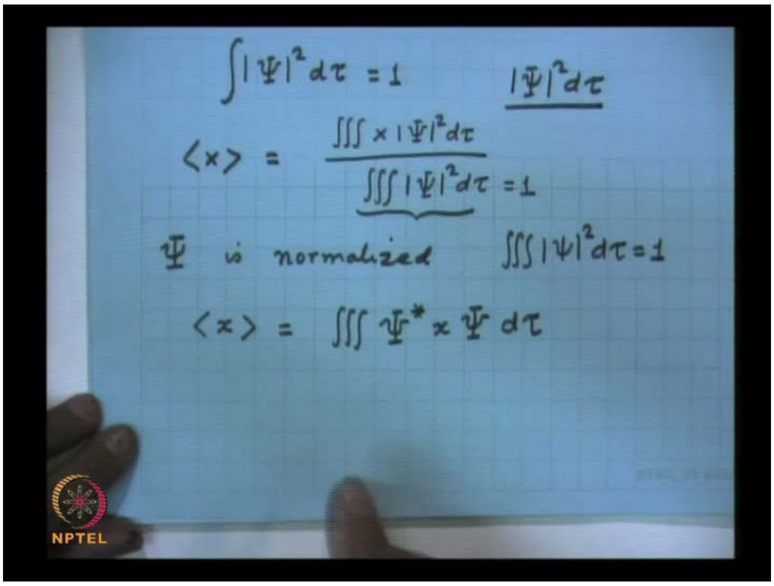

Actually we obtain that this is this should be proportional to the probability but then if we normalize this in the entire space, so then we can interpret mod side square d tau as the probability of finding the particle in the volume element d tau. So associated with the particle if I want to find out the expectation value of any quantity x then I just have to multiply by the probability density function and integrate over the dais space actually the integration is something like this that the all the integration is over the entire space x mod side square d tau divided by integral mod psi square d tau. Because mod psi square d tau is proportional to the probability but, if this integral is 1 which will assume from now on words so will assume from now on words that the function psi is normalized and if the wave function is normalized then mode psi square this integral over the entire space is 1 and therefore the denominator is one. So I will obtain x psi star psi and I will write this for reasons which will become clear in a moment as x is equal to integral psi star x psi d tau. Why do we write it this particular way it will become clear in 1 minute.

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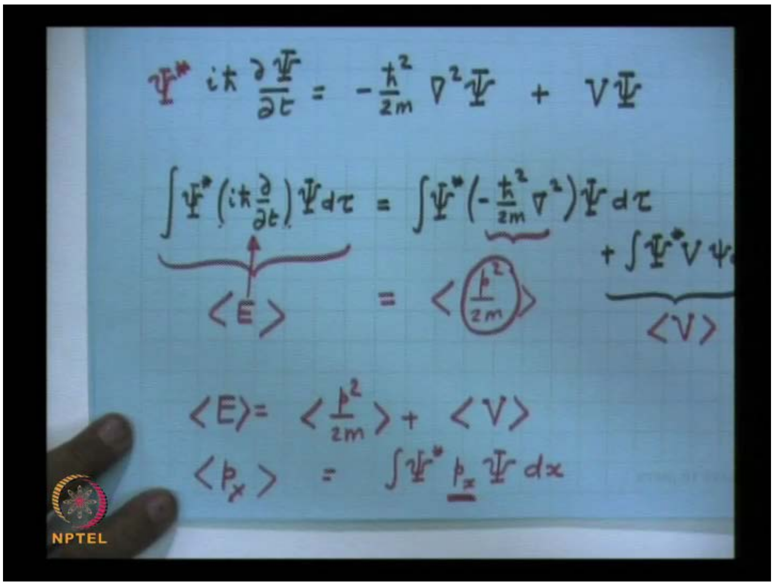

Now we have the time dependent Schrodinger equation with 3 dimensional Schrodinger equation i h cross delta psi by delta t is equal to minus h cross's square by 2 m del square psi plus V psi, what I do is that I multiplication multiply this equation by psi star and then integrate. So I obtain so I obtain on the left hand please see this carefully. This integration is over the entire space so the integral is really at 3 dimensional integral psi star multiplied by i h cross delta by delta t into psi d tau integration is over the entire space and then we will have psi star multiplied by minus h cross square by 2 m del square psi d tau plus psi star V times psi. On the last term this term is just the potential energy function multiplied by the probability density function integrated over the entire space, so this quantity is the expectation value of the potential energy. Classically we know that the total energy is the kinetic energy plus the potential energy so we should expect that the expectation value of the total energy must be equal to the expectation value of kinetic energy plus the expectation value of the potential energy. So therefore, this quantity should be the expectation value of total energy and this quantity should be the expectation value of the kinetic energy. And now we see that the quantity within the bracket within this within the bracket is the operator corresponding to the energy e. Similarly p square is p x square plus p y square plus p z square so this is minus h cross square by 2 m delta 2 by delta x square plus delta 2 by delta y square plus delta 2 by delta z square, so this quantity within the brackets is the operator corresponding to p square by 2 m. So therefore, we get the recipe that if I want to find the expectation value for example, p p x then what I have to do is I will write down psi star p x psi d tau where p x is the operator representation of p x. So therefore from above we obtain the recipe that if I want to find out the expectation value of x y and z this equal to this all these integrals are 3 dimensional integral psi star psi x d tau they are normalized, similarly for y, similarly for z for p x the expectation value of p x is equal to psi star p x psi d tau which is equal to psi star minus i h cross delta psi by delta x d tau

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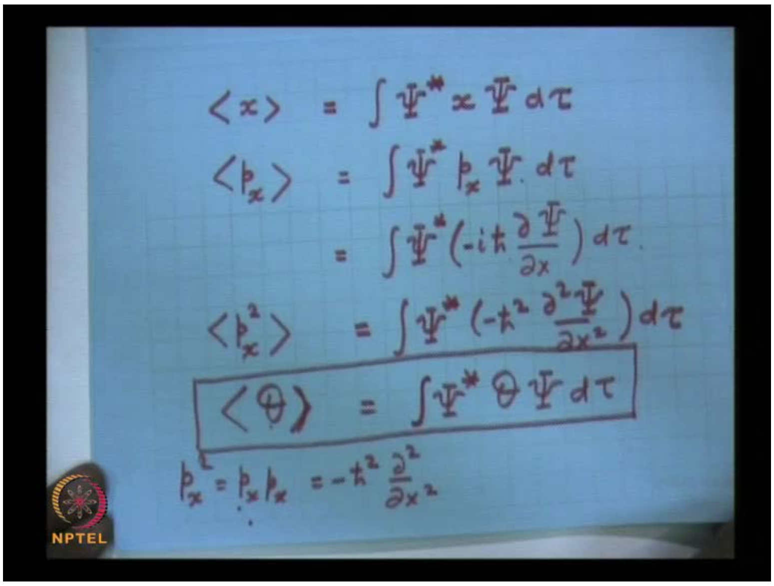

