Quantum Mechanics
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Lecture – 08
Bound States - II

But you already see something here, you get a power series which is even powers or a power series which is odd powers either or, cannot be both together okay, so it has some property; property is that what is that property?

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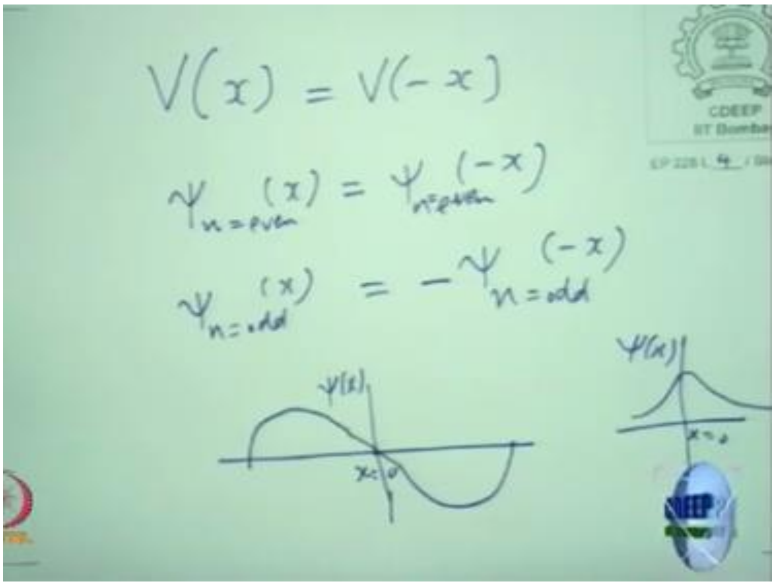

One of the property which we see is V(x) =V(-x), okay and we see that $\Psi_{n=even}(x)$ = $\Psi_{n=even}(-x)$, $\Psi_{n=odd}(x)$ = $-\Psi_{n=odd}(-x)$ will be in powers of odd powers, what are these functions called, you have studied this property, these properties are called even functions and odd functions, right. Even functions means it does not change sign and x going to any function, f(x), if it does not change sign when you make x to –x.

For example, cos function; cos of x is an even function, right but if it makes change of sign and x going to - x that is a odds function, okay, so you can have situations when it is an odd function suppose, you are looking at odd function at let us do the plot here, at x = 0, odd function has to be 0, do you agree, odd function has to go through 0, has to be 0 at x = 0. What about even function? Even function can be finite, something like this.

This is a well-defined even function, odd functions will be something like this, so there is always a node for an odd function and there is no such nodes for a n even function at x = 0, okay, so these are some things which you observe that if you have an odd power polynomial, you will have a node at x = 0 but you will not have a node at x = 0 for even functions, so I did not do anything, when I try to find the solution.

The property of V(x) = V(-x) squared forced the solution to be either even functions or odd functions, so that is the property of these symmetric potentials, I am sure you have all done this, you at least tried the double delta function which was given to you, right.

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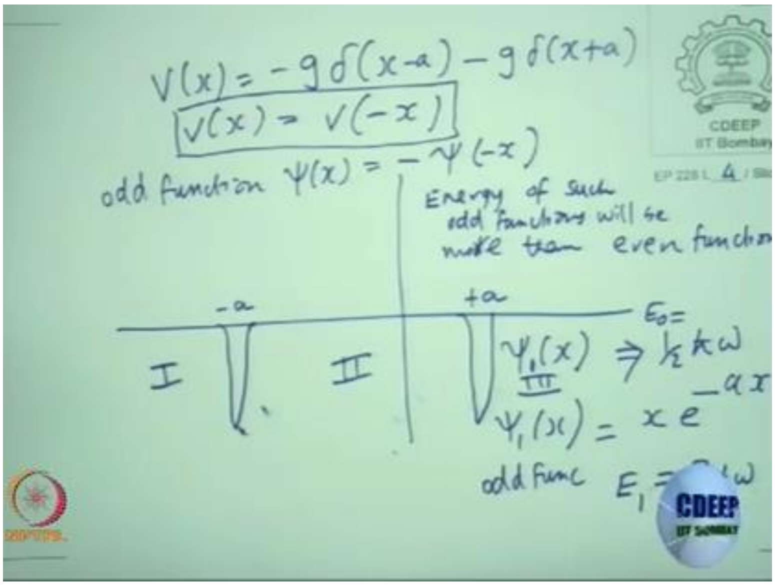

So, you have this potential V(x) is - g δ(x) - a - g δ(x) + a, so g is positive and what is the property of this potential, is that satisfy V(x) = V(-x); satisfies, what kind of solutions you can write here? Because of this property, we will prove also whenever, you have this property, the solutions will be either even functions or odd functions and even functions will not have a node at origin but odd constants will have a node at the origin, okay.

