Micro and Nanoscale Energy Transport
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Lecture - 07
Fundamentals of Quantum Mechanics Part 1

Good Morning. In today's lecture we will start little bit about the Fundamentals of Quantum Mechanics.

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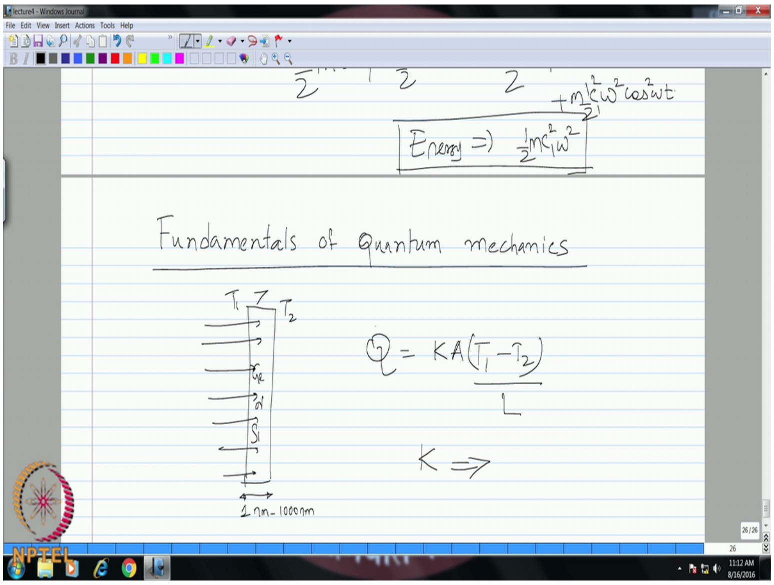

$+\frac{m c_1^2 \omega^2 \cos^2 \omega t}{2}$

$\boxed{\text{Energy} \Rightarrow \frac{1}{2} m c_1^2 \omega^2}$

Fundamentals of Quantum mechanics

$Q = KA\frac{(T_1 - T_2)}{L}$

$K \Rightarrow$

Now you should understand that we are not teaching quantum mechanics as a course. So, it is only a very small portion of the nanoscale energy transport. I will give you a, very brief over view solve a 1 or 2 examples and then, try to see were quantum mechanics is applied in the context of nanoscale energy transport. Since, till the end of the last lecture, we have l o ed in to an introduction about the nature of the microscopic energy carriers, the classification and also, the l o ing at the contribution of different energies.

The kinetic energy is if you l o at translational, rotational, vibrational from the classical prospective and from the quantum mechanical prospective. So, from the classical prospective, we can you know directly derive these energies from our knowledge of classical mechanics from the quantum mechanical prospective, I have given down the expressions.

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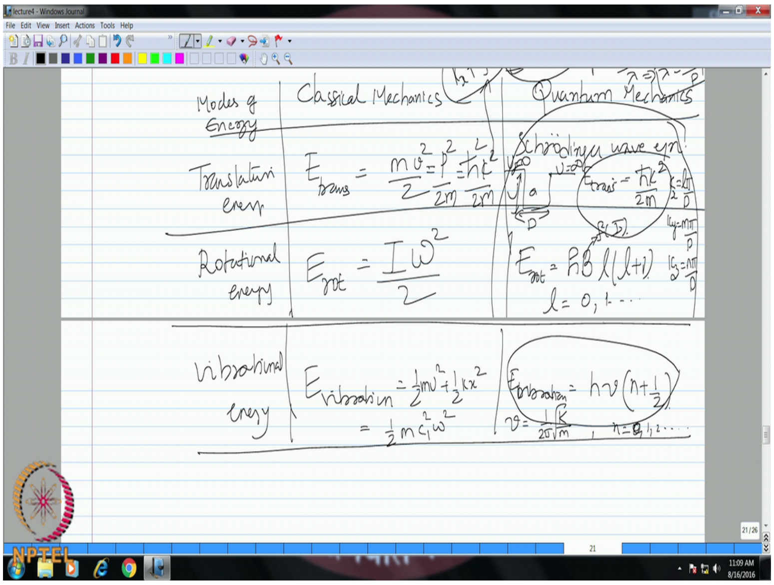

Modes of Energy	Classical Mechanics	Quantum Mechanics
Translation energy	$E_{trans} = \frac{mv^2}{2} = \frac{p^2}{2m} = \frac{\hbar k^2}{2m}$	Schrödinger wave eqn $V=\infty$ $V=\infty$ a D $E_{trans} = \frac{\hbar k^2}{2m}$ $k_x = \frac{l\pi}{D}$ $k_y = \frac{m\pi}{D}$ $k_z = \frac{n\pi}{D}$
Rotational energy	$E_{rot} = \frac{I\omega^2}{2}$	$E_{rot} = \hbar B\, l(l+1)$ $l = 0, 1 \ldots$
Vibrational energy	$E_{vibration} = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$ $= \frac{1}{2}mc_1^2\omega^2$	$E_{vibration} = h\nu\left(n+\frac{1}{2}\right)$ $\nu = \frac{1}{2\pi}\sqrt{\frac{k}{m}}$, $n = 0, 1, 2 \ldots$

I have stated the expressions for the energies, corresponding energies for translation, rotation and vibration all of them here. So, these are the things, that we will be deriving now the next few lectures.

Because you should understand that, when we talk about the really nanoscale energy transport, where the wave effects become dominant; we have to define these energies states based on quantum mechanics. So, that is way we need to understand little bit, we are not taking a separate course only on quantum mechanics to going to all the integrity details, but just a broad over view; because we are engineering students. So, we just should understand the basic concepts and how from there we go into statistical thermodynamics. So, beyond that it is not of our concern.

Now when we talk about where the quantum effects are to be felt in the nanoscale regime. I will just give you once again example; where we have for example, a thin film of some semi conductor material, let us say; it could be germanium or silicon these are the most commonly used semi conductor materials for building devices. Now, this film could be half the order of say several 100 nanometers, to ranging of the order of 1 nanometer say. So, let us say 1 nanometer to say several 100 nanometers or let us say 1000 nanometers.

Now you have the heat transport, across this thin film on one end you have a higher temperature, the other end you have lower temperature; and therefore, you have a heat transport, now if you use some method to measure the thermal conductivity of this particular film. So, in a classical case, you know how do you measure thermal conductivity is, you know the fixed temperatures, you measure the heat flux, by using the Fourier's heat conduction equation; then you extract the thermal conductivity.

