Electronic Properties of the Materials: Computational Approach
Prof. Somnath Bhowmick
Department of Materials and Engineering
Indian Institute of Technology - Kanpur

Lecture: 04
Solving Schrodinger Equation for Different Potentials

Hello friends we already have become familiar with quantum mechanics by solving quantum particle in a box problem. In this lecture we learn some classic problems by solving Schrodinger equation for different potentials.

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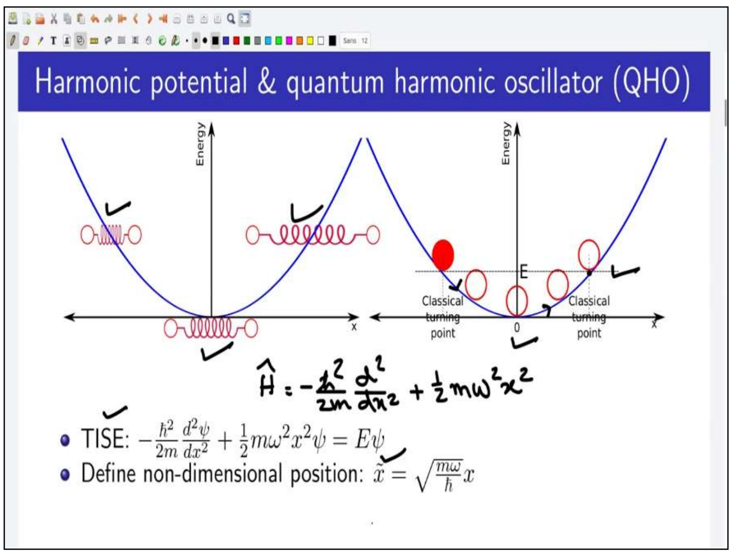

We start with harmonic potential you can think of a harmonic oscillator in equilibrium the potential energy is 0 as we stretch or as we compress the potential energy increases quadratically with x where x is the displacement with respect to the equilibrium. You can also think of a ball rolling down as shown in this figure at x equal to 0 it has 0 potential energy and kinetic energy is equal to the total energy.

The potential energy increases quadratically away from x equal to 0. Classical the maximum height can be climbed depends on the total energy E. So, this is the line indicating the total energy. At the highest point the kinetic energy is 0 and the potential energy is equal to the total energy. The ball cannot travel beyond this point and it turns back. So, at this point it will turn back this is known as the classical turning point.

Now let us see how do we solve this problem in quantum mechanical way. So, first let us write down the Hamiltonian or total energy operator.

$$\hat{H} = \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}mw^2x^2$$

Now let us define non-dimensional position

$$\tilde{x} = \sqrt{\frac{mw}{\hbar}}x$$

So, m omega by h bar if you take a square root of this, this term has a dimension of 1 over position and x is of course it has a dimension of position such that x tilde is non dimensional.

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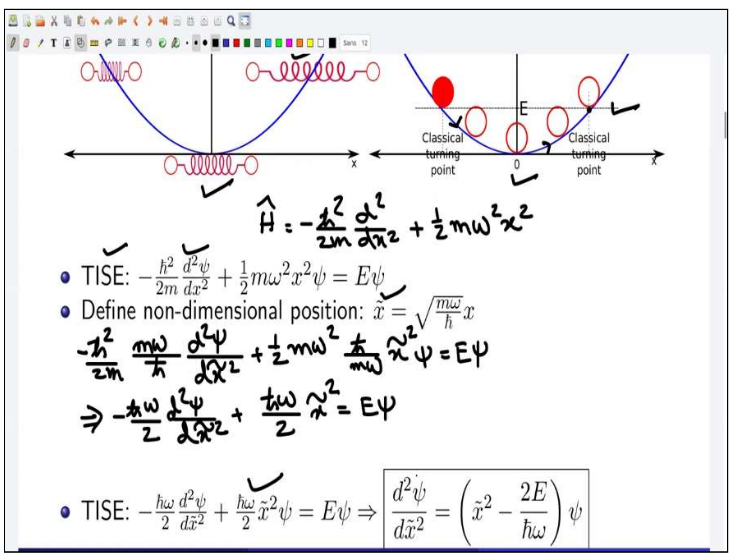

