Basic Quantum Mechanics

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Module No. # 02
Simple Solutions of the 1 Dimensional Schrodinger Equation
Lecture No. # 02
Physical Interpretation of the Wave Function

In our last lecture we discussed a Gaussian wave packet and as to how it propagates through through empty space today we will re derive Schrodinger equation, discuss the operator representation of momentum and also gives a physical interpretation of the wave function which is due to max born. Max born had given a probabilistic interpretation of the wave function and we will discuss that today in one of our earlier lectures we had given a heuristic derivation of the Schrodinger equation

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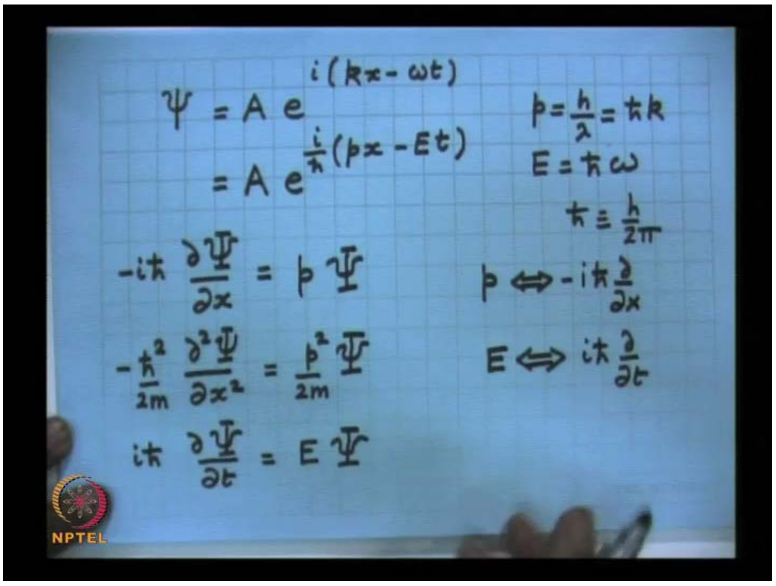

We started with a wave a classical plane wave which we represented as E to the power of I k x minus omega t. In this we replaced we used the wave particle duality which is equal to which is given de brogil relation h by lambda so this is h cross k where k is equal to two pi by lambda and then we introduced the Einstein equation that E is equal to h nu is equal to h cross omega, where h cross is defined to be equal to h by two pi. So if I substitute this we had discussed earlier that this wave function becomes E I by h cross p x minus E t then we have said that if we differentiate psi with respect to x and multiplied by h cross, so I'll get minus h cross delta psi by delta x this will be equal to minus I h cross times I by h cross. So h cross h cross cancel out I times minus I is plus 1 so this will be just p times the entire wave function psi so this will be psi. So this allowed us to interpret the p operator p to represent the momentum by its operator minus I h cross delta by delta x. If you differentiate it here we will obtain minus h cross's square delta two psi by delta x's square if you differentiate it again you will get p square by h cross's square into I square so this will become just p square psi, then we divide we divided two both sides by two m so p square by two m would represent the kinetic energy of a particle. When we differentiated psi with respect to time and if I multiply that differential with I h cross then we will obtain I h cross delta psi by delta t is equal to I h cross times I is minus minus minus plus so this will be just E psi.

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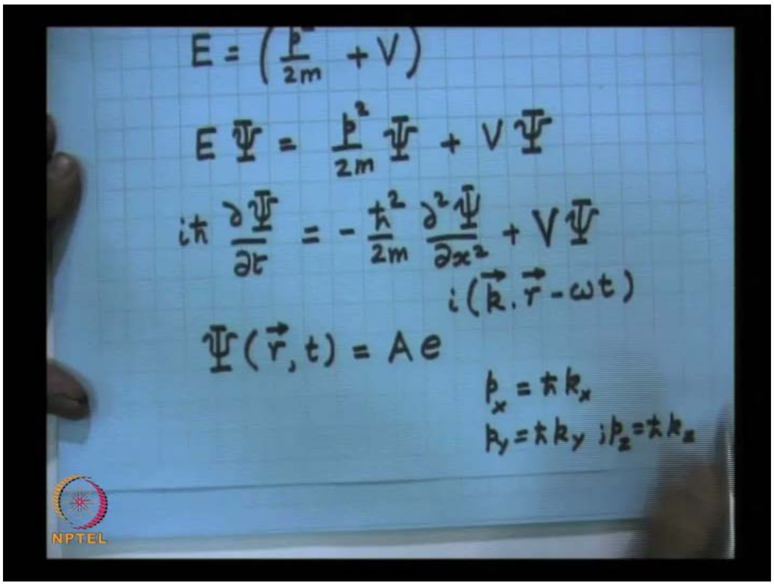

So we can using this we can represent the energy by the operator I h cross delta by delta t now since we have for a particle E is equal to p square by two m plus the potential energy, where v of x is the potential energy function. If we multiply both sides by E by psi then we get E psi is equal to p square by two m times psi plus v psi, but we have shown just now we had these two equation that E psi was equal to I h cross delta psi by delta t and p square by two m psi is equal to minus h cross's square by two m delta two psi by delta x's square. So I will write this as we have derived earlier I h cross delta psi by delta t is equal to minus h cross's square by two m delta two psi by delta x's square plus v psi. So this is the one dimensional Schrodinger equation for a particle which is inside a potential field described by the potential energy function v of x.

Now for a three dimensional wave this was one dimensional consideration for a three dimensional wave you will write we will write psi the wave function for a classical plane wave function where the vector r represents x y z and time. So I will have A into E to the power of I k vector dot r vector minus omega t this represents a plane wave propagating in the direction of the k vector. So now we will have we will define p x is equal to h cross k x and p y is equal to h cross k y and p z is equal to h cross k z.