If I want the expectation value of p x square then p x square as we know is p x times p x so minus I by h cross delta by delta x into minus i h cross that is minus h cross square delta 2 by delta x square, so the p x square the expectation value is psi star minus h cross square delta 2 psi by delta x square. And the general recipe if I want to measure a dynamical variable o then the expectation value of this I represent that by the corresponding operator and put between psi star and psi o psi d tau this is the general recipe for determining the expectation value. So therefore, we must remember these 2 3 equations the expectation value is of course very simple the expectation value of p x is psi star on the left and psi on the left right the p x represented by this differential operator representation and this is for p x square and if you want write the kinetic energy then I have to just divide by 2 m. In general if I want to make a measurement of a dynamical variable represented by o and if I want to find out the expectation value then all that I have to do is to integrate psi star o psi d tau. I am assuming that the wave function is normalized with this we will try to give an exact formulation of the uncertainty principle between x and p x that I in in statistical theories if there is a variation of a parameter then the spread is measured in terms of mean square deviation and that is delta x is defined as x square the average of x square minus x average square under the root so this is the spread the uncertainty in x

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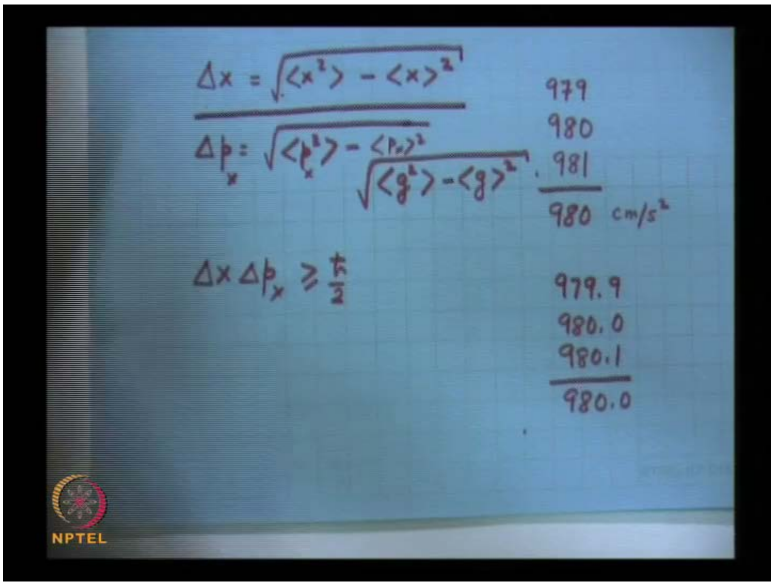

Now for example, let me give you an example of an experiment I measuring the acceleration due to gravity I use a simple pendulum and in three random measurement I change the length of the pendulum and in three random measurements I get nine seventy nine meter per second square nine eighty and nine eighty one. The mean of that is nine eighty centimeter per second square now I use a kater’s pendulum to make a measurement of acceleration due to gravity but, there I get 3 values like 979.99 80.0 and

980.1 if I take a mean of that again I will get nine eighty. But there is a difference between these two here the uncertainty is much more than this here the uncertainty of the order of 1 and here the uncertainty is the order of 0.1 how do we express this uncertainty this we express in terms of carrying out let us suppose the spread will be you will write down is will be the average value of g square minus the square of the average value and then take this square root. In this case it will come out to be point 8 or 0.9 and in this case it will come out to be 0.08 or 0.09 or 0.1 above something like that so this spread the variation if I make a large number of measurement the variation is usually expressed by this quantity delta x I take the average of the square minus square of the average. Similarly if I make the measurement of the momentum then I will write it as the square root of the average of the square of the momentum, I am considering only the x component I only considering the x component so p x square minus p x whole square I will show that for any wave function the product delta x delta p x is greater than or equal to h cross by 2 so this is an exact statement for the uncertainty relation.

Now in order to derive that we will first prove an inequality and this is known as Schrodinger inequality and inequality I have f star f d tau multiplied by g star g d tau where all functions f and g are well behaved square integrable functions

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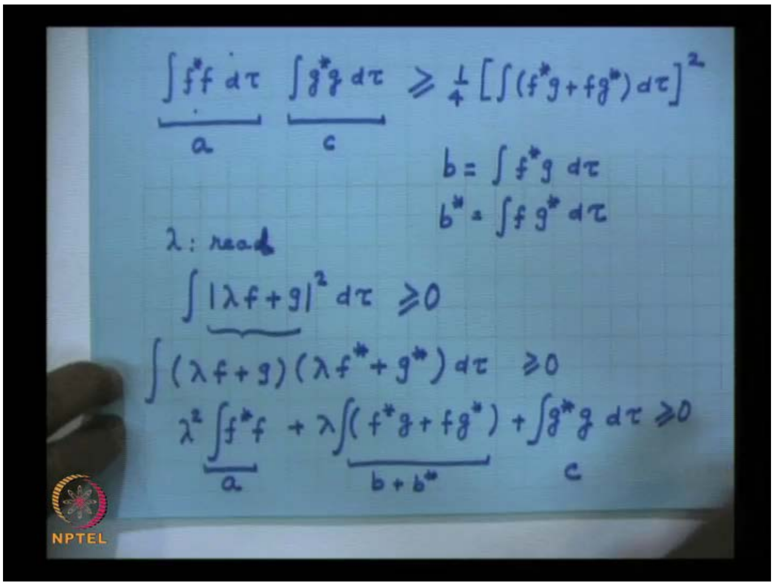