And typically, when you try to find the ground state energy okay, at least in a harmonic oscillator if you remember, when you try to find a ground state energy x = 0, V is 0, right classically, the potential energy, at that point there is a node for the odd wave functions which means, derivatives is going to cause some energy okay. So, let me try and tell you that if you have an odd function, ψ(x) = -ψ(-x), you will find the energy of such odd functions will be more than even functions.

Or equivalently, your ground states $\psi_0(x)$, energy was 1/2 $\hbar$ ω right, is that right, ψ_1(x) has odd powers to start with, so it is proportional to some xe^{-ax^2}, this energy; this is an odd function okay, whose energy you can work out by 2 methods. What is this one method; put this wave function in your time independent Schrodinger equation, compare powers of x, find the energies, right you can do that.

If you do that what will you get; $E_1$to be 3/2 $\hbar$ ω, so I am just trying to say that the lowest energy solution when you try to find for any system, the lowest energy solution will be an even function always, if you try to say that the lowest energy is an odd function, you are wrong, okay, so this is what happens in the harmonic oscillator, in the double delta potential which I have given in the assignment which I said we will discuss in class, we will do this in Friday.

But keep this in mind when you try to write the solutions for the double delta potential okay, so you have a potential here, a potential here which is - a and + a, the solutions which you are going to write; region 1, region 2 and region 3, at least in region 2, this is region 2, region 1. In region 2, you have to apply V(x) is same as V (- x) similarly, region 1 and region 3 are going to be relate, is that right, x; -a going to +a is this region, - infinity going to; so it is region 1 and region 3 are related to x going to –x, is that right.

So, keep this in mind when you are writing your solution that it should look like an odd function or an even function because of this property, the property is V(x) = V(-x), we will prove this, do you can also think about the proof, any one dimensional problems with the potential energy having the symmetric property, you all done particle in a box in a symmetric box, what happens to the solution?

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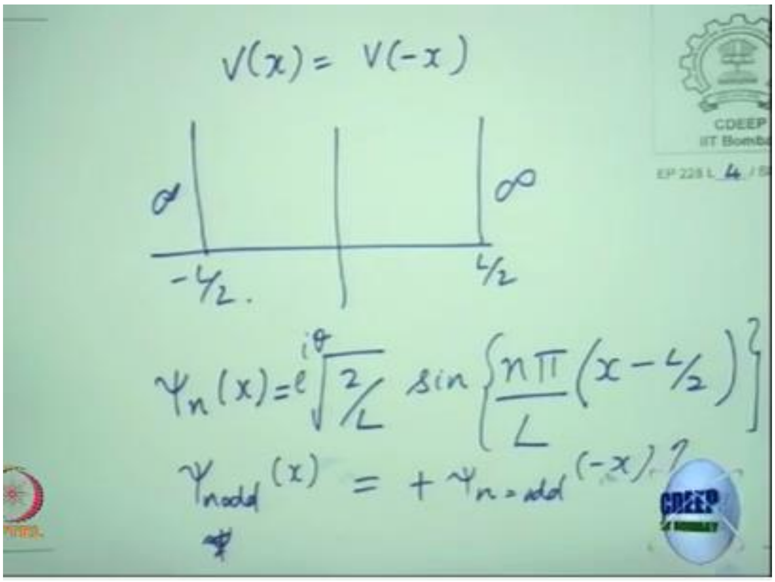

If suppose, I take infinity at L/2 and infinity at –L/2, what happens to the wave functions? No worries, you have done it know, how do you do this, you take the box and shift it, shift the box, so that your zero coordinate will become –L/2, how do you do that? If I had $\psi_n(x)$, I can write it as root of 2 over L, length of the box is still the same, coordinates of the box have changed.

So, sin(nπ/L), x is shifted to x – L/2, what you called as x, which was 0 becomes –L/2, x = 0 becomes –L/2, x = L will become L/2, nothing I did, I could do it this way, this is called shifting the box but equivalently, you can simplify this expression, can somebody simplify this expression for n odd and n even, what is it? $\psi_n(x)$ odd of x, is it – $\psi_n(x)$, is that right, yes or no, L, L cancels, it is n π/2.