Now if we replace this in this time independent Schrodinger equation then what we get is the following. So, minus h cross square by 2m and then I replace x tilde equal to this sorry that I get m omega by h bar d 2 psi dx tilde square plus half m omega square h bar by m omega x tilde square psi is equals to E times psi such that minus h cross omega by 2 d 2 psi dx tilde square plus h cross omega by 2 x tilde square is equals to E psi okay. So, this is what is written here and then we can just write finally this term.

$$\frac{d^2\psi}{d\widetilde{x^2}} = \left(\tilde{x} - \frac{2E}{\hbar w}\right)$$

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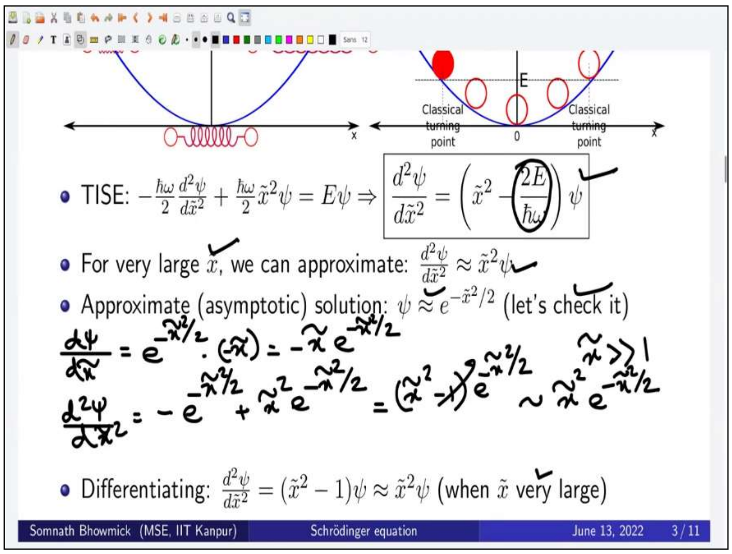

Thus, using non-dimensional position, we have converted the time independent Schrodinger equation in this form. Now for very large value of x tilde we can approximately write this equation as this because if x tilde is very large then we can ignore this part and we can just write this. Now approximate asymptotic solution can be written as

$$\psi \approx e^{-\widetilde{x^2}}\psi$$

So, if psi is this then d psi dx tilde is equals to e power minus x tilde square divided by 2 times minus x tilde is equals to we can just write it as and if we take the second derivative d2 psi dx tilde square is equal to plus x theta squared and we can write this as x theta square minus 1 e power. Now what we have assumed x tilde is very large correct. So, x tilde is very large. So, that means again we can ignore this star 1 such that we can write this term as x delta square x finder square by 2 which proves that this is a solution for this equation.

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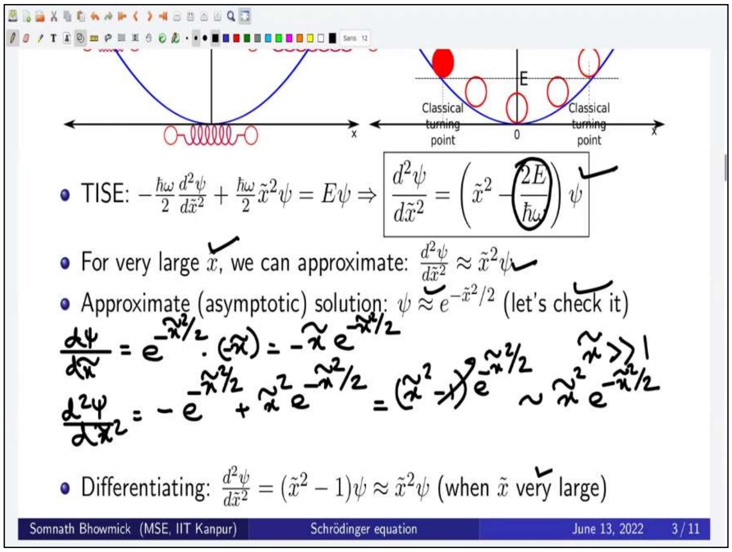