this is always greater than or equal to one by four brackets integral f star g plus f g star d tau whole square. Now this quantity we denote by a this quantity we denote by c and we write down that b is equal to integral f star g d tau therefore, b star is equal to the complex conjugate of this is f g star d tau. All this integrals are over the entire space and they are all three dimensional integrals. Now in order to prove this inequality where f g are all arbitrary function, arbitrary means single valued and integrable functions and in order to prove that I consider a parameter lambda which is real lambda I assume to be real and I have I consider the integral lambda f plus g mod square d tau. Now since lambda is real so this quantity is positive because it is the square of the modulus and integrated over the entire space so this must be always greater than or equal 0 positive always positive because this is the integrant is a positive indefinite quantity. So let me write down the integrant so that is equal to lambda f plus g multiplied by lambda f star plus g star, because lambda is itself a real quantity so I multiply this out so I get lambda square f star f I can write one before that lambda times f star g plus f g star plus g star g. So I multiply integrate this d tau and this is always positive definite, so I integrate it here I integrate it here so I integrate it here all integrals over entire space so this is always positive definite so this is a as I have renounced here and this is b plus b star and this is c, so I obtain lambda square a plus lambda b plus b star plus c will be always greater than zero.

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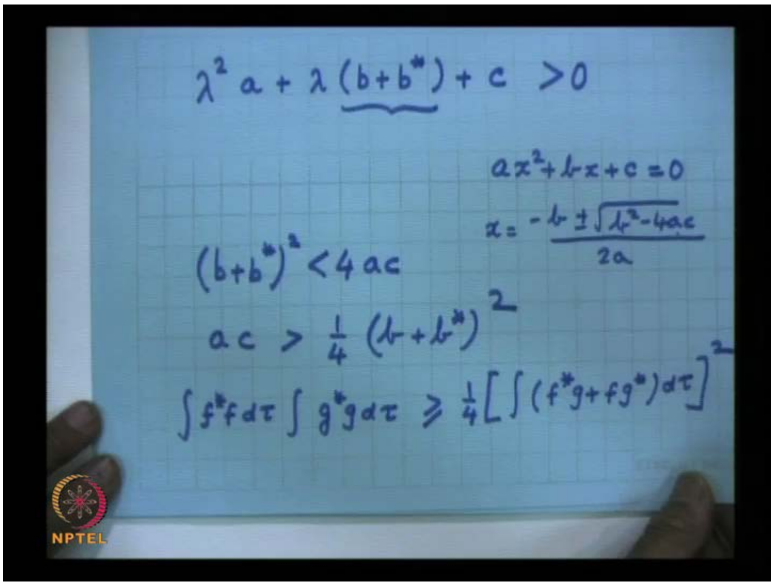

This means if you plot this as a function of lambda, it will have no zeros and therefore for example, as you will know that you see if I consider an equation like this a x square plus b x plus c the roots of this equation are x is equal to minus b plus minus under root of b square minus four a c divided by two a but, if this quantity is always positive then there are no real roots and therefore, this square must be equal to must be less than four a c. So that this quantity is negative and therefore, it will have no real roots, so this quantity b plus b b star whole square must be less than or equal to less than equal to four a c so you get a c must be greater than one by four b plus b star whole square and that is my inequality that f star a was equal to f star that is f star f d tau c was equal to g star g d tau this must be greater than one by four b plus b star whole square that is integral f star g plus f g star d tau whole square. So therefore, we have been able to to to derive what is known as Schrodinger inequality

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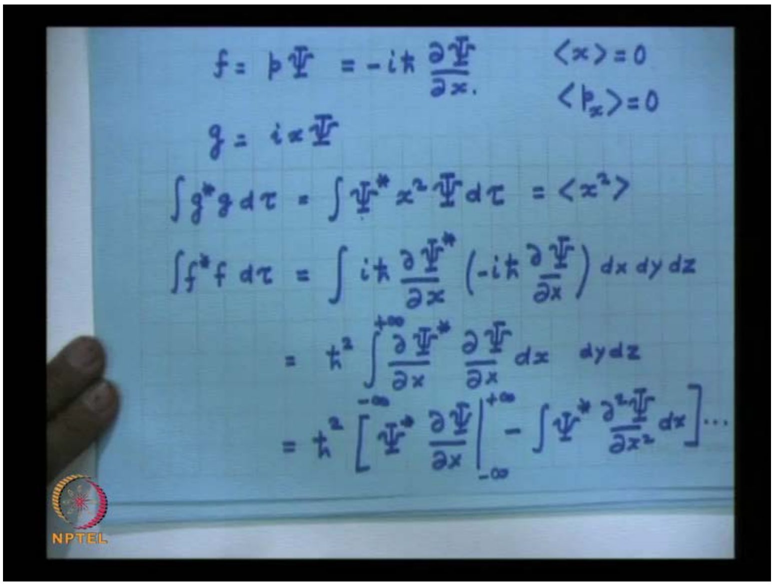

Now we assume that we assume that f is equal to p psi and p psi is equal to minus i h cross delta psi by delta x and g is equal to i times x psi, then you can see we will discuss the easiest case first g star g d tau g star s d tau g star will be i times minus i plus 1, so this will be g star will be x into psi star so this will be psi star x square psi d tau. So this is my the expectation value of x square we will we are considering the special case although the more general case can be considered very easily that the expectation value of x is 0 I can always choose the origin in such a way that expectation value of x is zero. we further assume the expectation value of p x is zero. So g star g d tau I x psi multiplied by minus i x psi star so i times minus i becomes one so psi star x square psi d tau so this is the expectation value of of x square. Similarly, f star f d tau will be equal to if you see this f star will be i h cross delta psi star by delta x multiplied by f that is minus ih cross delta psi by delta x multiplied by d tau that is d x d y d z. So I times minus i is one so h cross square if I take outside h cross square and I just consider the x part of the integration the y and z part is also there so I get delta psi star by delta x into delta psi by delta x d x actually into d y d z but, I omitting that in this moment. So this I integrate by parts and I obtain h cross square this I take as the integrating factor psi star delta psi by delta x from minus infinity to plus infinity minus integral psi star delta two psi by delta x square d x of course multiplied by d y d z and d y d z integrations are also there.