If n is even, what happens when n is odd, what happens; what happens did I write it correctly, so + occur, is it x + L/2 two that is okay that is a normalisation, should not matter that is fine but you could also shift it that way that is also not a problem, so this overall sign what you calling here that minus sign normalization, I can put it up to even a phase factor, I am sure you know that right, the wave functions can be complex.

Here, I can have an e theta, I theta, I can put that theta to be π that is not a problem, so what is this tell me, what is the ground state; ground state is n = 1 and ground state will be an even functions is what I said looking at harmonic oscillator, the lowest energy state should not have a node at the origin, okay because if you put a node, then the derivative operator because the node with continuity will have a slope, the derivative or momentum will become nonzero, energy will become nonzero, so it is little higher energy, once you have a node at the origin.

But if you do not have a node at the origin, then the lowest energy solution should not have a node, so that it has a lowest energy that is why the lowest energy solutions are always even wave functions and I have proved it for you for the particle in a box, you already seen by explicit solution that the ground state wave function is an even function, okay but this is the trend that when you do the double delta potential, I want you to keep this in mind, both the solutions are allowed.

You can have odds solutions as well as even solutions because of V(x) be = V(-x); V(x) = V(-x) even in the double delta potential, you have to incorporate the fact that is a solutions can be even functions or odd functions and when you do the explicit calculation, you will see that the even solutions will have a lower energy than the odd solution, will be even yeah, you can yeah, because of this $\frac{\partial^2}{\partial x^2}$ will be 0.

Because that will have a maximum there, so that is why that will have a low energy, the momentum operator do not have the node but it is a maximum point you see, you can prove it, even looking at the Schrodinger equation yeah, these are things I want you to think, see I am giving you the 2 examples; particle in a box and the harmonic oscillator and this double delta potential is another non-trivial problem to do it.

While doing this, you have to incorporate the information, if you have learned that is why I am trying to stress on these 2 simple examples which you have seen mechanically but I want you to get a feel of it in this fashion that whenever you have symmetric potentials V(x) = V(-x), you have to incorporate the fact that the solutions to the Schrodinger equation should be either even functions or odd functions, which you can prove, we will prove it also.

But this that lowest energy state will always be an even function, is also something which you can get a feel by looking at it; at the node of x = 0 and these are things which I want you to get a better picture, okay, so this is why I am trying to stress on these know things which you have already done but from a different perspective, is that okay, everybody with me, okay.

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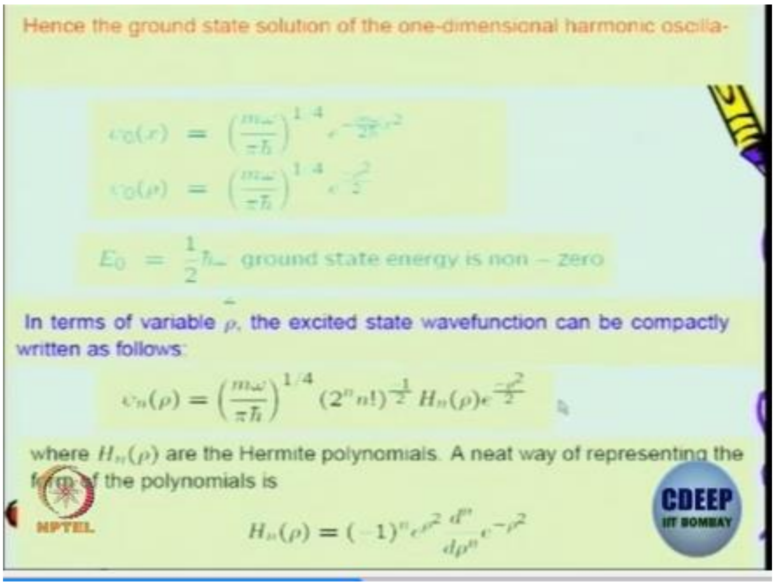

So, just to summarize the ground state solution is an even function as you see x going to –x, the wave function is the same, no sign and you can compactly write it in terms of the ρ variable for any n, this n could be odd or even, if n is odd, then this $H_n$will be odd powers in ρ, if n is even H_n will be only even powers in ρ, so there is a neat formula which is called as Rodrigues formula, I do not know whether you have seen it in your math course.