That means, you know the heat transfer rate q dot is equal to k times the surface area times t 1 minus t 2 upon l; where l is the thickness of this film. So, usually we will be supplying this q dot with some kind of an external power source. So, we will know the exact amount of q dot supplied, we will be measuring temperature at the source where the supply q dot and the other end is fixed at a given constant temperature t2, from this we calculate k. So, this is the classical way of measuring thermal conductivity.

So, this is a study state method, there are also transient methods to do this. However, what happens is if according to this particular example; whatever may be the thickness of the film, the temperature gradient in this particular case is fixed, for a given value of q dot.

So, if you increase your q dot, your temperature gradient will correspondingly go up such that your thermal conductivity will always remain constant value. So, that is your classical measurement, but surprisingly when you use another methods; there are several other methods apart from the classical method, where you do not measure temperature directly, but you actually measures some kind of (Refer Time: 06:04) temperature.

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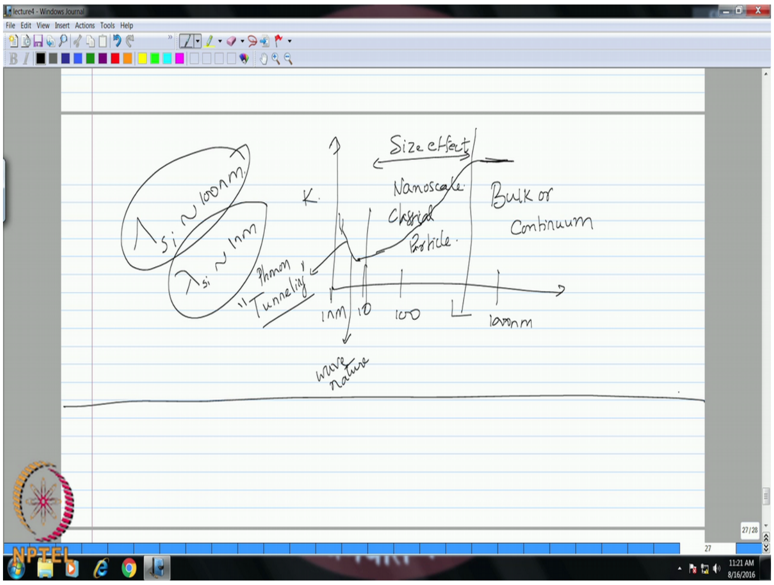

So, there are several methods, one of the most commonly used method is called 3 omega technique. So, you pass some kind of voltage, at a frequency omega u a c current and then you extract the third harmonic or 3 times omega component of this particular voltage and if you plug in into a transient heat conduction equation, we can show that this third harmonic is directly a function of your temperature rise across this film, which is the function of the thermal conductivity. So, you can measure this indirectly.

So, if you do that and you plot, the thermal conductivity as a function of l. So, suppose your L is of the order of 1000 nanometer here and something like 100 and you go to 10 and then somewhere it is 1 nanometer. So, you find that the value of k, will be somewhat close to the bulk value here, because this is where there are no micro scale or nanoscale effects. Your mean free path for example, if you take the case of silicon will be of the order of 100 nanometers. At this particular point, the (Refer Time: 07:39) number will be point 1 or less.

So, this value will approach the macro scale value of thermal conductivity and surprisingly as you keep reducing, you will find that this value keeps also dropping which is not a characteristic of bulk materials. Bulk materials thermal conductivity, is the constant value right so, but if you use this 3 omega technique, you will find that you will see that the thermal conductivity keeps dropping with reducing thickness. And finally, what happens if you go, what is the order of wave length, of phonons in silicon. Do you remember the order of wave length?

Student: 1.

About 1 nanometer; so when you drop reduce your film thickness to less than 10 nanometer now the wave effects will start appearing.

And surprisingly you know this thermal conductivity which was dropping. Now we will slowly start increasing again. So, this is the kind of a peculiar behavior that we will observe. Now, what is happening in this regime; it is all bulk or continuum transport right. So, in this particular regime, we use the Fourier's heat conduction equation to estimate thermal conductivity. So, this is the validity, this is the regime, were Fourier's equation is valid. Now if you take the length scale between 10 nanometers up to a few 100 nanometers.

So, this is where your size effect start appearing; that is thermal conductivity is the function of the thickness. So, this is where your nanoscale effects. So, why this drop is happening here, we will see this a little bit later in the lecture, but to give you a picture as your size becomes smaller than your mean free path. Now, you have fewer energy carriers within the bulk of the material. So, there will be chance that more of these energy carriers are colliding with the boundaries right, than with each other.

So, the diffusion will be very negligible compare to this catering at the boundaries. So, boundaries catering become the most dominant mechanism at nanoscales. So, in this case therefore, there will be a lot of temperature jump, created at boundaries because the boundaries are the sources of now non equilibrium. You are fixing the temperature at the boundaries, but this is not what that actual temperature of the energy carriers are, because the energy carriers do not have enough number density to sense this temperature at the boundaries.

Because this temperature can be sense only though diffusion process and since you have only a way very few energy carriers left, they directly come and hit the boundary and then realize this boundary at this temperature, but by the time it is too late and there will be a temperature artificial temperature jump; just like you have a shock wave. So, this is called Ballistic Transport. So, it is like your firing some energy carriers from this boundary, directly goes in hit is the other boundary and then senses the temperature there. So, because of this nature there is an artificial temperature drop. So, there is an additional boundary resistance; interface like you have inter facial thermal resistance, you have a thermal boundary resistance. Because of this temperature drop and therefore, this results in reduction in the thermal conductivity.

This temperature drop becomes more and more intense as you reduce the particular size, so on consequently what happens below 10 nanometers. So, ones wave effects start appearing so quantum mechanical effects now will come to picture. So, this phenomenon is attributed to phonon tunneling. This is the quantum mechanical picture we will see that. So, this is just where you know instantaneously phonon disappears and appears on the other side, nobody knows why it appears they attribute it to quantum mechanics. So, this will now reduce the thermal boundary resistance and you see that the conductivity now starts increasing, because of the transmission of phonons across these boundaries right.

So, you will see this more if you have an interface. So, we can see this tunneling process very clearly if you have an interface of 2 materials for example, you can have a germanium or silicon one side and you can have silicon or germanium. So, you have sandwich of this 2 materials and you will see the phonons can easily tunnel from one material to the other. So, they do not mind this barriers, they will be able to easily tunnel across them and were even for this kind of you know so, combination of 2 films composite films, you can see this kind of behavior of thermal conductivity rise .