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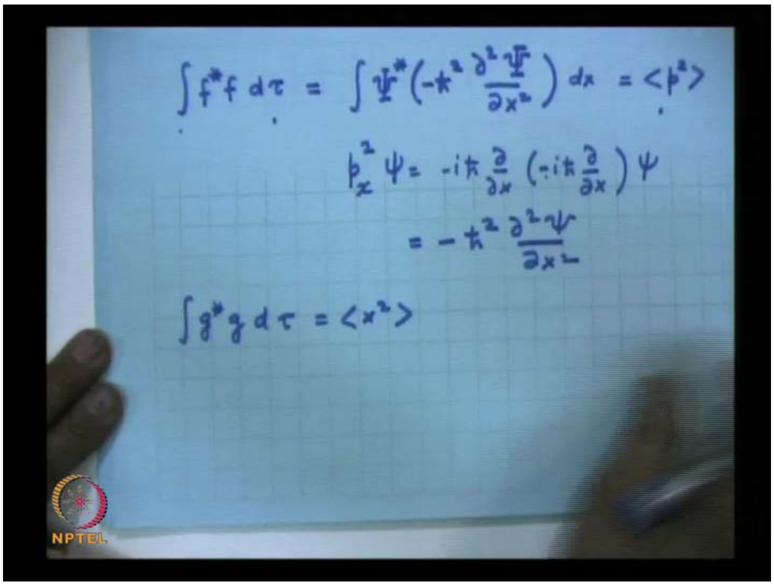

Now for a localized wave packet for a particle which is localized in a small region of space this wave function has to vanish at infinity so this term vanishes at the upper and lower limit and I obtain only this so I finally, obtain I finally, obtain integral f star f d tau is equal to psi star minus h cross square I take this inside delta 2 psi by delta x square d x similarly, d y and d z. So this is the expectation value of p x square because you remember that p x is minus i h cross delta by delta x and p x square will be minus i h cross d by delta x so p x square psi is minus i h cross delta by delta x into psi, so this will minus minus plus h cross minus minus plus and then this I square is minus so this is equal to minus h cross square delta two psi by delta x square. So this quantity becomes the expectation value of p x square but, I will just write p square and the third term on right side will be if you remember the therefore, so f star f d tau is p square g star g d tau we are just now obtained g star g d tau was equal to x square will be the term on the right hand side.

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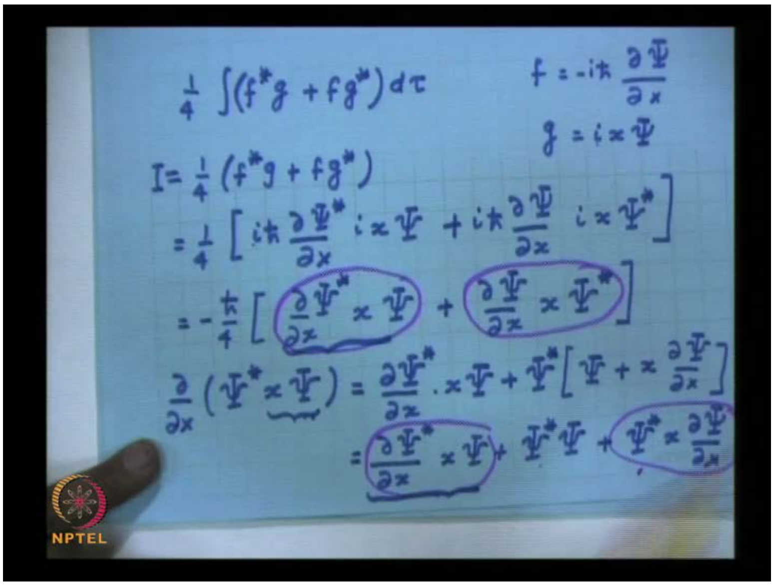

You see in the inequality we had we had 1 over this is f star f this is g star g is greater than equal to one over four f star g plus f g star so let me evaluate this so f star g let me do it in a fresh page that one by four integral f star g plus f g star again d tau is d x d y d z, so f as we may recall was equal to minus i h cross so f as you may recall was minus i h cross delta psi by delta x and g was equal to i x psi so you will have so let me just consider the integrant the integrant is equal to one over f star g plus f g star and this is equal to one over four f star that is i h cross delta psi star by delta x into g that is i x psi plus f that is f is minus I h cross delta psi by delta x you have to do this little carefully and g star is minus i so minus minus becomes plus so i x psi star, so this is i times i is minus one and this is i times i is minus one so this becomes minus h cross by four delta by delta x psi star x i plus delta psi by delta x x psi star.

Now if you write down this equation this expression delta by delta x psi star x i then this will be please see delta psi star by delta x into x i plus psi star into please see this carefully delta by delta x of these two terms the product of these two terms. And if I differentiate this if I differentiate this first I will get psi because the differential coefficient of x is one plus x delta psi by delta x. So you obtain so you obtain if you these two terms are appearing here if you see this carefully this is delta psi star delta x multiplied by x psi plus psi star psi plus psi star x delta psi by delta x, so if you see this this term is this term let me encircle them with red so this term is the same as this term and this term is the same as this term, so this plus this which is the quantity inside the square brackets here is this minus this.

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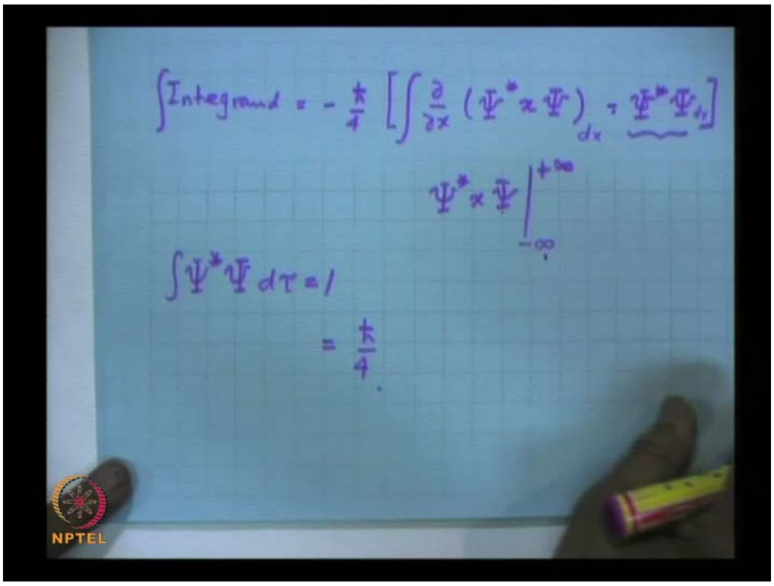

Therefore, a integrand will become the integrand will become minus h cross by for delta by delta x i has to just patiently work this out to straight forward but, it requires a little patience minus psi star psi. If I integrate this so I have to integrand if I had to integrate this with respect to x and this with respect to d x and then d y d z then the integration over x will be psi star x psi from minus infinity to plus infinity, so the wave function is going to vanish at both plus infinity and minus infinity therefore this term will be zero and if the wave function is normalized so psi star psi d tau is one is one if the wave function is normalized this your minus sign sitting outside so you will get h cross by four.