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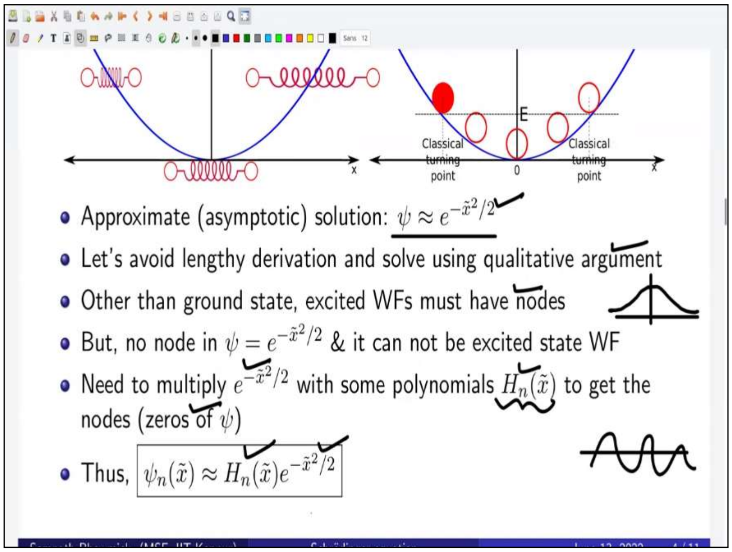

Thus the approximate asymptotic solution is this.

$$\psi \approx e^{-\widetilde{x^2}/2}$$

Now let us avoid lengthy derivation and solve using qualitative argument. We know that other than ground state excited state wave functions must have nodes this is what we have seen for particle in a box. The ground state wave function does not have any known the first excited state has one node the second excited state has two nodes and so on.

But the solution that we have derived so, far right this does not have any node because this is e power minus x tilde square by 2. So, the solution it looks like this correct it does not cross 0 line at any point like this. So, that means this wave function does not have any nodes. So, this can be a ground state wave function but this cannot be excited state wave function. Thus we need to multiply this function with some polynomial which at this point of time I just write it as H n of x tilde right. So, this is some polynomial which will be having some nodes. So, that means this will be some polynomial which will cross this line 0 at several points correct depending on the energy state and this polynomial will be having nodes and if I multiply this part with this polynomial then the net wave function will also be having same number of nodes as H n of x. So, we have to multiply e power minus x tilde square by 2 with some polynomials to get the nodes or 0s of psi of x. So, at the moment we can just

$$\Psi_n(\tilde{x}) \approx H_n(\tilde{x}) e^{-\widetilde{x^2}/2}$$

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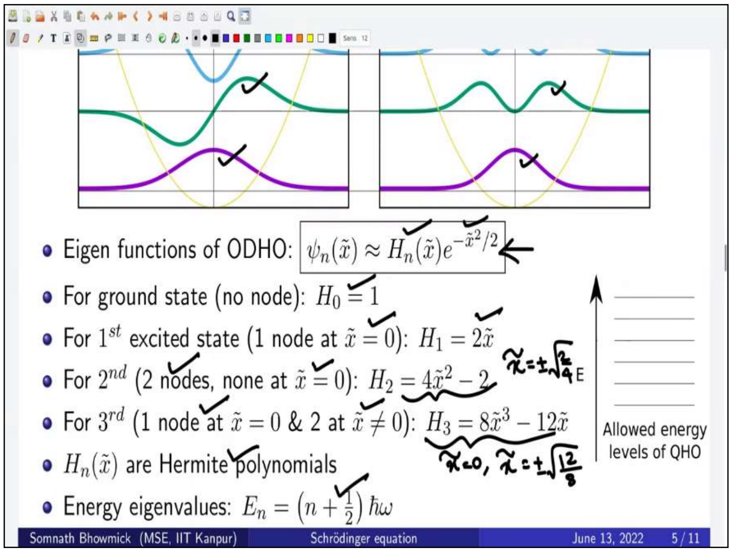