Therefore, this is where we have a classical nanoscale picture, this is the classical nanoscale picture where we can use particle based approach and here you have to go to wave nature, pure quantum mechanics, you understand. So, within the nanoscale; we have two distinct regimes. So, on that is why we have to use both the mean free path as well as the wave length to distinguish between the two. Now, I will just give you a summary of some basic nature of waves, before we because quantum mechanics is all about waves.

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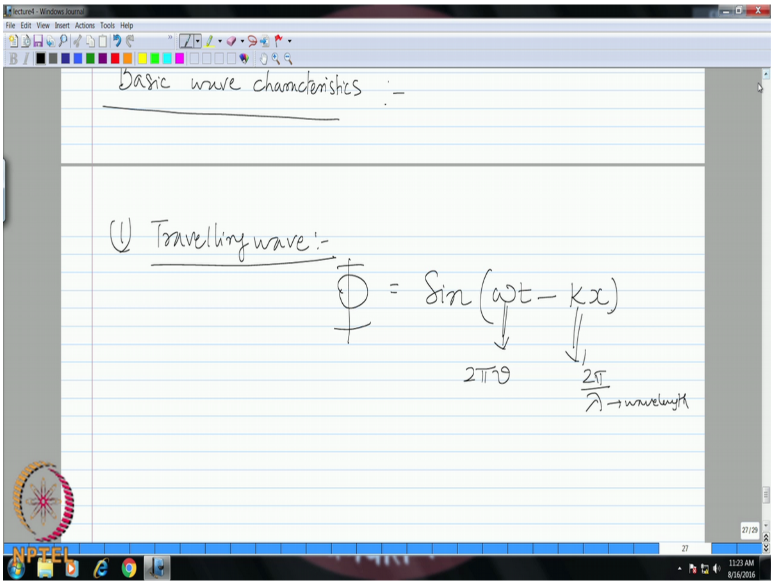

Basic wave characteristics :-

(1) Travelling wave :-

$$\Phi = \sin(\underset{\underset{2\pi\nu}{\downarrow}}{\omega} t - \underset{\underset{\frac{2\pi}{\lambda}}{\downarrow}}{k} x)$$

$\lambda \rightarrow$ wavelength

I will just give you a basic overview of wave characteristics. So, you should understand that waves we have 2 classifications; one is called a traveling wave and for a traveling wave the wave function, could be a sinusoidal or a cosign distribution function, if you assume a sine distribution function; these wave function phi can be assumed to be sin distribution both in time and space.

A traveling wave will definitely have certain characteristics over time and over space. So, over time we use the angular frequency to represent the characteristics and over space we use the wave number. So, you can say minus k x; x could be a vector and then your this k could become a you know a wave vector also, but right now we can see an 1 dimensional space and k is a wave number, t is time and omega is the angular frequency. So, why did we use omega t minus k x and not plus k x, we will see that. So, therefore, if you l o at this particular wave here, so this is nothing but 2 pi times mu e, this is your linear frequency which is one over the time period right. And this is your wave vector, which is related to your wave length as 2 pi by lambda and this is your wave length.

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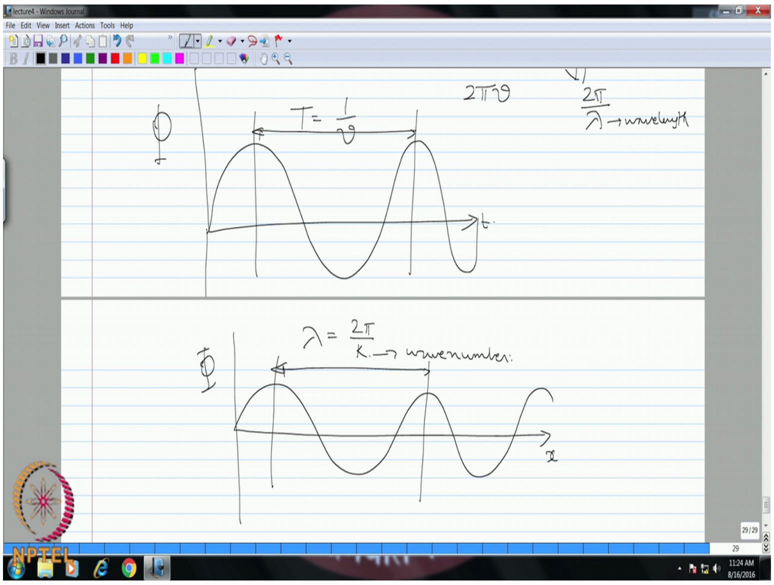

So, if you plot this particular wave with respect to space first let us (Refer Time: 16:58) with time, you have sinusoidal distribution in time and this particular separation between the peaks is given by the time period which is one over frequency right. So, this is characteristics in time, the other in space, you can plot it over x and you have again a sinusoidal profile here and what is this separation between 2 peaks in space.

Student: Wave length.

Wave length lambda, this is nothing but 2 pi by k. The k is your wave number. So, you can also have a combination of sin and cosine functions to form these waves. These waves could be electromagnetic waves. So, electric field or magnetic field or it could be any wave an energy carrier; phonons, electrons, all of them can be represented by these functions. So, you can also have a complex representation of waves. So, you can.

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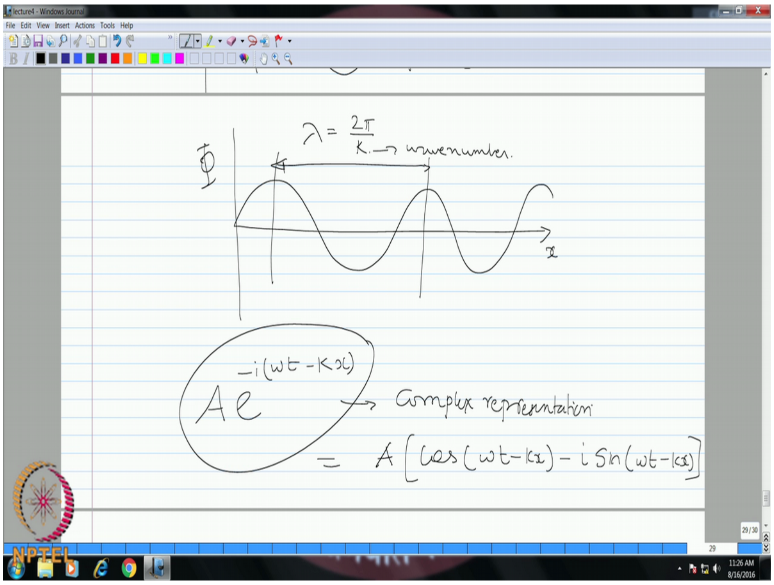

$\lambda = \frac{2\pi}{k} \rightarrow$ wavenumber.