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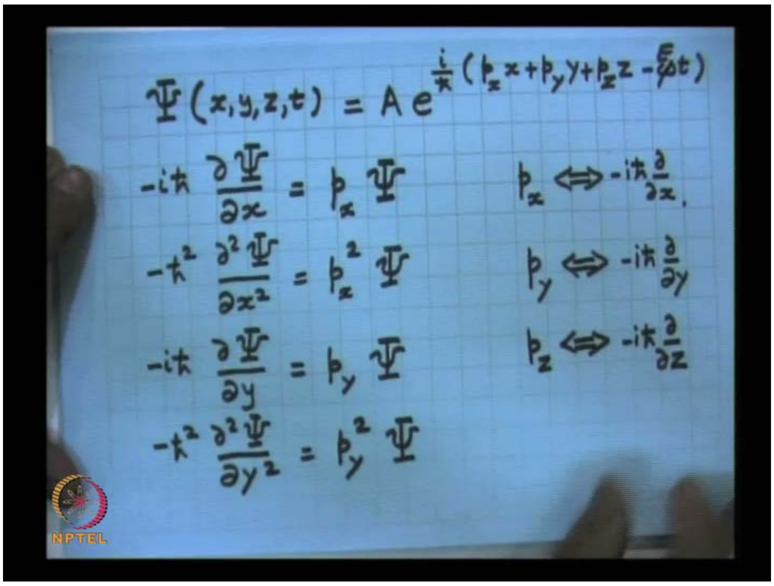

So instead of the one dimensional formula we will have psi of I can write as r t or x y z t this is a three dimensional plane wave, so this will be A E to the power of I by h cross p x x plus p y y plus p z z , p y y plus p z z minus omega t. If I now apply the same method as we did last time and differentiate first with respect to so sorry this will be E so this will be E. So E is equal to h cross omega so first with respect to x and multiplied by I h cross. So I will obtain minus I h cross delta psi by delta x is equal to p x times the whole thing so this is p x psi so I can associate the operator p x with the differential operator minus I h cross delta by delta x. And similarly, if I differentiate it again I will get minus h cross's square delta two psi by delta x's square is equal to p x's square psi I can differentiate with respect to y so instead instead of p x psi we will obtain p by psi. So we will obtain minus I h cross if I differentiate partially with respect to y, so then we will obtain p y psi. Now we can associate with the operator p y with p y the differential operator minus I h cross delta by delta y and I can differentiate it again and I will obtain minus h cross's square delta two psi by delta y square is equal to p y square times psi. In an exactly similar manner I can differentiate with respect to z and I will obtain for p z the operator minus I h cross delta by delta z.

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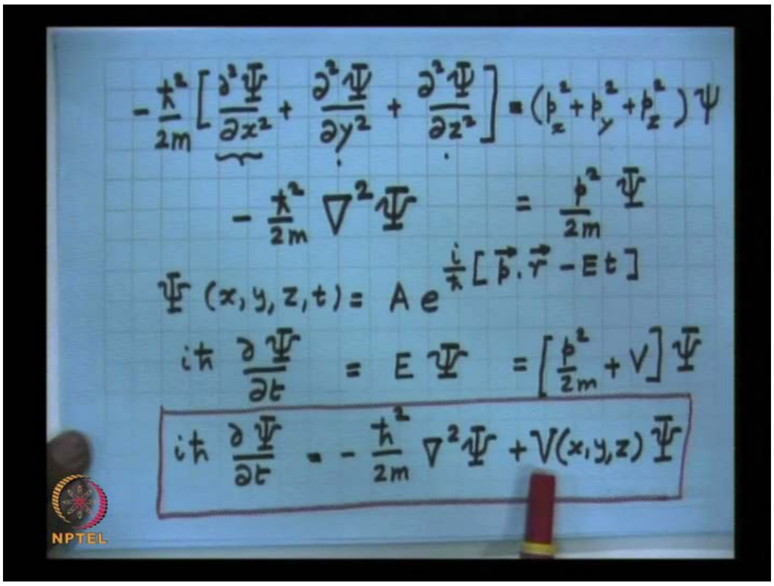

And we will finally, obtained that minus h cross's square delta two psi by delta x's square plus delta two psi by delta y square plus delta two psi by delta z square so this will be p x's square psi plus p y square psi plus p z square psi. So we can write down p x's square plus p y square plus p z square psi. And therefore it is equal to p square psi, if I divide both sides by two m where m is the mass of the particle then I will get p square by two m psi. So in the one dimensional equation we just obtain the first term in the three dimensional equation we obtain minus h cross's square by two m del square psi, where del square psi in the Cartesian system of co ordination is equal to delta two psi by delta x's square plus delta two psi by delta y square plus delta two psi by delta square. If I now differentiate the wave function if you recall our wave function was given by psi x y z t was equal to A E to the power of i by h cross p x x by p y y plus p z z is easier way to write that p dot r minus E t this is my wave function. So we will have i h cross delta psi by delta t if I differentiate this so I times I becomes minus one minus minus becomes plus h cross h cross cancels so you get E psi and since E psi is equal to p square by two m plus b, so E psi will be E psi will be so much. So I will obtain E psi is I h cross delta psi by delta t is equal to p square by two n times psi is minus h cross's square by two m del square psi plus v psi.

Now we here we will assume it will be now a function of x y z psi. This is a very important equation and this is known as the three dimensional Schrodinger equation three dimension 1 three dimensional time dependent Schrodinger equations and the major portion of non relativistic quantum mechanics is the solution of this equation for different potentials. And we will be discussing the solutions for different forms of the potential function b of x y z, now before we get solutions we would like to we would like to obtain a physical interpretation of this wave function and as I have mentioned earlier this is due to max born.

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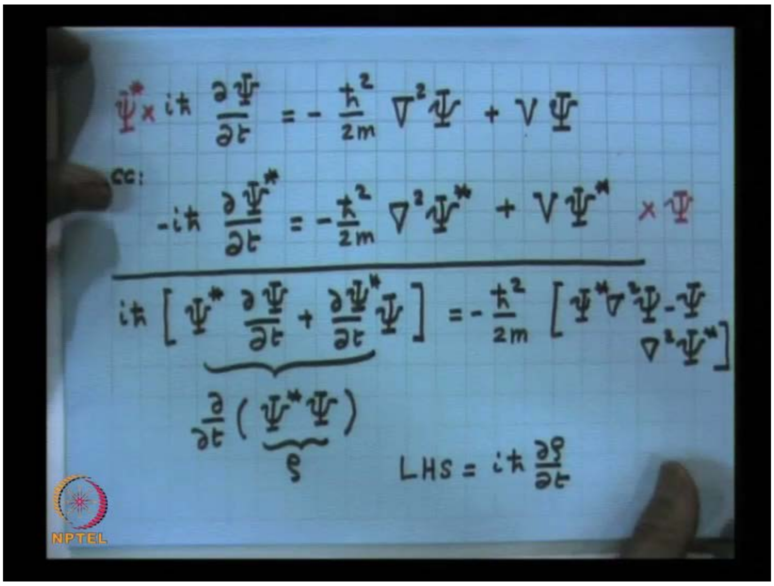