If you have not seen, there is no need to memorize H_n(ρ) but you could try and do this systematically by working out the nth derivative operator on, $e^{-\rho^2}$, so for n = 0, this derivative operator is not there, you get directly 1, if n is 1, the derivative will be d/ d ρ on, $e^{-\rho^2}$ that will give you a – 2 ρ become 2 ρ and so on. So, this is a very compact you know, Rodrigues formula is what we say, where you could directly derive all the polynomial powers for any n using this ρ.

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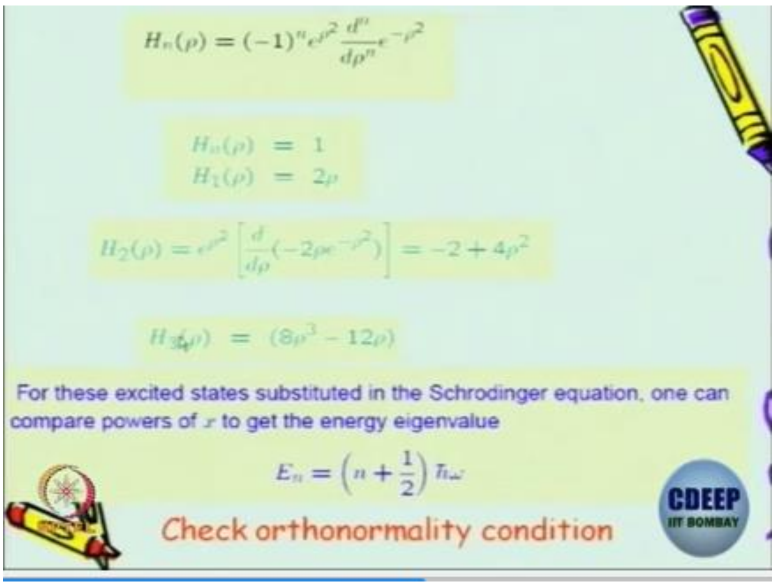

So, just to list a few, $H_n(\rho)$ will be; sorry this would have been 0, $H_0(\rho)$ should be 1, $H_1(\rho)$ is 2 ρ and $H_2(\rho)$ will be again only even powers, there would not be any odd powers, so there is a constant + 4 ρ square, so this I have already showed that once you put a truncation in the series, you automatically find that the energy has to be quantized and wherever we truncate, if we put an + 2 to be 0.

Then, the corresponding energy we call it as E subscript n that will be (n+1/2) $\hbar$ ω and you will go up to a polynomial series up to that okay, H_2 will have the highest polynomial power which is ρ square, if you want to write H_4 the highest polynomial power will be ρ power 4 and will be only even powers. I hope I have given you a flavour of how to see the solution and how to get a handle on writing these power series using these Rodrigues formula, okay.

It is a very nice compact, you should just play around and see how you get all the polynomial powers, that is one thing I have not done here, just like in a particle in a box, I want you to check the orthonormality condition for the wave functions, where the orthonormality of $H_n(\rho)$ will play a crucial role. This $H_n(\rho)$ even though, I have not really specified, they are called hermite polynomials in the literature, so please check the orthonormality condition.

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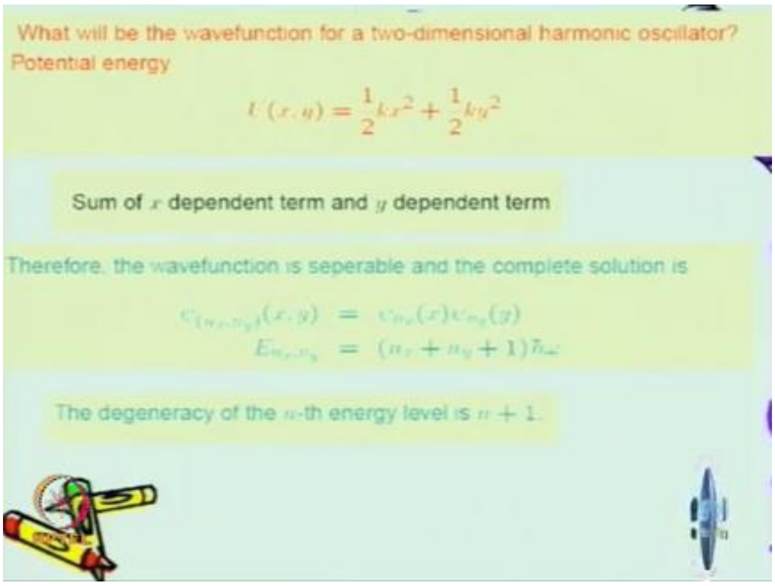

So, same procedure if you want to go beyond one dimension; to two dimensional harmonic oscillator, they are separable or not separable, they are separable right, they are separable then you can write your solution as with 2 quantum numbers n_x and n_y and you could write the total solution of energy also as (n_x + ½) $\hbar$ ω + (n_y + ½) $\hbar$ ω, they can be added to give you (n_x + n_y + 1) $\hbar$ ω and there is a product of 2 wave functions.