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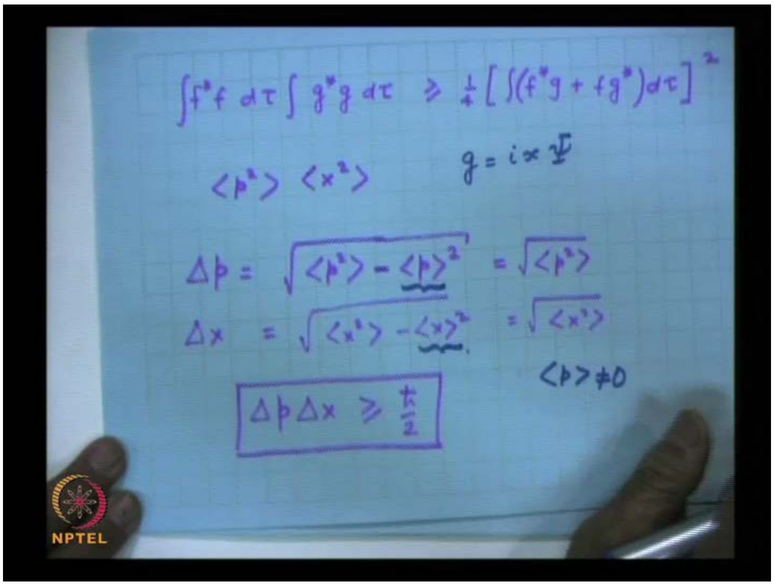

So you will get the relation that a that a if I substitute that in a let me let me put it that f star we had obtained that f star f d tau multiplied multiplied by g star g d tau is greater than or equal to one fourth of this integral f star g plus f g star d tau whole square. So you will obtain so you obtain that that this was equal to if I remember it rightly that one was g star g was equal to I have found that out g star g was equal to x's square and this was equal to p square. So as you know that delta p is equal to under root of p square minus p average whole square i'm assuming p average to be zero therefore, this is equal to I am taking the special case of p average being zero, so this is square root of p square and delta x is equal to under root of x's square minus x average square which is under root of x's square I am assuming I can this I can always choose the origin of my coordinates such that the x average is zero. So this from if I substitute this here I will get the uncertainty relation that delta p delta x is always greater than or equal to h cross by two this is the uncertainty relation that we have proved from the first principles and let me let me give you a few examples. So from the Schwarz's inequality which is written here we have and then by assuming that f is given by g is given by i x I, g was equal to i x i and similarly, we had assumed an expression for f we have been able to prove that only thing that we have assumed is that the expectation value of p is zero and expectation value of x is zero but, expectation of value of x zero is does not mean anything because you can always choose the origin to be such that the expectation value of x is zero but, expectation value of p is zero one can also generalize this for the case when the expectation value of p is not equal to zero.

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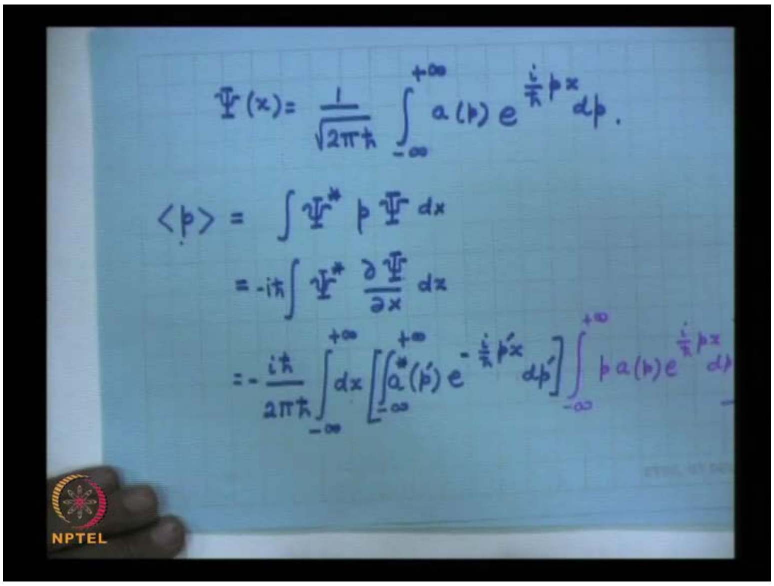

Now let me go back having proved the uncertainty principle let me go back to a simple wave packet so the simple wave packet is a one dimensional packet that we had considered that psi of x is equal to I consider this as a super position of plane waves under root of two pi h cross minus infinity a one dimensional wave packet a of p E to the power of i by h cross p x d p. Now the expectation value of p as we had discussed earlier is equal to psi star p psi where p is the operator representing p the variable p and as we all know now that what we have been discussing that this is equal to minus i h cross minus i h cross psi star delta psi by delta x d x so what I do is I substitute for psi star here I substitute for psi here it is little complicated but, if you work this out it is worth it. So I psi star will be complex conjugate of this so let us do do this carefully i h cross and then two pi h cross will come here two pi h cross. And now there are three integrals one for psi star another for psi and the third one is on d x, so please see this first integral is over d x going from minus infinity to plus infinity then we write down the expression for psi star psi star will be two pi h cross I have already taken outside so this will be a star p a star p E to the power of minus i by h cross p x d p the limits are from minus infinity to plus infinity and then delta psi by delta x so let me do it with a red pen so two pi h cross, I have already taken outside so I will have minus infinity to plus infinity, if I differentiate with respect to x then I will get a p inside so I get p times a of p e to the power of i by h cross p x d p. Now here I have to be very careful till now it is all right if I first integrate this and then integrate this and then carry out this integration but, I am going to jumble up the integration then this p has to be distinguished from this p and therefore, I put a prime here now I can write all the three integrals together then this p prime will not get confused with this p.