$\boxed{Ae^{-i(\omega t - kx)}} \rightarrow$ complex representation

$= A[\cos(\omega t - kx) - i\sin(\omega t - kx)]$

For example, use e power minus I omega t minus k x, this is a complex representation of wave. So, this is nothing but if you expand this is a times cos omega t minus k x, minus I times sin omega t minus k x. So, you can also represent waves like this and sometimes rather than sins and cosines, you might prefer the representation in terms of exponential functions. They might be easier to handle differentiation or integration some times. So, you can interchangeably use them, either trigonometric functions or exponential functions.

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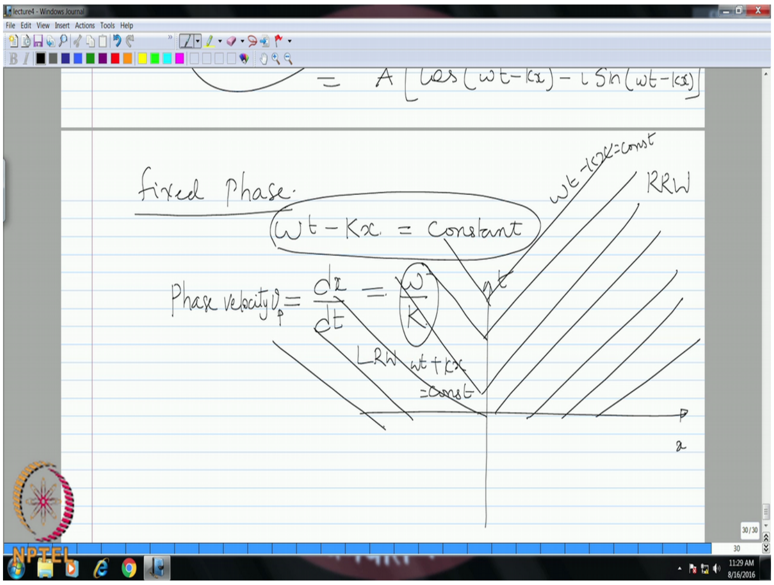

$= A\left[\cos(\omega t - kx) - i\sin(\omega t - kx)\right]$

fixed Phase.

$\omega t - Kx = \text{Constant}$

$\text{Phase velocity } v_p = \frac{dx}{dt} = \frac{\omega}{K}$

If you therefore look at this particular term omega t minus k x; so for a fixed phase; that means, a wave with a fixed phase will have the value of omega t minus k x is equal to constant typically. Therefore, if you differentiate this; so what do you get? What will be d x by d t? What do you get?

Student: Omega.

Omega upon k; so this d x by d t for a fixed for a wave with the fixed phase this is called the phase velocity. We represent v subscript p phase velocity for a constant phase plane. So, this tells you what is the speed of the propagation of the wave. So, and that is related to your ratio of angular frequency to your wave number right. Therefore, if you plot therefore, a wave with a fixed phase omega t minus k x is equal to constant, you get a positive slope which tells you to that in a phase plane, if you plot phase plane of x t verses x, time on 1 axis and x. So, how do these waves go, in which direction do they go? So, they run on towards the right side. These waves you can represent them over different position and time space like this.

These are all waves with positive slope. So, these are called right running waves. Running waves and typically the fixed phase is omega t minus k x is equal to constant. So, the slope is given by the ratio of omega upon k.

Similarly, if you take the waves which are omega t plus k x is equal to constant. So, that the slopes are negative. So, they will be running on the other side. So, you have these are called left running waves. Omega t plus k x is equal to constant. So, these are some basics most of you might already know this, I am just again revisiting. Now these are all the characteristics of what we call as travelling waves, the travel in position and time. So, you can actually use 2 traveling waves.

So, one traveling towards the right, and 1 traveling towards the left and create what is called as standing wave. We can super impose 1 wave traveling towards the 1 wave traveling towards the left super impose these 2. And finally, what happen, the wave now cannot move to this way or this way this will be just fixed in phase. So, these are called standing waves. So, we will know l o at the characteristics of standing waves.

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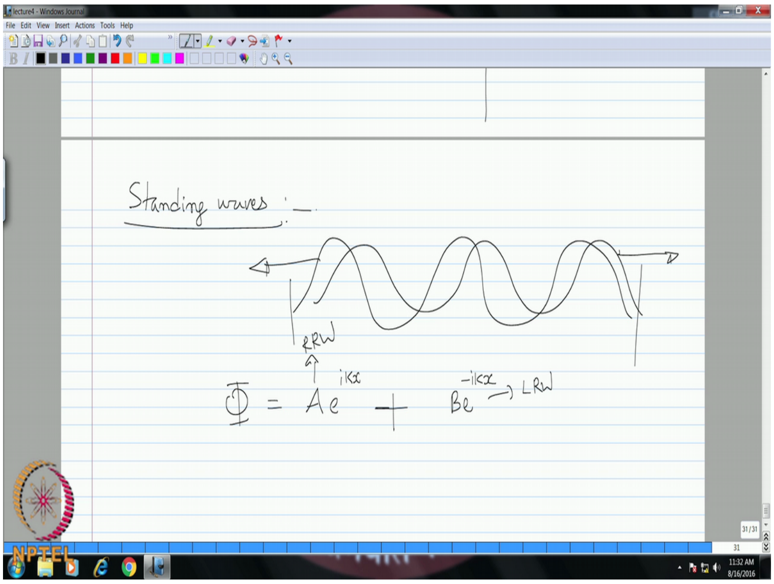

Standing waves :-

$$\Phi = \underset{\uparrow\,\text{RRW}}{Ae^{ikx}} + Be^{-ikx} \rightarrow \text{LRW}$$

So, in standing waves typically you have a right running wave which is moving in this direction and you have a left running wave, which is moving in this direction you see super impose these 2, assume a linear super position of the waves. So, the wave which is now let us l o at only the coordinate, the position space, not the time. Let us look at only position and therefore, the right running wave will be indicated by e power I k x left running wave will be b e power minus I k x right. So, we linearly superpose these 2 and we create this standing wave. So, wave functions are described like this. Because in the complex representation. So, for the case of right running wave in a special coordinate it is e power I k x. So, the left running wave will have e power minus I k x. If you superpose these 2 you create, standing wave with these particular wave function. So, this is the right running wave; this is your left running wave.