So, far we have seen that the eigen functions of one-dimensional harmonic oscillators are given in this form psi n of x tilde is equals to h and x tilde. So, these are some polynomials multiplied by e power minus x tilde square divided by 2. What we do not know is what are these polynomials H n of x tilde. So, for ground state there should not be any node just H tilde will be equal to 1 for the first excited state there has to be a node at x tilde equal to 0. So, that means this polynomial H of 1 will be equal to 2 x tilde because this has a node 2 x tilde has a node at x equal to 0. For second excited state we need 2 nodes right and none of them should be at x tilde equal to 0 note that this is something which is very similar to what we got in case of particle in a box. So, now to meet this requirement that we need two nodes and none of them at x equal to 0 you can just check that this polynomial will meet those requirements. Because you will get two nodes in this case at these two points okay. Similarly for the third excited state we need one node at x tilde equal to 0 and two nodes at x tilde not equal to 0 and then you can see if you look at this polynomial you have one node at x tilde equal to 0 and you have two more nodes that x tilde is equals to plus minus square root of 12 by 8. So, and then soon right we can even derive this for even higher excited steps. And $H_n(\tilde{x})$ these are known as Hermite polynomials and I have shown some wave functions in this plot. So, this is the eigen function for the ground state this is for the first extinguisher this is for the second state and this is for the third one and these are the corresponding probability densities. Now we can prove that the corresponding energy eigen values are given by this.

And note that similar to particle in a box all the energy eigen values are not allowed and here I just schematically show the allowed energy levels of quantum harmonic oscillator.

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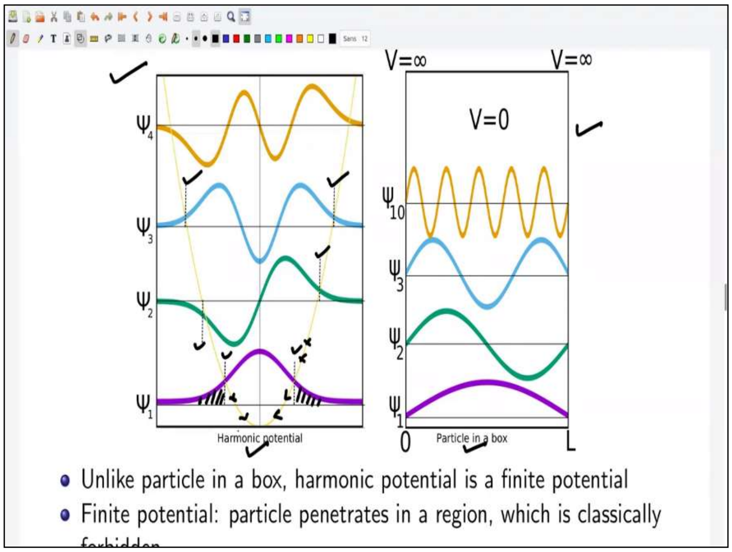

Let us compare between harmonic potential and particle in a box. Unlike particle in a box harmonic potential is a finite potential this remains finite for finite value of x for finite potentials a quantum particle can penetrate in regions which are classically forbidden however this is not possible for some infinite potential. For example, in case of particle in a box problem particle remains confined inside the box whether you treat it classically or quantum mechanically.

As you see here the wave function remains completely confined inside the box. This happens because the potential becomes infinite at the box edges. Since harmonic potential is finite for finite x we find some small probability of finding the particle beyond the classical turning point shown by these dotted lines. So, these dotted lines are the points from where the particle is supposed to turn back in this region okay. The particle is not classically you are not supposed to get the particle in these regions that is beyond these dashed lines you are not supposed to get the particle classically. Thus classically the particle should turn back from these dashed lines and start rolling down the potential in this way. Existence of the particle beyond the dashed lines is classically formal. However a quantum particle can exist there you can see that you have some probability. Although this is very small but still you have some finite probability of finding the particle beyond the classical turning point. This is related to quantum tunnelling which we are going to discuss towards the end of this lecture.

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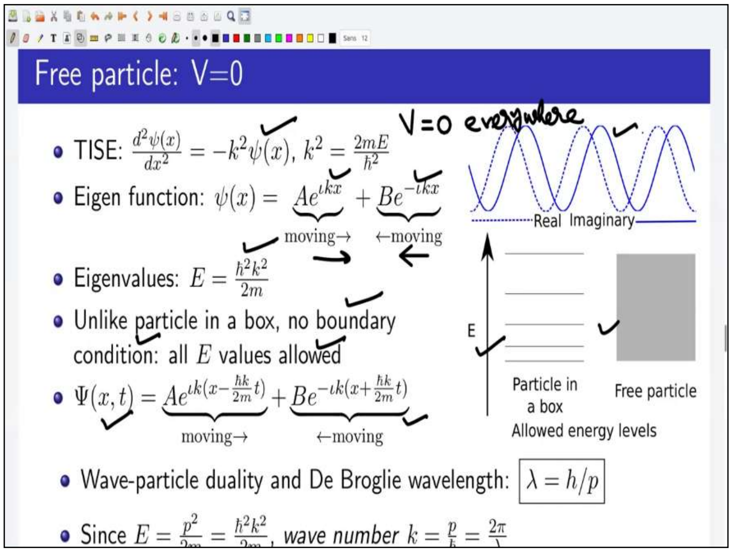