The forms are exactly similar to your one dimensional harmonic oscillator, only variable x will be replaced by variable y and the appropriate quantum number, so there is one more feature once you go to 2 dimensions, what is the feature? So, degeneracy of any level given in an integer n; $n_x + n_y$, I can call it as some integer n, it is actually a whole number, it could also be 0, you can try to tell me how to divide 2 pieces out of it.

So, to divide 2 pieces, you put one partition right, given an integer n, take a number line with integers and you put a partition somewhere in between, so where you put this partition; there are how many possibilities are there; n + 1 possibilities are there, so you have the total n can be split up into 0 and n, 1 and n - 1 and so on, so that depends on where you put the partition, so you get n + 1 as a degeneracy, is this clear to you.

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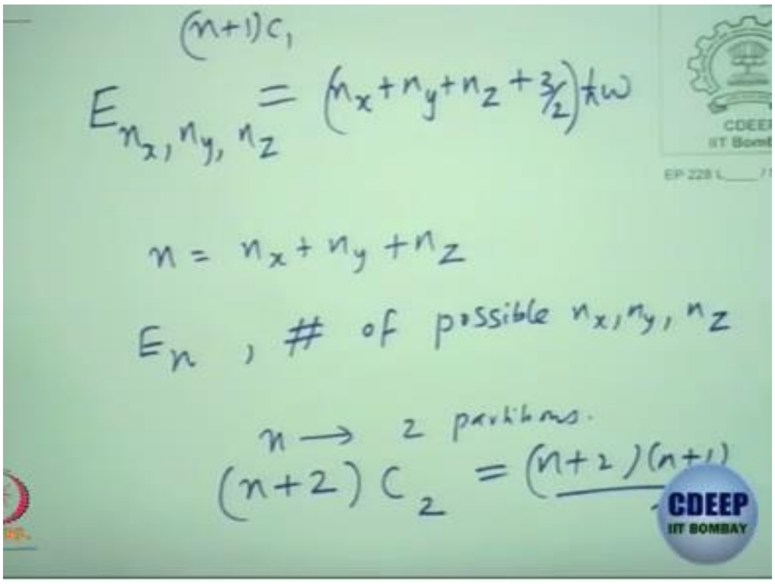

If you want to do 3 dimensional harmonic oscillator, what will be the energy eigenvalues; tell me, is that right, I can call n to be n_x+ n_y + n_z, so if I want to find for a specific energy E_n, what is the number of possibilities; someone said (n + 2) C_2, do you understand, so given an integer n, you need 2 partitions, right then you can split it up into n_1, n_2, n_3, first partition can be put in n + 2 possibilities including this partitions right.

And you will have the second one in n + 1 and then you can swap these partitions also, so you will have a (n + 2) C_2, so this is and you can actually extrapolate to any dimensional harmonic oscillator, it will become (n + r) C_r, r is dimension. For 2 dimension, you had (n + 1) C_1, for 3 dimension, it is (n + 2) C_2, is that clear. So, one of the features which happens beyond one dimension is that even the bound state solutions will become degenerate.

But in the case of one dimension, you found that the bound state solutions are always non-degenerate, okay.