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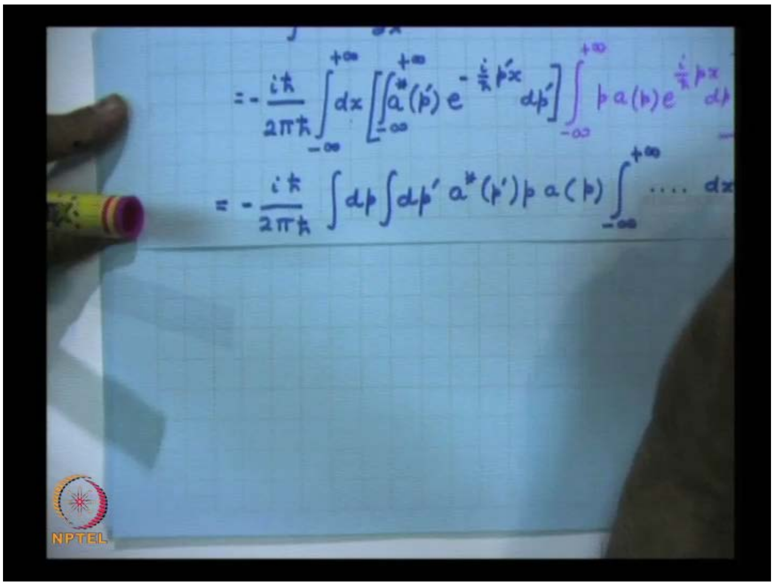

So let me write it down that that this p p will be equal to minus i by h cross by two pi h cross, I carry out this d p and then d p prime collect all the terms which involve only p and p prime and these are a star p prime p a of p and then there is an integral over x, let me write this down what is the integral over x.

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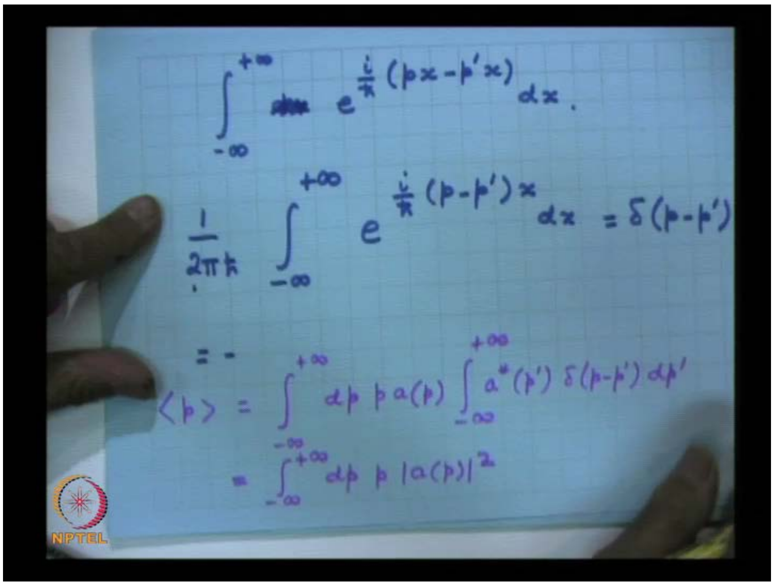

So the integral over x is minus infinity to plus infinity d x e to the power of i by h cross p x minus p prime x d x. So if I take the factor to pi h cross this will be minus infinity to plus infinity I am sorry I have written d x twice so e by e to the power of i by h cross p minus p prime into x into d x and this as you know is delta of p minus p prime. So therefore, in this integral in this integral I have taken this factor here and this factor this integral and I obtain I will obtain minus I am sorry in I i that is what I made a mistake that when I differentiated delta psi by delta x I will not get just p I will get I by h cross p so this will be i by h cross sorry. So so i by h cross, so that I i will multiply by i will become minus one and this will become plus h cross h cross I hope you understand what I am trying to say that we had here delta psi by delta x and when I differentiate this with respect to x then I will get an i by h cross times p into E to the power of I by h cross p x. So I had forgotten the factor i by h cross so i times i is minus one minus minus is plus and the h cross will cancel out with this and then so this two factors will go away and this will become plus and this will become two pi h cross.

Now this two pi h cross I have taken here so I will obtain for expectation value of p this remarkable result that minus infinity to plus infinity d p and if I write down p the a p star a star p prime then delta of p minus p prime d p prime so if I carry out this integration over p prime then this is just a star p so I get this as minus infinity to plus infinity d p p mod a p square.

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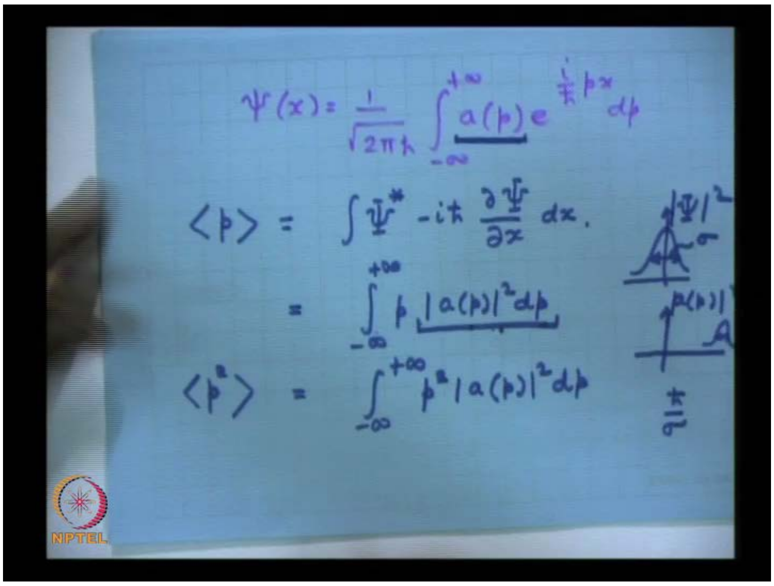

So so we have for any wave function psi for any wave function psi if I write as one over two pi h cross integral a p e to the power of i by h cross p x d p from minus infinity to plus infinity then then the expectation value of p will be given by psi star p psi that is minus i h cross delta psi by delta x into d x and if you we just carried out the entire manipulation entire algebra and we found that this is equal to p into a of p mod square d p therefore. Similarly if I calculate p square I will find that this is equal to minus infinity I leave this is an exercise you have to differentiate this twice it is very easy it is very straightforward and you will have a p square d p.