So, to observer it will look like this wave is particularly pined and this is not moving at, suppose you confine this wave with in a particular domain. For example, this boundary, at the boundaries of this domain, since the domain is stationary the wave will be appear to be pinned to this domains and it cannot move either right or left. So, the typical value of this wave function will be 0 at these boundaries. Therefore, now if you l o at the standing wave of in a particular domain.

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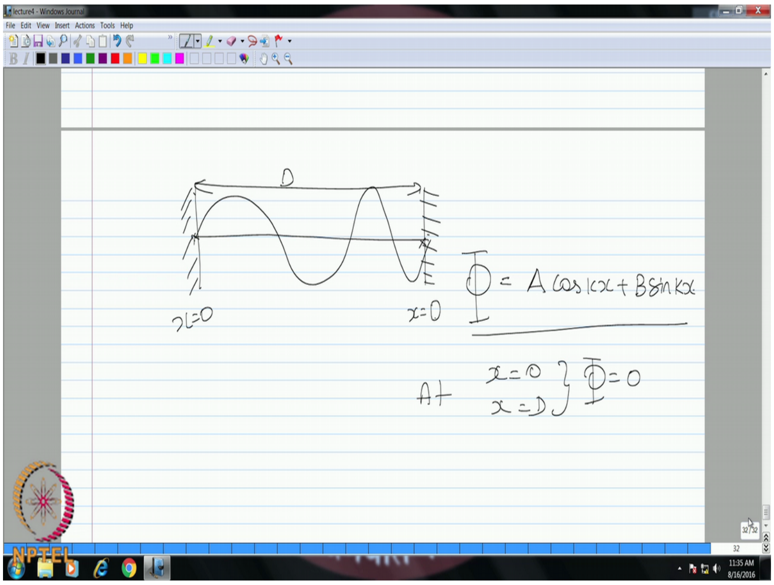

Let us take a domain like this and you create a standing wave. You can have standing wave might l o something like this, the wave function will be 0 at the boundaries. Now if you want to write this complex representation in terms of exponents, exponential functions, we can always convert this back to trigonometric function. So, we can always write this also has a cos k x plus b sin k x so, we can always flip back and forth between exponential, representation and trigonometric representation.

Let us now start with the trigonometric representation of this wave, a cos k x plus b sin k x and at the boundaries; let us say x is equal to 0 and this is x is equal to D, where d is the length of this particular confinement; which produces the standing wave. So, at both these boundaries, the value of wave function will be equal to 0. Therefore, you can apply the boundary conditions. So now; you can calculate what does this? What are the constants and also the corresponding Eigen values? So, can all of you can do this and let me know.

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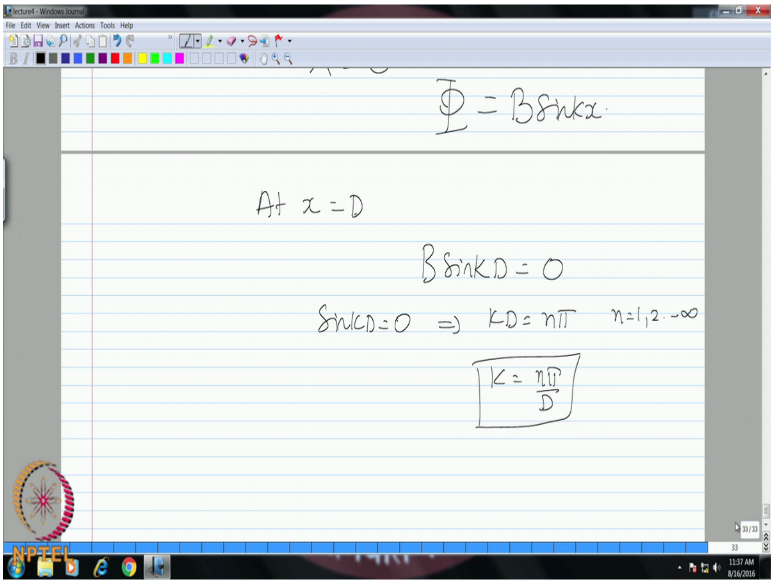

$$\Phi = B\sin kx$$

At $x = D$

$$B\sin kD = 0$$

$$\sin kD = 0 \Rightarrow KD = n\pi \qquad n = 1, 2 \ldots \infty$$

$$\boxed{K = \frac{n\pi}{D}}$$

So, therefore what will be A, A will be 0 and therefore, you are phi will be b sin k x. So, if you apply the second condition, at x equal to D you have B sin k D will be 0, if B is 0 the entire solution becomes to be (Refer Time: 29:47). Therefore, sin K D should be equal to 0 which means that K D should be equal to n pi.

Again n cannot be 0, if n is 0 again the solution become (Refer Time: 30:01) so, n should be equal to one total infinity therefore, your K becomes n pi by D. So, with this now we can calculate, what is the energy of these waves. It could be an electron wave or a phonon wave or a photon wave, which is within this particular element of thickness D. So, what is the energy?

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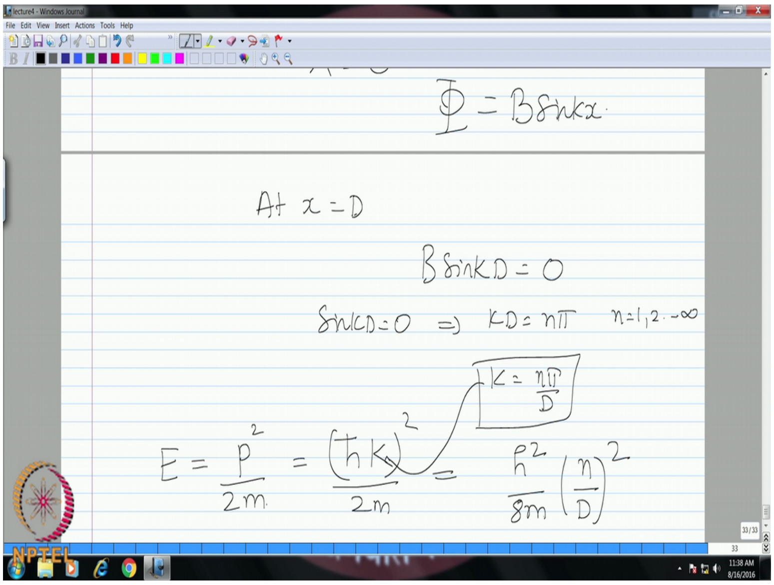

$$\Phi = B\sin kx$$

At $x = D$

$$B\sin kD = 0$$

$$\sin kD = 0 \Rightarrow kD = n\pi \quad n = 1, 2 \cdots \infty$$

$$\boxed{k = \frac{n\pi}{D}}$$

$$E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m} = \frac{h^2}{8m}\left(\frac{n}{D}\right)^2$$

So, if you take the particle nature, your energy is nothing, but p square by 2 m, where p is your momentum, particle momentum. Now, we just convert this particle picture to wave picture. So, how is p related to the wave number h bar k is p. You have seen this in the last class.