So I rewrite the Schrodinger equation and this i h cross delta psi by delta t is equal to minus h cross's square by two m del square psi plus v psi. V is the potential energy function which is necessarily real, I take the complex conjugal of the above equation the complex conjugal of the above equation will be I will be replaced by minus i h cross delta psi will be replaced by its complex conjugate delta psi star by delta t this is equal to minus h cross's square by two m del square psi star v, v is the real function what we now do is multiply this equation by psi star say psi star we multiply the first equation by psi star and multiply the second equation by psi. And then subtract if you subtract that then this term will be psi star v psi and this will be psi star v psi so these two terms will cancel out and if I multiply the first equation by psi star the second equation by psi and subtract so the left hand side becomes i h cross psi star delta psi by delta t plus delta psi star by delta t into psi.

This is my left hand side and the right hand side becomes minus h cross's square by two m psi star del square psi minus psi del square psi star. So this quantity as you see is just delta by delta t of psi star psi, I represent this by function rho so I obtain on the left hand side so the left hand side is just equal to i h cross delta rho by delta t this is the left hand side and if I take the minus sign inside

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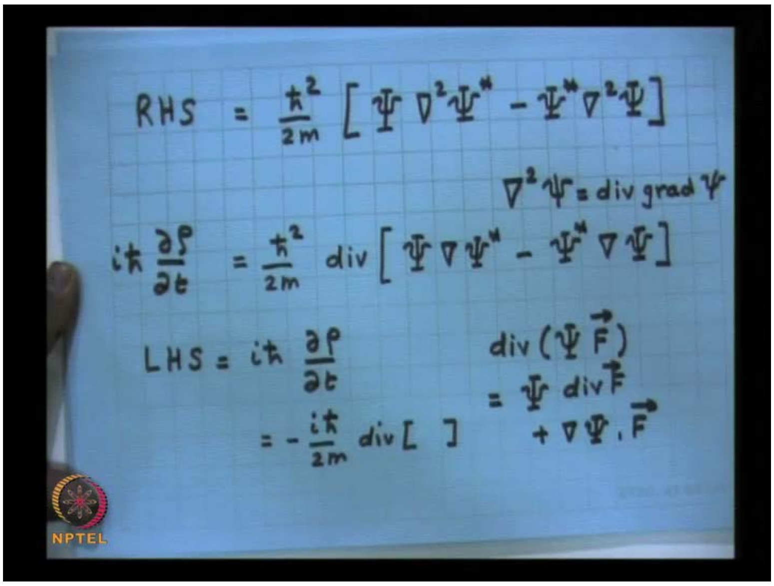

Then the right hand side will become and the right hand side will become the right hand side will become h cross's square by two m I take the first term psi del square psi star minus psi star del square psi.

Now the operator del square is actually del square operating on any function on any scalar psi is equal to divergence of the gradient divergence of the gradient of the psi. So I can write this down as h cross's square by two m divergence of psi grad psi star, this is gradient of psi star minus star gradient of psi, because divergence of a scalar times a vector this is equal to psi divergence of F plus grad psi dot I grad psi is a vector. So if I take the divergence of this function first term will be psi divergence of the gradient psi star then there will be a term which is grad psi dot grad psi star which will cancel out with this term. So therefore you will obtain this so this left hand side was equal to i h cross delta rho by delta t, so I write this down as i h cross delta rho by delta t is equal to so much. So if I divide by i and h cross so this will become the right hand side will become minus i h cross by two m into divergence of the quantity without this within the square brackets and then I will obtain this particular equation.

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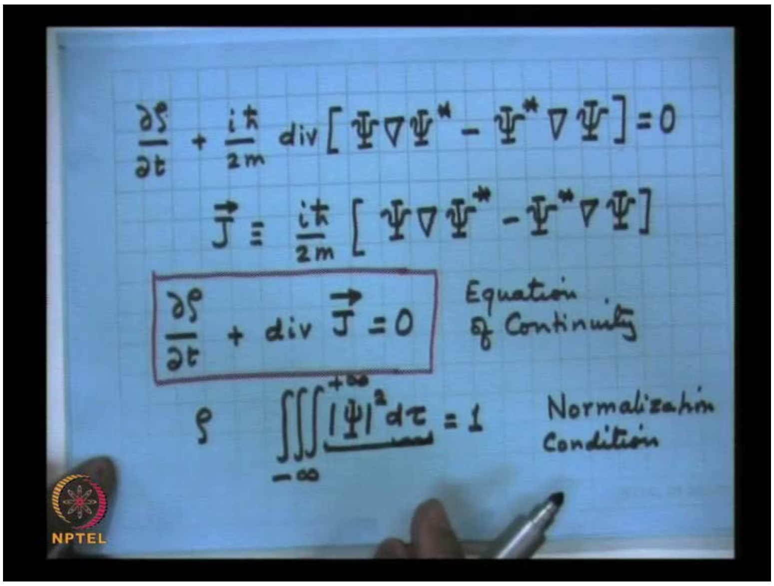

So on simplification this becomes delta let me write it carefully delta rho by delta t I bring the left hand side right hand side to the left hand side plus i h cross by two m divergence of psi gradient of psi star minus psi star gradient of psi. This is equal to zero, I define a vector J which is defined to be equal to you see this i h cross by two m psi gradient psi star minus psi star gradient. If I define a vector J given by this equation then from the Schrodinger equation we are able to derive the equation of continuity, delta rho by delta t plus divergence of J is equal to zero this equation this is a very important equation in any fluid flow this is given this is known as the equation of continuity and I will give a physical explanation in a moment this is known as the equation of continuity.