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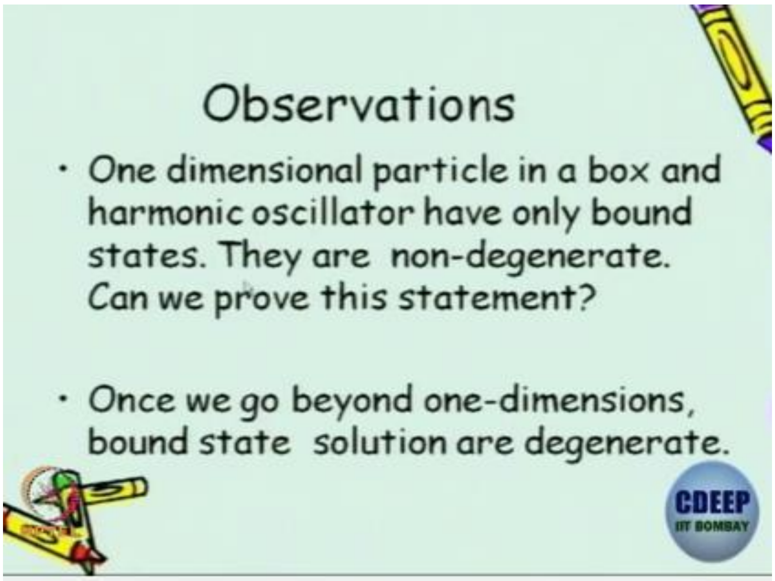

Okay, so observations, what are the observations, is this correct; one dimensional particle in a box and harmonic oscillator have only bound states that we have seen that this condition that the energy will always be < V at + or – ∞, right, +∞ and V at – ∞, if you also absorb that the solutions are non-degenerate, what about free particle in one dimension, is it degenerate or non-degenerate?

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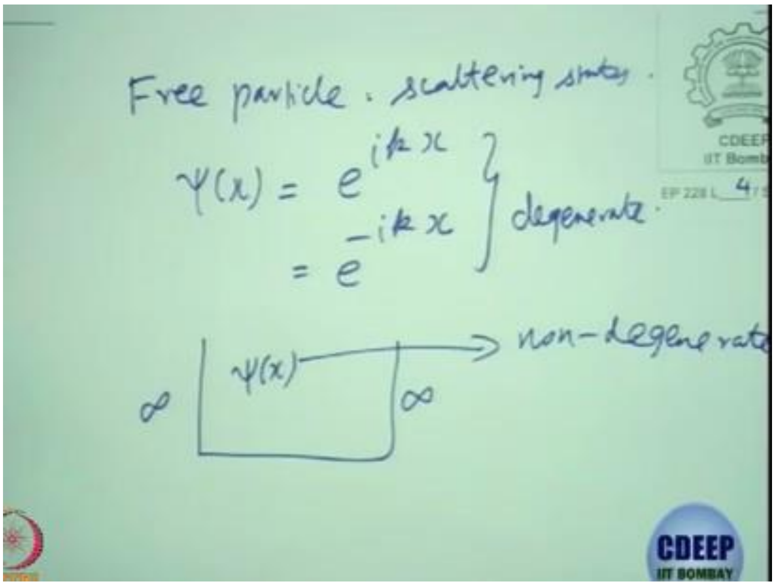

Someone, yes, free particle; free particle solutions ψ(x) could be e^{ikx} can also be e^{-ikx}, they could be degenerate, this is scattering states right, you all agree, scattering states; scattering states can be degenerate but once I put them to be bound inside the wall, then it becomes a bound solution which is non-degenerate, can have 2 solutions, so can we prove the statement and bound state solutions in one dimension are always non-degenerate can you prove, that okay.

Once we go beyond one dimension, we have seen two dimensional harmonic oscillators and three dimensional harmonic oscillator, we see that the solutions are degenerated okay, sorry I do not know, I put that okay, so this is also something which I want you to know.

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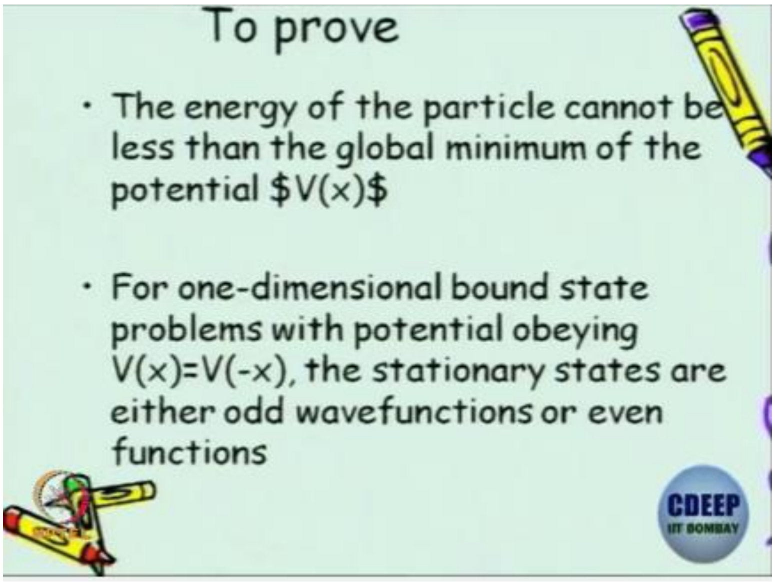

The energy of the particle, okay can be less than the local minimum but not the global minimum, what do I mean by that?