So, far we have discussed about particles confined by some potential for example harmonic potential or particle confined within a box. Now we are going to learn about particles which are not confined by some potential but travelling. The time independent Schrodinger equation is d psi by dx square is equals to minus a square times psi of x it looks exactly like the particle in a box problem. However now potential is 0 everywhere in case of particle in a box we had infinite potential at the box edges but now v is equals to 0 everywhere. Now the eigen functions are given by psi of x is equals to Ae power ikx + Be power minus ikx. So, this is the case of a particle moving from left to right and this is the case of a particle moving from right to left. And if you put the this eigen function in this equation. Then we get the eigen values as e equal to h cross square k square divided by 2m. Unlike particle in a box problem there is no boundary condition in this case. Thus all the energy values are allowed. So, this is what is shown here schematically in case of a particle in a box problem all the energy values are not allowed whereas for free particle all the energy values are allowed. And now we can write down once we have the eigen functions as well as the eigen values using them we can write down the time dependent wave function like this. And you see the eigen functions are now complex. So, we can separately plot the real part and the imaginary part as shown here.

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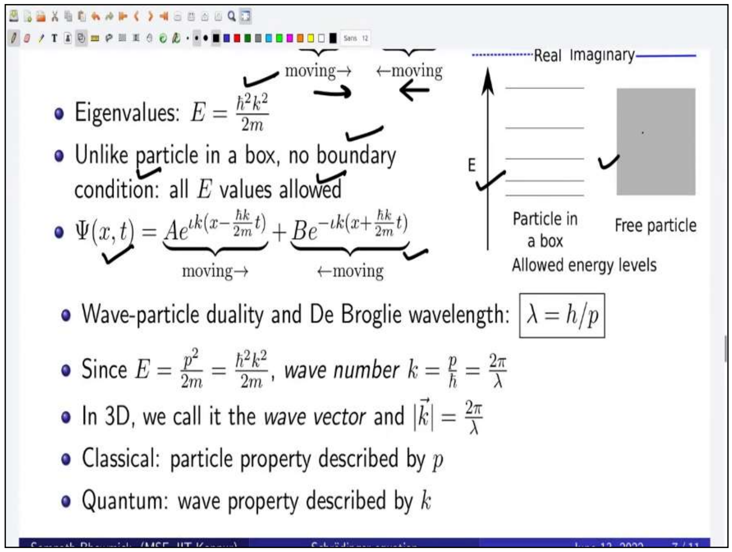

Now the wave particle duality and the wrongly wavelength they are given by this lambda is equals to h by p. So, if we know the momentum we can define some wavelength and if we know the wavelength we can find some momentum and so on. Now classically the energy is given by equal to p square by 2m and we have seen the energy eigen values to be like this h plus square k square by 2m. So, if we equate them, we can define something called a wave number k which is given by 2 pi by lambda. In 3D we call it the wave vector and magnitude of y vector is given by 2 pi divided by lambda where lambda is the wavelength. Thus, classical property of the particle is described by its momentum. Similarly, quantum mechanical the wave property is described by its wave vector k.

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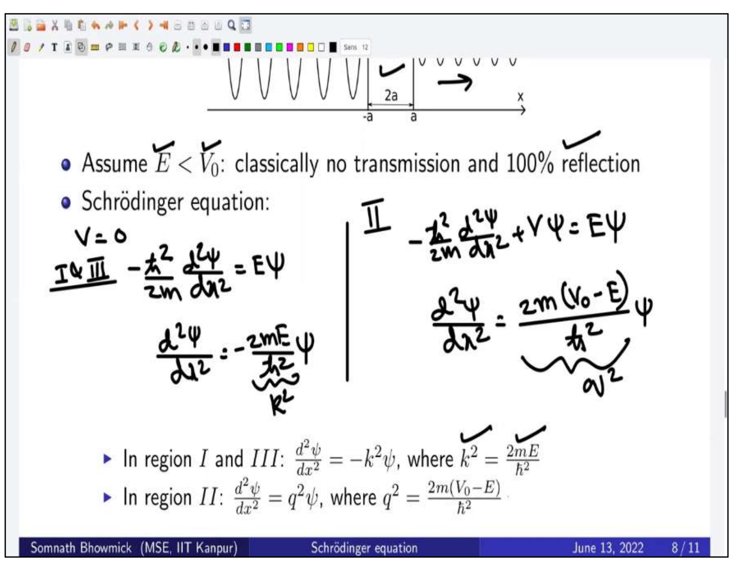