And therefore, we may assume rho to the proportional to the position probability density so we associate rho as the position probability density per unit volume ,so if we interpret psi square D tau as the probability of finding the particle in the volume element D tau and the particle has to be found somewhere, so therefore the integral over the entire space it is a three dimensional integral over the entire space must be equal to one this condition is known as the normalization condition Normalization condition. And physically if you represent a particle like an electron or a proton by a wave function psi then we will interpret psi square D tau as the probability of finding the particle in the volume element D tau and since the particle has to be found somewhere psi should be such that the total integral should be one. The Schrodinger equation is linear therefore, if psi is a solution multiple of psi is also a solution and we can choose the multiplicative constant in such a way that this condition is satisfied where all limits are from minus infinity to plus infinity, let me for a moment discuss the physics of the equation of continuity.

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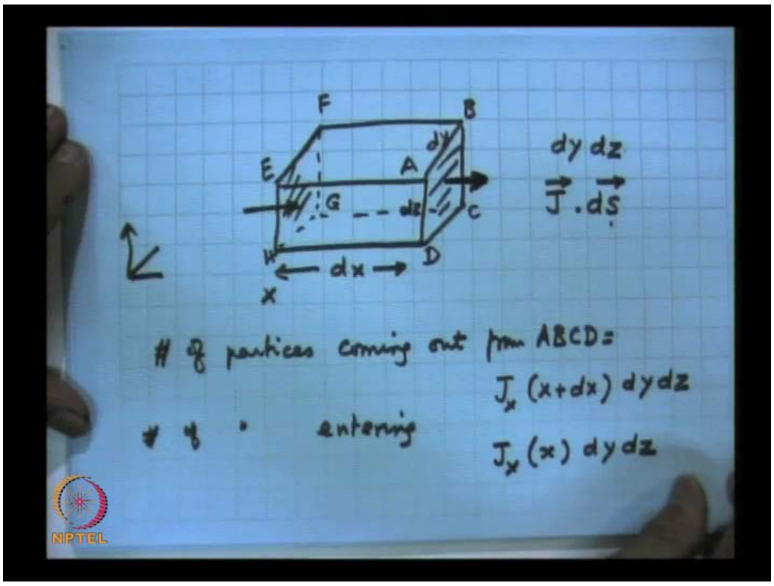

Let us consider a room in which particles are flowing, so we inside the room we consider a small volume element let us suppose D x D y D z so I have here this length this axis let us suppose this x axis so this suppose D x and this length is D y and the this is so x y and z so this is a box. Now there are particles in the room let me try to find out the number of particles that are coming out of this surface of this surface the area of this surface is D y D z and the normal to the area is along the x direction. So if there is a current density J which represents number of particles crossing per unit area per unit time then J dot D s will represent the number of particles crossing the area D s per unit time so since s the D s vector normal to the surface is along the x axis and this is at the point suppose this is the point x so this is the point x plus D x. So if this area I represented by A B C D so number of particles coming out per second from the area in A B C D is equal to J x evaluated at x plus D x multiplied by the area and the area is D y D z. Similarly if this area I represent by E F G H then the area of this surface is also D y D z, so the number of particles which are entering the surface so number of particles entering entering the area E F G h will be equal to J x at x into D y D z. So the net outflow from these two surfaces.

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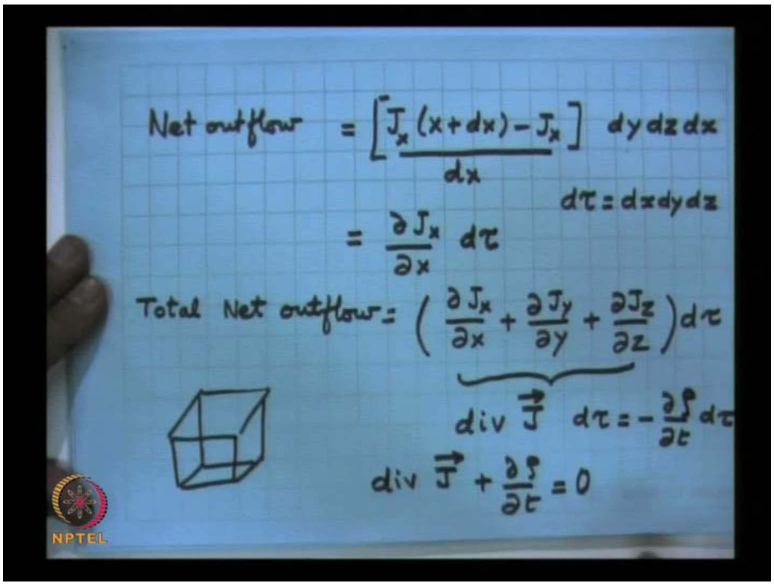

So the net outflow from the two surfaces will be equal to J x at x plus D x minus J x into D y D z I multiply the numerator and denominator by D x, so this quantity becomes delta J x by delta x into the volume element. Volume element is D tau so where D tau the volume element of the box is equal to D x D y D z. We had considered particle coming out of this surface and particles entering from this surface similarly, you will have four more surfaces 1 perpendicular two perpendicular to the z axis two perpendiculars to the y axis. So we can write that down in exactly similar way so the total net outflow the total net outflow from the volume will be equal to delta J x by delta x plus delta J y by delta y plus delta J z by delta z into the volume element D tau. This quantity is known as the divergence of the vector J and it represents a four of of of particles and since I consider a volume element if there is a net outflow then the particle density inside this must be reducing.

If there is a net inflow then the particle density will be increasing so divergence of J into D tau must be equal to of the minus the delta rho by delta t where rho is the number of particles per unit volume times rho D tau is the number of particles in the volume D tau, since this represent the net outflow so there is a minus sign from which we get if there are no sources and sinks in the room so we get the equation of continuity.