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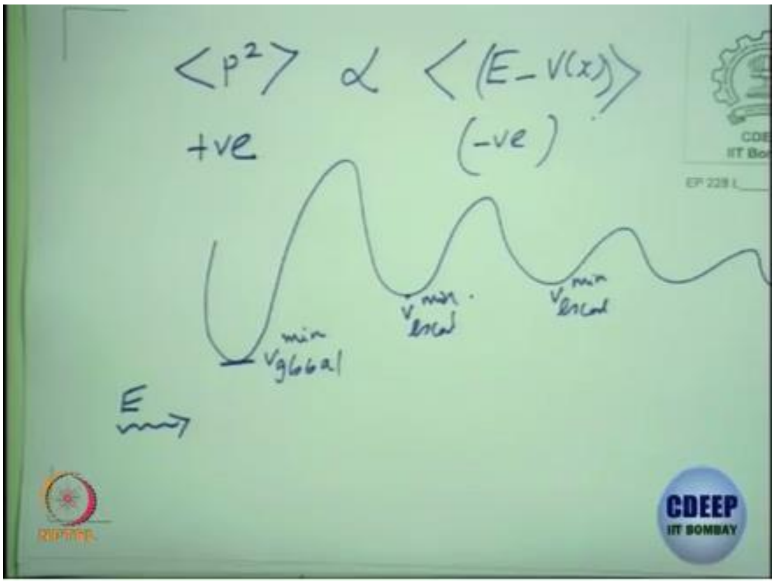

If suppose, I have potentials like this which is the global minimum, this one is V global minimum okay, these are V local minimum okay, they are all local minimum, they are not global, this is the global minimum, suppose this is the whole range of the region I am taking, the lowest potential energy will give you the global minimum, if the energy of the particle which is coming is less than the global minima, is there a solution possible, you have proved this some point.

How did you prove it? You can do it for a simple step potential, how do you prove it? Remember, so if you try to do expectation value of p^2 that will be proportional to expectation value of E - V(x), in Schrodinger equation, $p^2/2m$ in Schrodinger equation expectation value will be same as trying to find the expectation value of E - V(x), what is this quantity for this energy?

It is negative right, so this expectation value will always be negative, what about left hand side; p squared expectation value can it become negative, why? p^2 is positive definite, right it is not an imaginary number, p was not imaginary, p^2 will always be positive right, so if you try to find the expectation value of squares of any observable operators, it will always be positive.

Schrodinger equation says that this should be proportional to this in fact, the proportionality constant is a positive number okay, not writing it for you, please go and fill in this gap, right hand side is negative, left hand side is positive which is a contradiction which means you cannot have energy of a particle to be less than the global minimum as an allowed solution, so that brings me to a simplest question for you.

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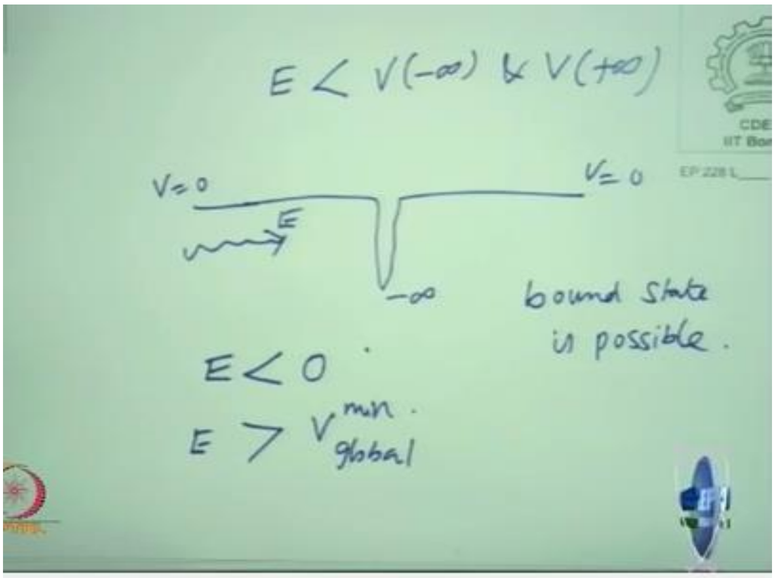

If suppose, I have a delta function potential, what is the global minimum; global minimum is like minus infinity if you want, so can we have bound states here, allowed or not allowed, why are you confused, you have done it so, it has a bound state right, you have done it, so energy will be less than 0 but it is definitely greater than V global minimum, you all agree at plus or minus infinity, the potential is 0 let us take okay.