Thus we can interpret a p square d p as the probability of finding the momentum between p and p plus d p, I must add probability of finding the x component of the momentum between p x p and p plus d p therefore, this is also physically obvious because what is an integral integral is the superposition of this wave functions and therefore, in this case e this represents the momentum spread of the wave function the the the quantity a p square represents the momentum spread of the wave function. So if a particle is localized within a distance of the order of sigma if this is the wave function then the corresponding momentum spread function a of p mod square this is say mod psi square the mod p a p square will be localized also within a distance within momentums spreads function will be of the order of h cross pi sigma.

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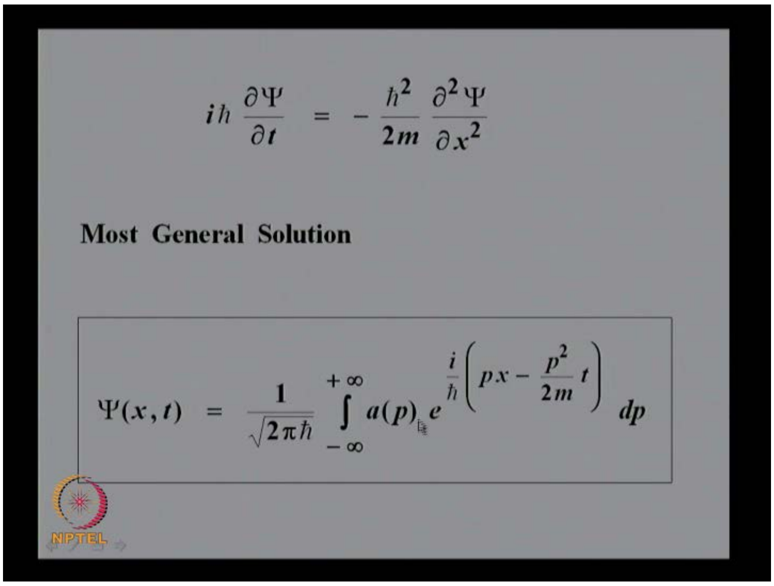

So therefore, let me we note down the two terms back we wrote down for the free particle the most general solution was given by this of the time independent of the time dependent Schrodinger equation and here a p represents we have now physically interpreted a p represents the momentum distribution function.

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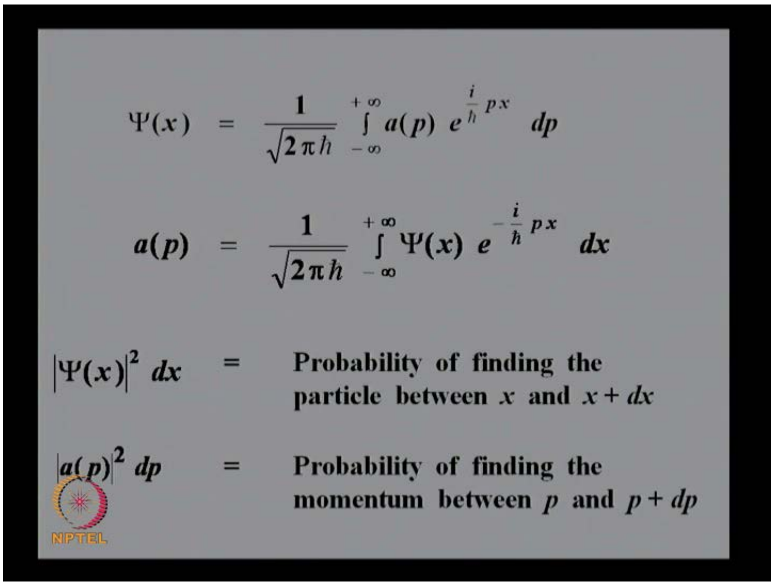

And this is how from the given form of psi of x I can determine the corresponding a of p by taking the inverse Fourier transform and interpret psi of x mod square d x as probability of finding the particle between x and x plus d x and a p square d p will be the probability of finding the particle or finding the momentum between p and p plus d p.

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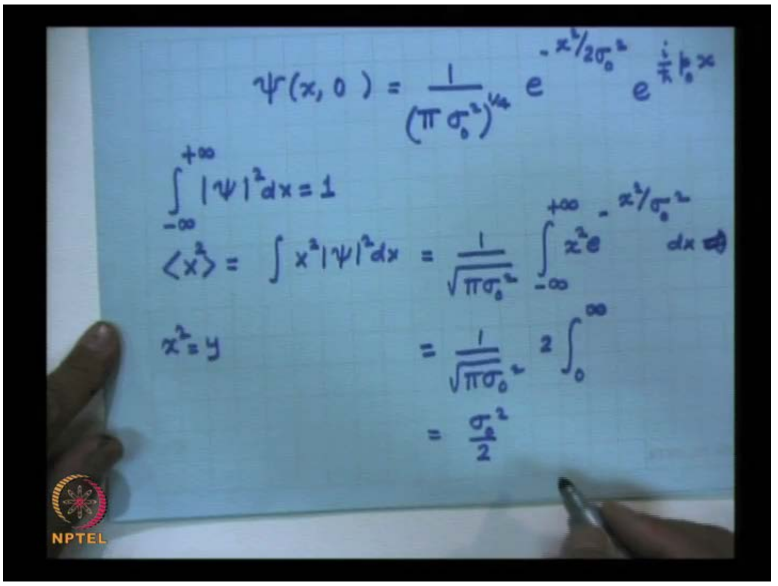

I conclude today's talk by writing the wave function which is psi x at t equal to 0 let us suppose we wrote down that we we consider this two terms back pi sigma zero square raised to the power of four e to the power of minus x's square by two sigma zero square e to the power of i by h cross p naught x. If you calculate this first of all you can easily show that minus infinity to plus infinity mod psi square d x is one so the function is normalized I have done this quite a few times I do not want to do. Secondly the expectation value of x will be the will be x times mod psi square d x so mod psi square will be e to the I can write down under root of pi sigma zero square and then x into x E to the power of minus x square by sigma naught square the mod square of this function. This is this will become one and this will become e to the power of minus x square by sigma this limits are from minus infinity to plus infinity and of course, this is an odd function of x and therefore, the integral is zero.

So the expectation value of x is 0 the expectation value of x square is x square here x square here and here you can easily integrate this in terms of gamma function and then you will get one over under root of pi sigma zero square two integral zero to infinity and then if you put x square is equal to say y and then carry out the integration you will obtain this to be equal to sigma zero square pi two.