Next, we discuss quantum tunnelling. We are dealing with a free particle which is propagating from left to the right it hits the potential barrier at this point. Now let us assume that the barrier height is more than the energy of the particle. Thus classically no transmission is possible and the particle is reflected from this point. However as mentioned before quantum particle can penetrate in regions forbidden for classical particles. We shall find the probability that the particle tunnels through the barrier in region 2 and emerges in region 3 to continue its journey. Now let us write the Schrodinger equation in region 1 and region 3. So, in region 1 and region 3 V is equals to 0. So, that means we can write the Schrodinger equation as this is like in region 1 and region 3 okay. So, that we can write the Schrodinger equation as minus h cross square by 2m p 2 psi dx square the potential energy part is equals to 0.

And this is equal to E times psi such that we can just rewrite this in this form d2 psi dx square is equals to minus 2 m E by h square. Now in region 2 we can write the Schrodinger equation as minus h plus square by 2 m d 2 psi dx square plus v of psi is equals to g of psi and we can rewrite this as d 2 psi dx square is equals to 2m V naught minus E divided by h cross square psi okay and we define k square as 2 m E by h cross square and that means this term is defined as k square and this term is defined as q square. So, q square is equals to 2m V naught minus E divided by h cross square.

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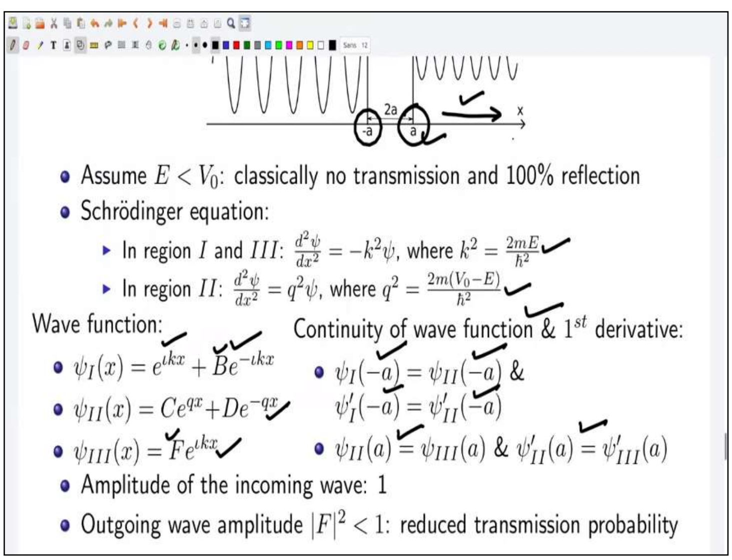

So, far we have defined the Schrodinger equation in different regions. Now we have to write down the eigen functions. So, in region 1 we see that the particle is propagating from left to right and then it hits the potential barrier here and then a part of it will be reflected back. So, this is the part or this is the function which is like propagating from left to right and this is the portion which is reflected back. And in part two we do not have some propagating solution and in part three we again have some propagating solution but now in this case it is propagating from left to right there is nothing that is getting reflected back. So, that is why this e power minus ikx part is not present in region 3. So, now we have the wave functions in three different regions part one part two and part three. Now the wave function and its first derivative must be continuous and we just have to maintain the continuity at x equal to minus a as well as x equal to plus a. So, that means at x equal to minus a we must satisfy psi i of minus a is has to be equal to psi 2 of minus a and similarly the first derivative psi 1 dash of minus a this should be equal to psi 2 dash of minus a correct. And similarly at this boundary that is at x equal to plus a we must satisfy this conditions. Note that this constant right; in front of these functions these are the amplitudes. For example amplitude of the incoming wave is equal to 1.