Therefore, the whole square divided by 2 m. Now, we got the expression for k, as n pi by D, you can substitute into this and you will be getting the expression, this is if you rewrite in terms of just normal planes constant; you have h square by 8 m into n by D the whole square. So, I am just plugging in for k, what we got from there into this is it clear? Now, if you represent therefore, different modes of these waves if you are n is equal to 1 how does this wave appear.

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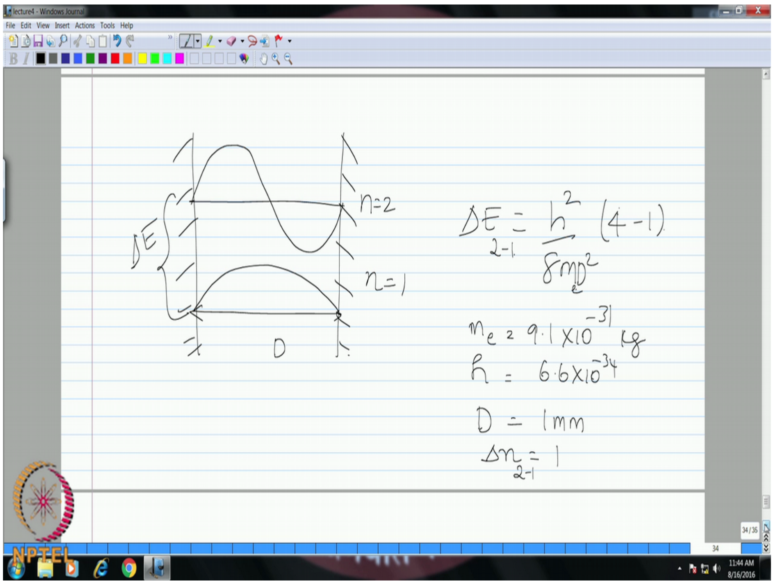

$$\Delta E_{2-1} = \frac{h^2}{8 m_e D^2}(4-1)$$

$m_e = 9.1 \times 10^{-31}$ kg

$h = 6.6 \times 10^{-34}$

$D = 1$ mm

$\Delta n_{2-1} = 1$

So, let us draw the confinement and this is your separation distance D, if your n is equal to 1. In this case, k is equal to pi by D. So, how will the wave l o. This is how the standing wave will look. Now if n is equal to 2, your wave number will become 2 pi by D. So, you will have therefore, a peak and a trough. Similarly if n is equal to 3, 4. So, you have multiple modes; n is equal to 1, 2 infinity. So, all this possible waves are there, all these possibilities exist for the standing wave.

Once you put the standing wave within a particular confinement this wave now appears to be discretize, into infinite number of waves of different modes. So, infinite number of standing waves are created within this particular confinement and each of this will have a particular energy and that energy is given by this expression, Therefore, what is the discretization of the energy levels, between n equal to 1 and n equal to 2, 2 to 3, 3 to 4 and. So, on that is the delta e. The delta e is now given by h square by 8 m, delta n by d the whole square; therefore, if you take the case of electron.

Student: (Refer Time: 34:17).

But h is the constant, m is the constant, d is the constant. So, the delta is only due to the delta in n.

Student: (Refer Time: 34:29) delta of n.

Delta of n square that is true. So, you mean, you want this to be written, I take the d square out like this right. Now, let us take the case of electrons. So, we will call this mass associated mass of electron. We want to see, what is the jump in the energy levels between 2 successive modes? So, m e will be equal to 9.1. 10 power minus 31 kg's planes constant h 6.6 into 10 power minus 34. Let us take the example of confinement which is 1 millimeter. And let us take delta n to be equal to 1; changes jump in the energy level. So, what do you get for delta e? This is substitute this; can somebody check that we want to now l o at the jump in energy level from 1 mode to the second mode yeah. So, it should be actually delta of n square right.

Student: (Refer Time: 36:04).

Yes should be delta n the whole square. The delta n is basically in this case unity; we want to look at the change in the energy between.

Student: 0 to 1.

0 to 1 or 1 to 2 not 0.

Student: (Refer Time: 36:28).

It should be.

Student: 4 minus 1.

Yeah. 4; no that is what, it should be in this case. I think no, this cannot be delta of n square for sure. If you then l o at, 2 2 1. Then this is 4 minus 1. For example, let us go from 2 2 1, then you can calculate and let me know. So, this will be therefore, 4 minus 1 right. So, let us say 2 2 1. So, what do you get?

Student: (Refer Time: 38:04) 1.8 sorry 1.7.

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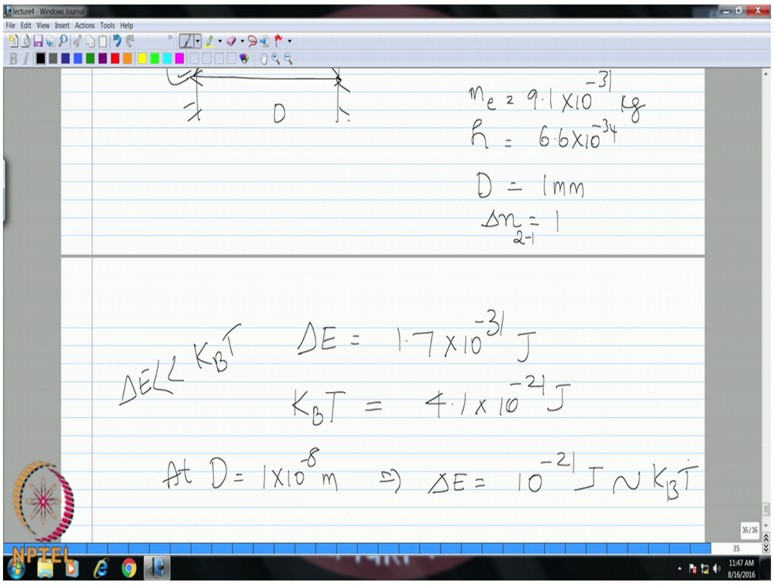

$m_e = 9.1 \times 10^{-31}$ kg

$\hbar = 6.6 \times 10^{-34}$

$D = 1$ mm

$\Delta n_{2-1} = 1$

$\Delta E << K_B T$

$\Delta E = 1.7 \times 10^{-31}$ J

$K_B T = 4.1 \times 10^{-21}$ J

At $D = 1 \times 10^{-8}$ m $\Rightarrow \Delta E = 10^{-21}$ J $\sim K_B T$

1.7 9, just a moment; 1.7 into 10 to the power minus.