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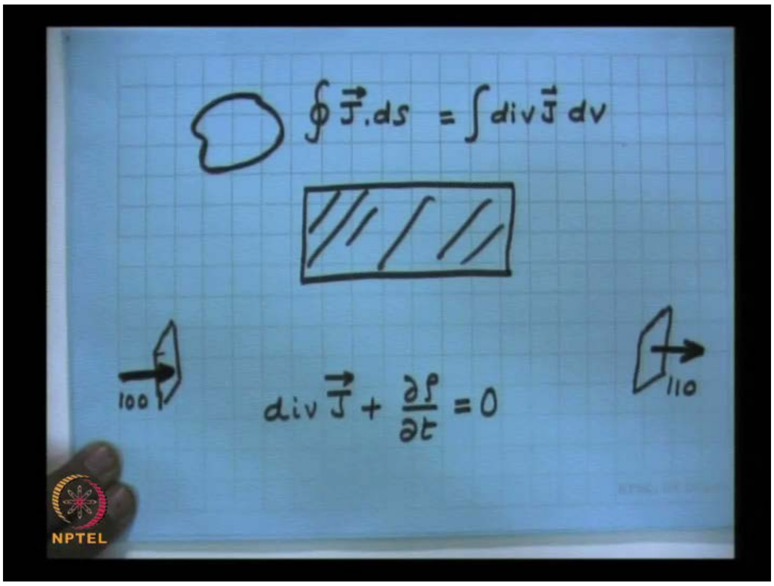

So let me explain this once again if I have a close surface s then the total number of particles that are going out will be equal to J dot D s integrated over the entire surface the entire surface and this will be equal to divergence of J into D v, integrated over the this is known as the Gaussian theory. Another example which will clarify the concept of the divergences let us suppose that there is a there is a room which contains a painting this is a painting on the wall this is a big painting in the wall. And in this room there is a door here and there is a exit door here and people are entering this room looking at the painting and going out if the number of people entering there is a constant flow of people, if the number of people entering the door per unit time is the same as the number of people going out then the population of people inside the room will remain constant.

The divergence of current is zero so therefore delta rho by delta t is zero on the other hand if there is a net inflow that is if hundred people are entering the room and only ninety people are coming out then the density of people inside the room will increase. So there is a net divergence of the current because of which the population will increase. Conversely if there are hundred people entering and hundred and ten people leaving then the population inside the room will go on decreasing. And we are assuming that no person is born or die inside the room so there are no sources or sex, so whenever there is an outflow the population density will decrease and whenever the outflow is negative there is a net inflow then the population density will increase.

So this is represented by the equation of continuity divergence of J which is an equation of tremendous importance in fluid dynamics divergence of J plus delta rho by delta t is equal to 0 and what we have been able to do is that starting from the Schrodinger equation starting from the Schrodinger equation.

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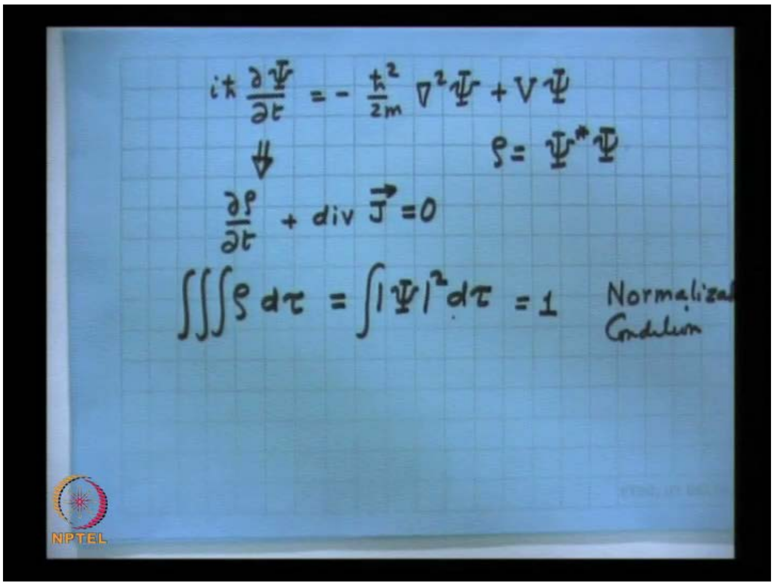

There is i h cross delta psi by delta t is equal to minus h cross's square by two m del square psi plus v psi then we took the complex conjugate and subtracted one from the other and we have been able to derive that delta rho by delta t plus divergence of J is equal to zero. Since this equation represent a equation of continuity, therefore we physically interpret rho as the position probability density as you know rho was we have put equal to psi star psi. So we we interpret physically interpret rho D tau which is equal to mod psi square D tau as the probability of the finding the particle in the volume element D tau. And we in this equation this is a linear equation if psi is the solution then the multiples I is also the solution and we choose the multiplication factor such that this integrated over entire space this is actually a three dimensional integral three dimensional integral is one. And as I have mentioned earlier this is known as the normalization condition.

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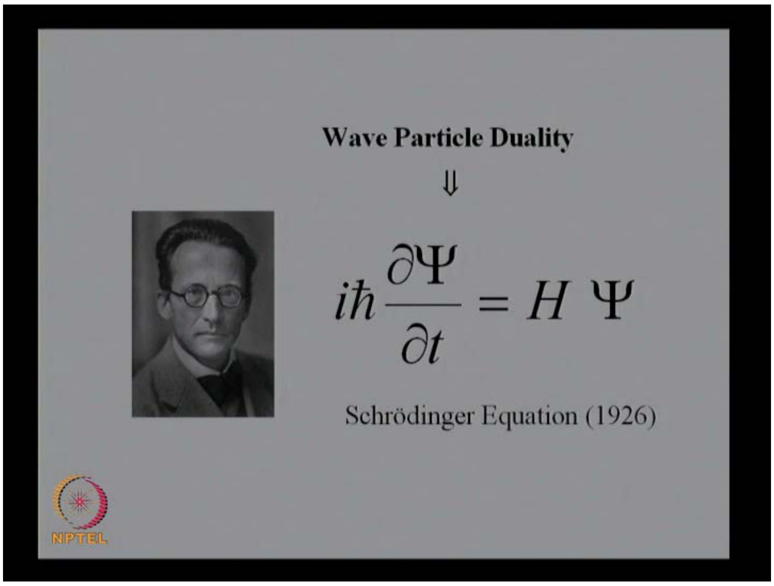

So you know the wave particle duality let us to the Schrodinger equation we made a heuristic derivation of the Schrodinger equation and we gave a physical interpretation of the wave function.