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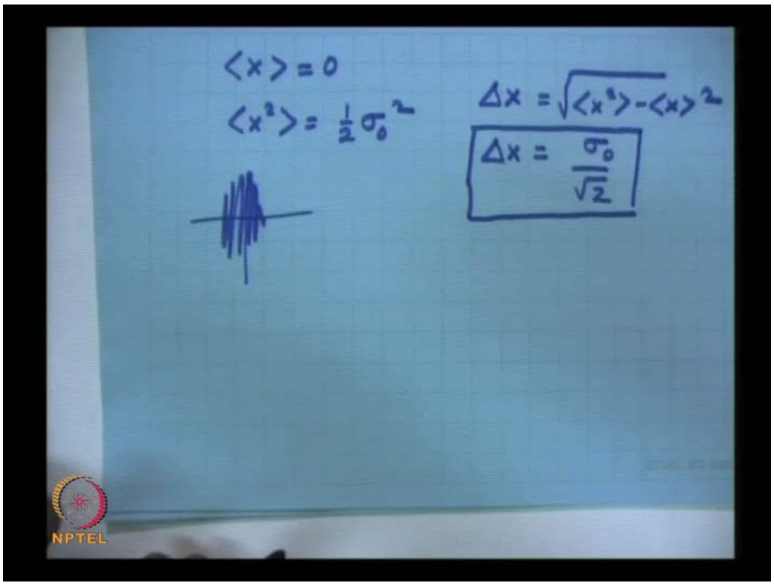

So we had we had x average is zero and x square average is half sigma zero square therefore, uncertainty in x will be under root of x square minus x average square so this is zero, so this will be sigma zero by root two this is the uncertainty that if you make a measurement of the x coordinate of the particle then it will be I showed you a wave packet. So the wave packet is such that that it is localized within a distance of sigma zero.

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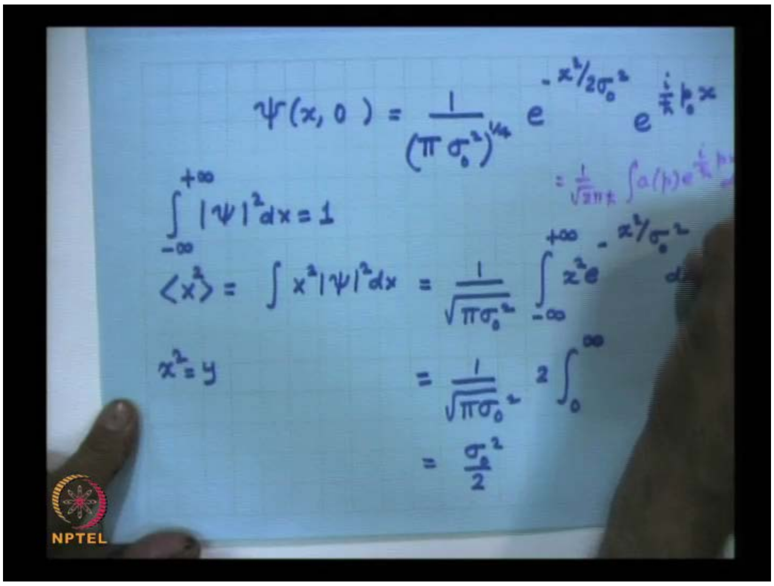

Now for the wave function that I had written down for the wave function I can write it as I can write it as equal to one over two pi h cross integral a p E to the power of i by h cross p x d p and then take the inverse Fourier transform of of the function.

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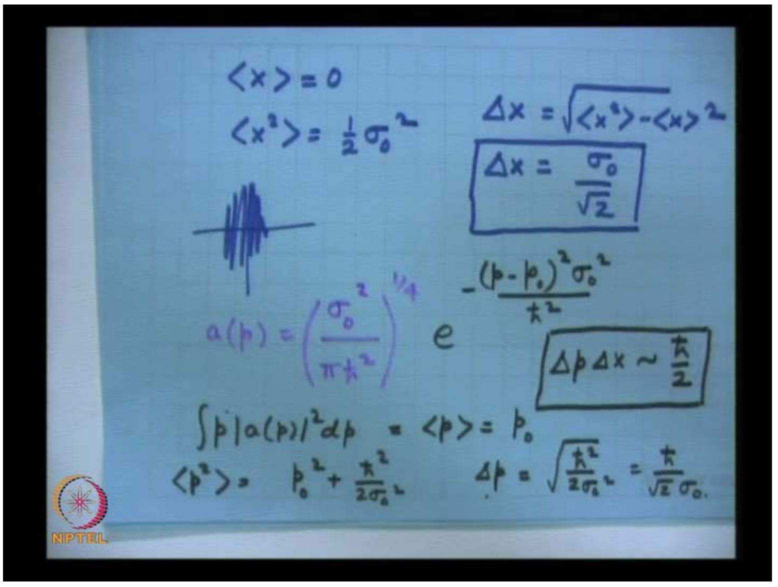

And you will finally, get a p is equal to sigma I leave that an exercise sigma zero square raised to the divided by pi h cross's square raised to the power of one by four raised to the power of one by four e to the power of minus p minus p 0 whole square sigma naught square by h cross's square. So this is if you plot the momentum distribution function then you will find that p mod a p square d p. This will be the average value of p this will come out to be p naught and average value of p square will be p square of this thing and if you carry out this integration one can show that this will come out to be p 0 square plus h cross's square by two sigma naught square, so delta p will be this minus square of this so delta p will be under root of h cross square by two sigma naught square. So this will be h cross by a root to sigma naught, so if I take the product of the two so delta p delta x it will be of the order of h cross of two, so the uncertainty principle the uncertainty principle is contained in the solution of the wave function. So I end by showing the wave packet that I had shown last time that this is the let us suppose I increase the so the particle is described by this wave function which evolve with time as shown in this diagram as shown in this in the evolution of the wave packet the particle is localized somewhere here and as it propagates it broadens with time that I have not explicitly shown. But you can you can carry out the calculations and show that that how the wave function will evolve with time and at each step the product of delta x and delta p is always greater than each cross by two. So we have considered the the the definition the the of the uncertainty principle we have proved the uncertainty principle given a physical interpretation of the wave function through the equation of continuity and interpreted the wave function corresponding to a Gaussian wave packet . Thank you.