Student: 31.

31. This is in Joules and now what is the energy associated with room temperature; for example. That is your k B times T where k B is a Boltzmann's constant. So, this at room temperature comes out to be 4.1 into 10 power minus 21 Joules. So, what this means is, if your order of D is around 1 m m. So, your delta e that is the difference between the energy levels, due to this quantization due to the discreteness will be less than your disenable energy. Because you are normal energy level at room temperature itself is 10 power minus 21. And this is much smaller than. So, you cannot even sense it, you cannot even feel this certain shifts in the energy, due to the quantization at room temperature.

Whereas, if you now, put your D to the order of nanometers. Let us calculate the same thing, with D as 1 into 10 power minus 8 meters. 10 nanometers, what happens to delta e? So, this we have D square in the denominator now. So, as your D is reducing, that should increase 1 over D square. So, this goes to 10 power how much.

Student: Minus 21.

Minus 21; now, you see that the order of delta e is comparable to k B t. Now, you can really go and measure; the change in energy level from mode n equal to 1 to n equal to 2 and these are significant values compare to k B t. So, it depends on what is the size of this confinement you are looking at, if you are confinement size is very large, then the shift in the or the spacing between these energy levels are so small that you can almost neglect the discreteness or quantization, whereas if your confinement length becomes smaller and smaller this shift becomes very large. And therefore, the real quantization happens. So, all waves in principle have some discreteness even at room temperature.

But it depends on the size of the confinement. We are talking about waves, maybe which are the order of nanometer confinement, so there it becomes very significant. Whereas, if you are talking about millimeters, centimeters, there you can completely ignore this quantum effects, so this is a very nice simple example, to tell to illustrate, what happens to standing wave in a confinement and what happens to the shift in energy levels when the confinement size reduces. I think this expression what we have derived for energy you will have to just mark it just, because the way we have derived now is very less regress; we have just used simple wave equation and then we have derived this e, but now next what we will do, now we will introduce Schrodinger wave equation .

So, that is the more regress for describing quantum mechanical waves and from there we will also derive for a simple confinement and we will see that the expression comes out to be the same, but we will do it in a more regress way using this Schrodinger equation. So, we may not have much time to solve anything today.

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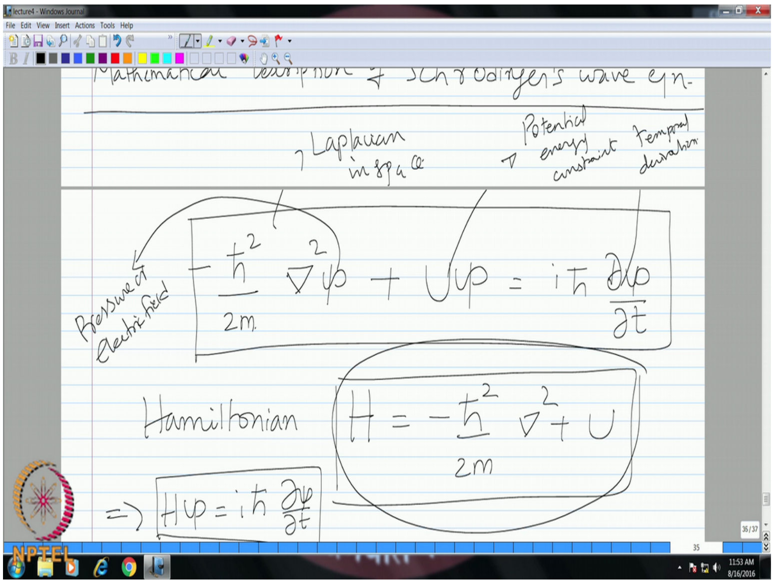

Mathematical description of Schrodinger's wave eqn.

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = i\hbar\frac{\partial\psi}{\partial t}}$$

Hamiltonian $\boxed{H = -\frac{\hbar^2}{2m}\nabla^2 + U}$

$$\Rightarrow \boxed{H\psi = i\hbar\frac{\partial\psi}{\partial t}}$$

But I will at least introduce you the mathematical description of the Schrodinger equation. So, in fact when Schrodinger first; I mean when you first describe this wave nature through this particular equation. So, he did not understand the meaning of the wave function. So, he wrote the mathematical form of this wave function as minus modified plants constant h square by 2 m times Laplacian of wave function psi.

So, we will call this as psi 2 say that this is a wave function we will see what it is. Plus you have a potential energy constraint u times, wave function, which is equal to I modify planes constant times d psi by d t. So, this is your Schrodinger wave equation. So, generally what people do is; the use an operator call the Hamiltonian operator, Hamiltonian, they use this operator h to signify this entire term minus modified planes constants square by 2 m, del square plus u, this entire operator is called Hamiltonian operator. And they write this in a very compact form therefore, as h psi is equal to I h bar d psi by d t.

We will see what is this Hamiltonian and this is actually the indicator of the energy possessed by the particular wave. We will see that, but right now we will just state it, later on we will prove that, this is nothing but, the indicator of the energy processed by the wave. So, Schrodinger basically stated the wave characteristic like this. So, this is it could be the psi could be a wave function which indicates either a pressure wave for example, or a electric field, could be anything. If you are talking about electron, this is a basically electric field; wave it could be pressure waves, molecules, pressure waves, so whatever field that you consider. So, this is the corresponding wave function for that. So, therefore, the first term here, this is the Laplacian operator in space and this is the function of only the space where as the second operator here. It is the potential energy constraint and this is your temporal derivative. So, that is your wave function is a function of both position and time.