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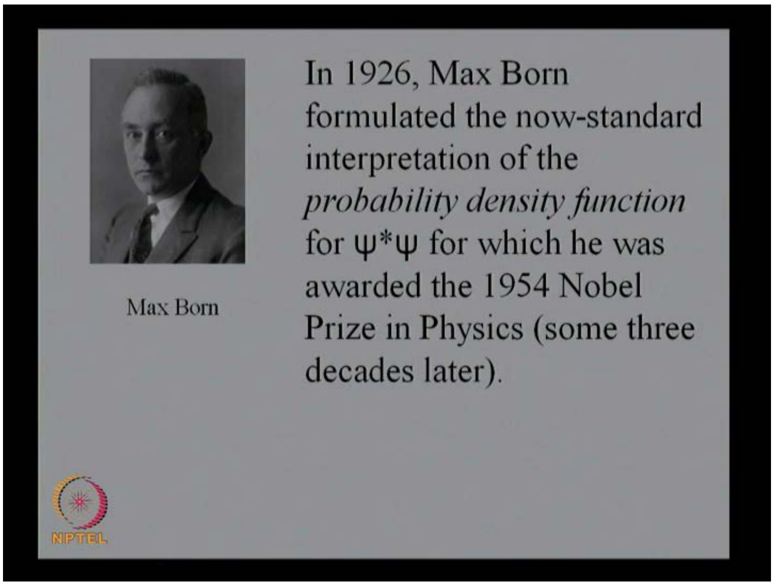

Which was given by max born in nineteen twenty six he formulated what is now the standard interpretation of the probability density function for psi star psi for this contribution he was he was awarded the nineteen fifty four the Nobel prize physics about thirty years after he had made that announcement.

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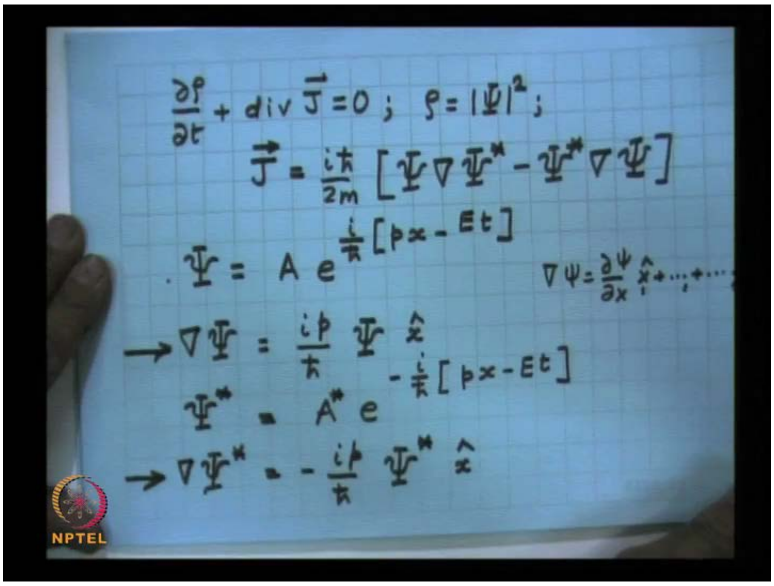

Now now let me give you one example that we had obtained we had obtained that delta rho by delta t plus divergence of J is equal to zero, where rho is equal to psi star psi or psi square and J is the current density, so this is equal to i h cross by two m i h cross by two m then we will have just one second i h cross by two m psi grad psi star minus psi star grad psi. Let me consider as a very simple example the plane wave solution, so the wave function is given by psi is equal to A into E to the power of i by h cross p x minus E t so and then psi so grad psi this depends only on x so if I write down delta psi by delta x so this will be i p by h cross i p by h cross times the whole function so that is equal to psi. If psi is given by this equation then psi star I assume it to be real but it a can be complex also A into E to the power of minus i by h cross p x minus E t, I am sorry gradient of psi is a vector so this is multiplied by the unit vector. You see gradient of a scalar function is gradient of psi is equal to delta psi by delta x into x cap plus delta psi by delta y into y cap plus delta psi by delta z into z cap, where x cap y cap and z cap as you all know are the unit vectors along the x y and z directions respectively. So this is my gradient of psi.

And similarly gradient of psi star let us make a complex so a this is a star so if I differentiate this with respect to x so I get minus i p by h cross so minus i p by h cross and the whole quantity is psi star multiplied by the unit vector in the x direction. So I have gradient psi this expression gradient psi star this expression and of course, I have psi here and psi star here I just substitute these four quantities in this equation. It is a very straightforward substitution and you will get you will get for J is equal I h cross by two m psi grad psi star.

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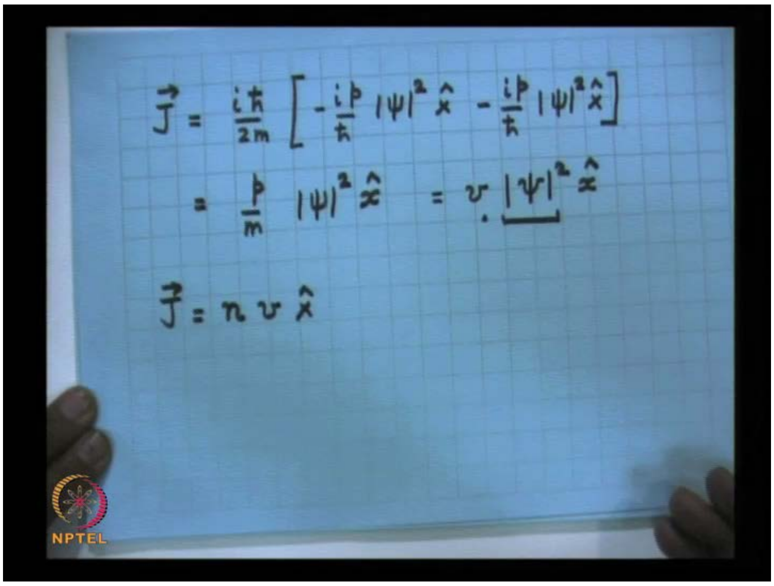

So therefore, this will be minus i p by h cross psi psi star that is mod psi square x cap and the second term again the same minus i p by h cross mod psi square x cap so the current density is in the x direction so these two terms are equal I times minus I is 1 h cross h cross cancel out and there is a factor of two coming in because these two numbers these two quantities are equal. So the two cancels out and I will get p by m psi square into x cap so momentum of mass into velocity so I get v psi psi square, so as you know that if I have a probability if I have a number density n and if all the particles are moving in the x direction with velocity v then the current density is given So here if we have the probability density associated with the particle multiplied by v, similarly I can also, this is the for a for a infinitely extend plane wave which is really a practical impossibility because it is not normalizable.