And then the amplitude of the reflected wave will be given by mod of B square and similarly the amplitude of the outgoing wave that is mod of f square this is and then we expect this to be less than 1 how less we do not know so, far and then that is why right you see in this diagram since the amplitude of the transmitted wave it it reflects the transmission probability. So, this has to be less than whatever was there for the incoming waves.

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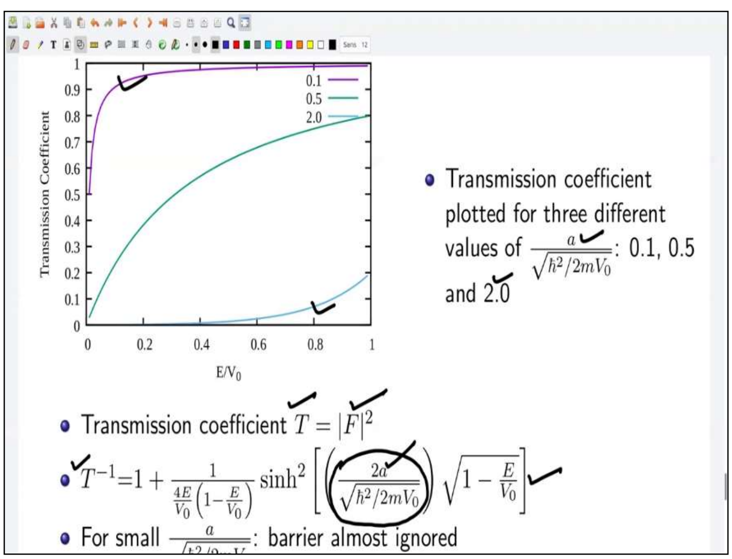

Using the conditions for continuity of the wave functions and their first derivatives we get four equations and solving those four equations we can get mod F square which is equal to the transmission coefficient and inverse of transmission coefficient can be represented in this form. Now we are going to plot T using different values of this parameter note that a is the or 2a is the width of the potential barrier. So, that means this also has to be the term in the denominator also must be having some dimension of length. So, now in this plot we have plotted the transmission coefficient for various different values of this parameter. So, for example 0.1, 0.5 and 2.0 and what do we see for small value of this parameter say for example 0.1 the transmission coefficient is almost 100%.

So, that means the barrier is almost ignored whereas if you take this parameter to be very large then the transmission coefficient is very small that means there is almost no transmission. And for some value in between for example 0.5 the transmission coefficient looks like this.

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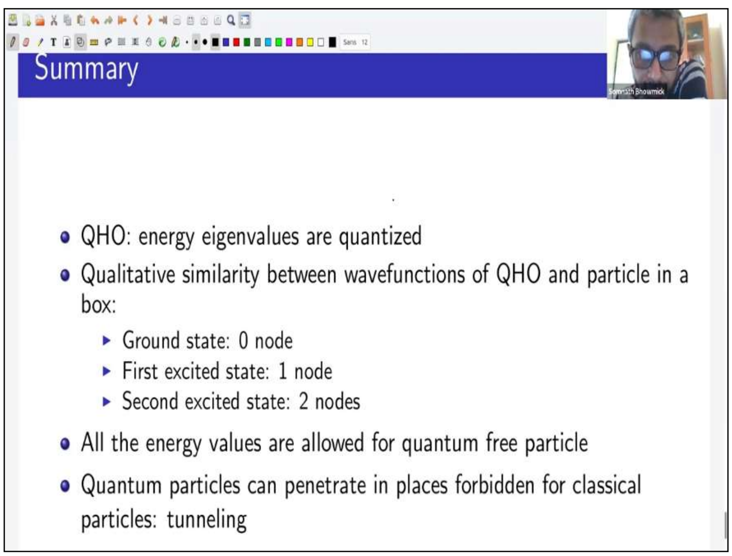

Let us summarize what we have learned in this lecture we have solved three classic problems in quantum mechanics. So, it started with quantum harmonic oscillator and we found that the energy eigen values are quantized and we also have noticed the qualitative similarity between wave functions of quantum harmonic oscillator and particle in a box. For example the ground state has 0 node the first excited state has one node the second excited state has two nodes and so far. Then we learned about quantum free particle and then we found that the energy eigen values all of them are allowed because there is no boundary condition. And the third problem that we have learnt is tunnelling we found that quantum particles can penetrate in places forbidden for classical particles, thank you.