So, this is a partial differential equation. Now you can compare this for example, if your potential energy constraint is 0. If you there is no potential energy constraint, the particle is say or the wave is free to move without any constraint on the potential energy so; that means u is 0.

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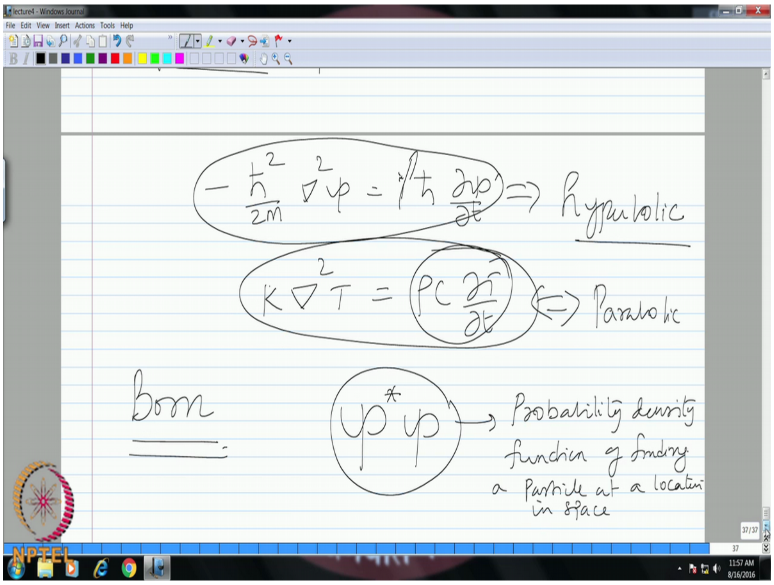

$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial\psi}{\partial t} \Rightarrow$ Hyperbolic

$K\nabla^2 T = \rho c\frac{\partial T}{\partial t} \Leftrightarrow$ Parabolic

Born

$\psi^*\psi \rightarrow$ Probability density function of finding a particle at a location in space

And therefore, the equation will be minus h bar square upon, 2 m del square psi equal to I h bar d psi by d t. Now compare this to your energy equation that we derived. So, how does your macroscopic energy equation look for conduction; you have k into del square t is equal to row c in to d t by d t.

So, it l o s like a similar structure, what is the mathematical nature of this; heat conduction equation here. This is parabolic. Because of the temporal derivative, if there was no temporal derivative it would be, elliptic equation, is governed only by the boundary conditions. Now it is governed by also the initial conditions. So, it becomes a parabolic equation. You see structurally this looks similar if your h square by 2 m is replaced with k and this by rho c, but what is the nature of this wave equation? This is called hyperbolic equation.

That is why it is a wave equation. Any wave equation is hyperbolic. So, what is bringing this hyperbolic nature is this imaginary number I. If there was no imaginary number, this equation would be parabolic right. So, what brings the hyperbolic nature to be Schrodingers equation is essentially this imaginary number without it; it is not a wave equation so.

Basically, when what is interesting in histories that Schrodinger himself did not come up with a correct explanation for this wave functions psi. He did not understand what to do with a solution for psi, so later on it was born; b o r n. So, so this scientist, he understood that there is a significant to this wave function; only if you multiply the complex conjugate of this wave function. I denote the complex conjugate as psi superscript star. For example, if psi is equal to a plus I b, a complex conjugate will be a minus I and if I take the product of this complex conjugate of the wave function at this, then together this product is nothing but, the probability density function, of finding a particle at some position in space of finding a particle at a location in space.

So, by itself the wave function does not have any physical meaning but if you take the product of complex conjugate of the wave function with a wave function. So, this gives the probability of finding a particle at some location, you know and if there is a particle it has to be found somewhere.

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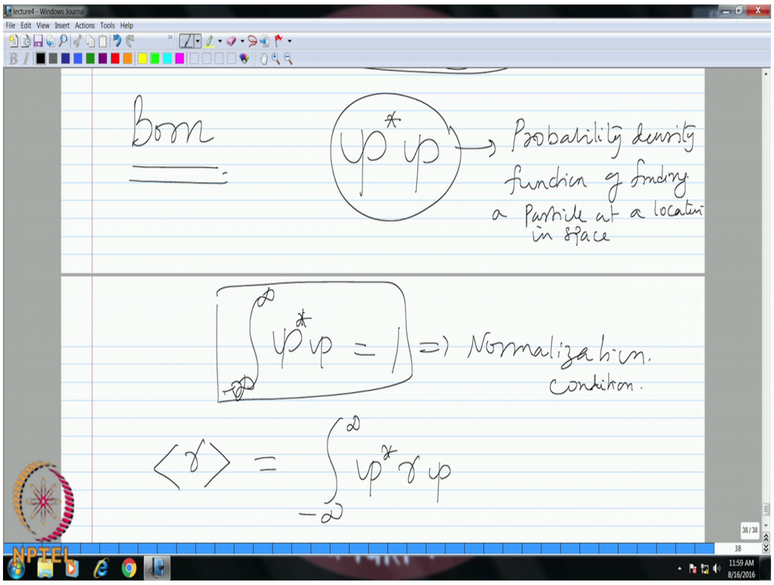

Born

$\boxed{\psi^* \psi}$ → Probability density function of finding a particle at a location in space

$$\boxed{\int_{-\infty}^{\infty} \psi^* \psi = 1} \Rightarrow \text{Normalization condition.}$$

$$\langle r \rangle = \int_{-\infty}^{\infty} \psi^* r \psi$$

Therefore, according to the normalization what should happen? Between these spaces 0 to infinity, the product of psi star psi should be equal to 1. Because the particle has if, there was a particle it has to be found somewhere in the infinite space. So, therefore, this condition has to be satisfied this is called Normalization Condition. So, this should be sorry minus infinity to plus infinity. Because this space now you do not have coordinate system 0 to infinity. There is minus infinity all the wave to infinity normalization.

So, this now bond brought out the proper way of interpreting the solution. So, with this we can actually find outs important things like for example, the exact coordinate of a particle, by using this we can find out, any expected value; now in quantum mechanics everything is an expectation nothing is 100 percent sure. So, we always use an operator like this to show that this is an expected value.

So, the expected value of position; for example, is denoted by this particular operator r is nothing but, minus infinity to infinity psi star r psi. So, based on this operator, you can find out what is the probable location where the expected location or expected coordinate of this particular particle. Similarly you can do that for momentum and energy. So, we will continue that tomorrow. We will see what are the operators for momentum and energy.

Thank you.