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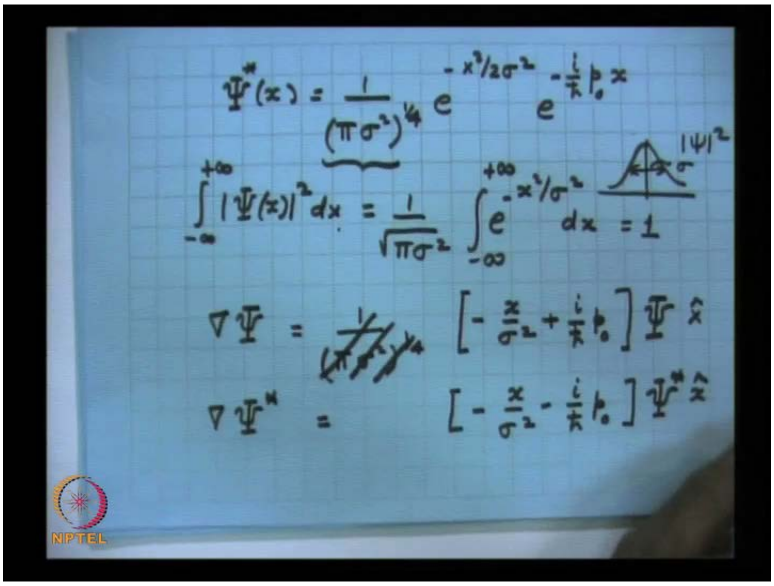

So my normalizable wave function is a something like a Gaussian wave packet we had discussed earlier and we have for the wave function let me suppose I consider a wave function psi of x which is equal to pi sigma square raise to the power sigma four E to the power of minus x's square by two sigma square E to the power of i by h cross p naught x this is a Gaussian wave packet, which is located around if you plot the probability function then it is looked spiked around x is equal to zero. This is psi square and whose width is of the order of sigma so this is the localization of the particle. The particle is localized within a distance of the order of sigma and using the formula that I have given two three turns back 1 can show that minus infinity to plus infinity mod psi x whole square D x if I do that then this will be one over under root pi sigma square and this will be E to the power of minus x's square by sigma square D x. And this integral is obvious you remember the formula that we have given and so this will be 1. So therefore this factor is such that the wave function is normalize and therefore, we can interpret psi of x's square D x as the probability of finding the particle between x and x plus D x. And then we we write down what is gradient of psi psi depends only on the x coordinate so I differentiate this with respect to x so I get 1 over pi sigma square raise to the power of 1 by four etcetera and if I differentiate this I will get minus two x by two sigma square. So minus x by sigma square plus i by h cross p naught and then the whole function. So therefore that is psi I remove this because this factor is contained inside multiplied by x cap. Similarly if I take the complex conjugate of this equation you see if I take psi star then this becomes minus and you'll have gradient of psi star. Gradient of psi star will be equal to minus x by sigma square minus i by h cross p naught psi star x.

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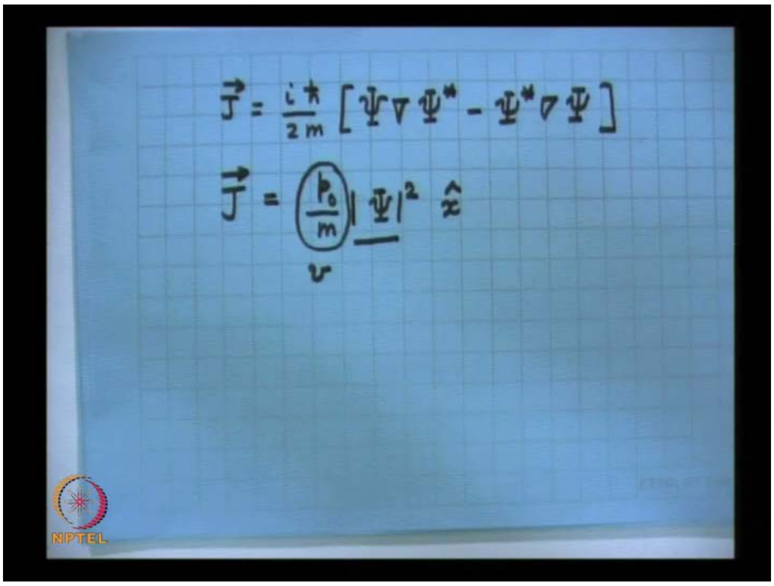

And then I substitute this these two expressions in the in the equation that J equal to the current density i h cross by two m and then you have psi grad psi star minus psi star grads psi if I substitute these two I leave it as an exercise for you you will get p 0 by m psi square psi square into x cap. So this is the velocity average velocity of the particle this is the velocity this is the position probability density and so therefore we obtained the expression for the for the current density. So from the solution of the Schrodinger equation we have been able to derive obtain a physical interpretation of the wave function and we interpret it psi such that mod psi square D tau represents the probability of finding the particle in the volume element D tau.

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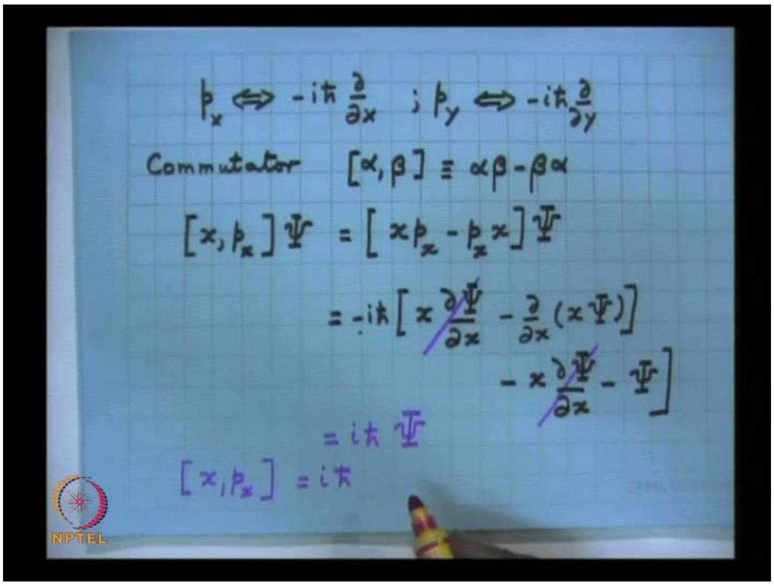