The global minimum is - infinity for bound states, E should be < V at + ∞ and V at – ∞, is that correct, for the bound state E should be < V at - ∞ and V at + ∞, so E at + ∞ and - ∞ are 0, E should be negative but E should be > global minimum, so you can have energies of the particle like this, so bound state is possible, right, you all agree. Let us make this attractive to a repulsive delta function let us do that.

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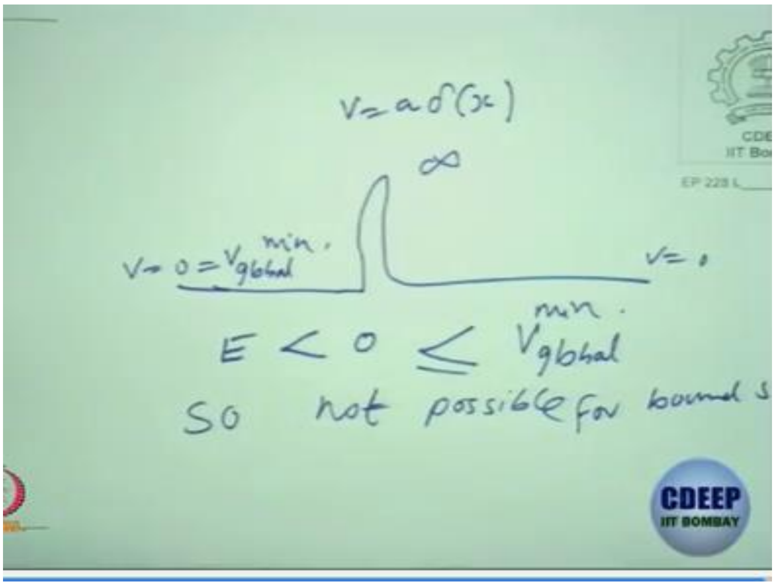

What will happen? Now, tell me will it have a bound state, can this have a bound state, what is V global, this is also V global minimum, for bound state E should be < V at + ∞ and – ∞, so E < 0 is < V global minimum, so not possible, so I did not do anything, I use the earlier theorem that you cannot have an energy of a particle to be less than the global minimum, I tried to see contradiction between the condition for bound state and that it does not satisfy energy, right.

And showed that bound state for a delta function repulsive potential, it is not possible, mathematics when you do, you can still do it for the delta function you will see that the result is dependent, I am sure some of you would have done, it is whatever is this weightage factor which we write as a times $\delta(x)$, you will see that the amplitudes reflection coefficients are all proportional to a squared and so on.

So, you will think that making an attractive to repulsive should not change the situation mechanically because the final result which you find for your reflection coefficient or transmission coefficient is a function of a squared, you should go and check it, so a going to – a, it will appear that you will have a bound state possible but technically, you know that it violates the theorem, repulsive delta function potential will not allow for a bound state.

So, some of these things do not memorize, sit yourself, used the rules and understand, okay, so let me just finalize the final one, so some of these things, I have already proved for you the first one or at least given you an indication, find the expectation value of P squared showed to be expectation value of E - V(x) and you can show that it is impossible for the energy of the particle to be < V global minimum.

And for an one dimensional bound state problems with potentials obeying V(x), this is said to be proven, we will do it in the next class, you can show that the stationary state, at least for the particle in a box, a symmetric box – L/2 to + L/2 and also for the harmonic oscillator; one dimensional harmonic oscillator, I have tried to show you that the solutions are either odd functions or even functions.

But we still have to prove this, we have also not proved that a bound state solution in one dimension is non-degenerate, so these 2 we will try to prove and also we will do the double delta function on Friday, please try and think about it and come to the lecture, so that we can have a active participation, one is bound state one dimensional bound state problems are non-degenerate.

Other one is the solutions to V(x) and V(– x) are odd and even functions, third one is the double delta symmetric attractive potential which will allow for a bound state and we want to understand that which one will be the allowed functions; odd functions or even functions and what is the regime and which it is part, okay.