In the process we had also obtained an operator representation of p p x p y and z so we found that p x can be associated with the operator minus i h cross delta by delta x and p y with the operator minus i h cross delta by delta y. And similarly, t z with minus I h cross delta by delta psi this allows us to calculate what is known as the commutator. The commutator between two operators alpha and beta is written as alpha beta within two square brackets and that is defined to be equal to alpha beta minus beta alpha alpha beta minus beta alpha. You must have read in the theory of matrices that two matrices may not commute so here you have let us consider that alpha is x and beta is p x so I want to calculate the commutator x comma p x operating on any wave function psi. So this is equal to we operate at x p x the commutator of x p and p x is x times p x minus p x x operating on psi p x I replace by the operator minus i h cross delta by delta x so this is minus I h cross x delta psi by delta x, I have taken minus i h cross outside so I will get delta by delta x operating on x psi if I expand this then I will get minus x delta psi by delta x minus just psi because delta x by delta x is one so this term this term cancels out with this term minus minus plus. So this becomes i h cross psi since this is valid for any psi so I obtain the commutation relation x comma p x x and p x do not commute and we have this as the commutation relation.

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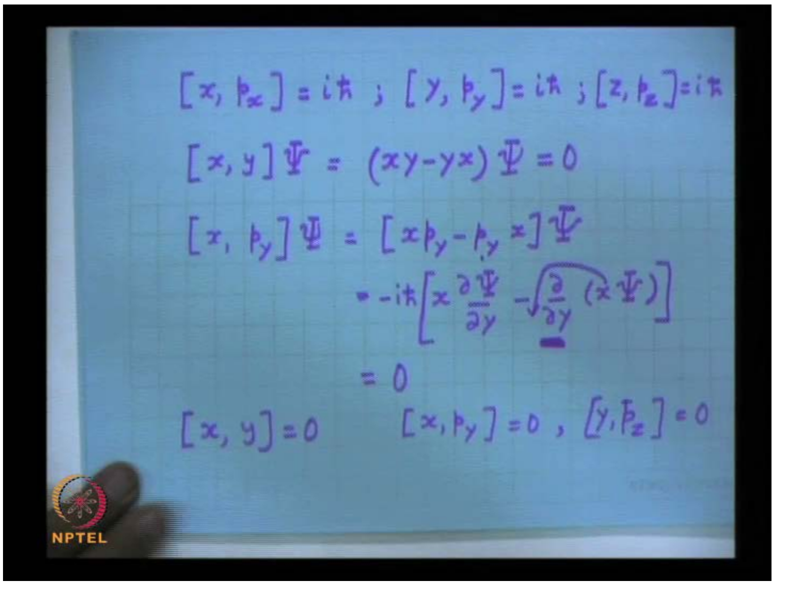

So using the differential operator representation of p x p y and p z. I have been able to derive x does not commute with p x and commutator is equal to h cross i h cross similarly, y does not commute with p y this is equal to h cross. And similarly z does not commute with p z is equal to I h cross I leave it an exercise for you to show that x will commute with y because x this is equal to x y minus y x operating on a wave function and these two are equal. So x commutes with y x commutes with z y commutes with z and so on, even x will commute with p y x commute with p y because psi is equal to x p y minus p y x psi. So this is a differential operator with respect to y and when I use this differential operator on x x can be treated as a constant. So let me write it down carefully so this is minus i h cross x delta psi by delta y and minus delta by delta y into x psi. So since the differentiation is with respect to y I can take the x outside and then these two terms will cancel out so I obtain using the operator representation that x commutes with y is equal to 0 x commutes with z x commutes with p y similarly, y commutes with p z and so on. The only two quantities which do not commute are x and p x y and p y and z and p z.

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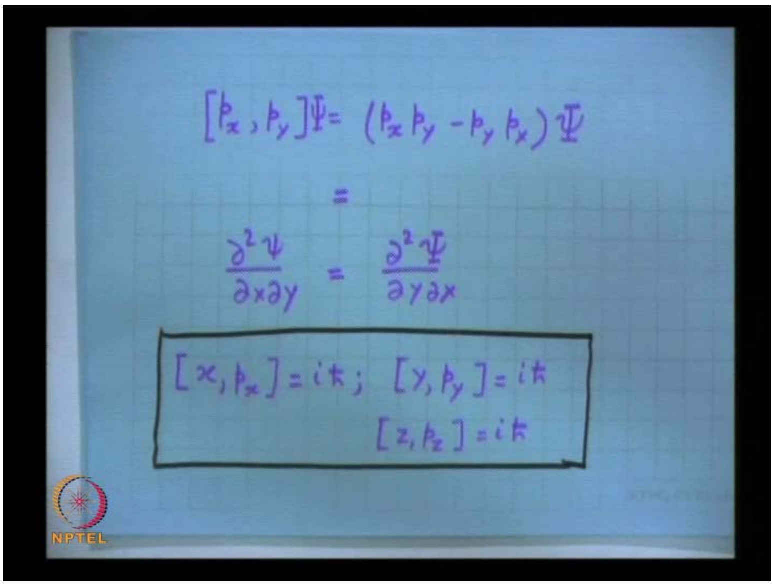

T x and t y also commute and that follows from the fact that p x comma p y will be equal to operating on psi will be equal to p x p psi minus p y p x operating on psi and this will be both will be equal. Because delta two psi delta x delta y for any well behaved function is equal to delta 2 psi delta y delta x because of that p x and p y p x and p z p y and p z commute so only the three important commutation relations are which operators which do not commute and this you all must remember that x p x is equal to i h cross y comma p y is also equal to i h cross and z comma p z is equal to i h cross. And this follows from the differential operator operator representation of p x p y and p z. So these are the commutation relation because of the differential operator representation of the operator p x, p y and p z