Quantum Physics

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Lecture No. # 10

I could write down arbitrary Hamiltonians but there is no guarantee that this would actually represent a realizable physical system. Our approach rather has been to say that all the physical systems we know of are assumed to be Hamiltonian systems and then we try to model the physics of the systems by model Hamiltonians. So necessarily Hamiltonians are abstractions trying to approximate some reality.

Now most physical systems have a lot of interaction with other physical systems and therefore one of the crucial and important points one has to find out is how to include these interactions in a reasonable manner and this is a nontrivial problem. So it's a problem of modeling and then of course there is no guarantee that given a Hamiltonian, you can actually find the eigenvalues and eigenstates analytically. that's a separate question and for that you have to solve the Schrödinger equation and as you know the number of solvable integrable classical mechanical problems is itself small and the number of integrable quantum mechanical problems is even smaller, it's not immediately doable. Let me give you an instance of precisely this point. You know that if you took the1dimensional simple harmonic oscillator, it's integrable.

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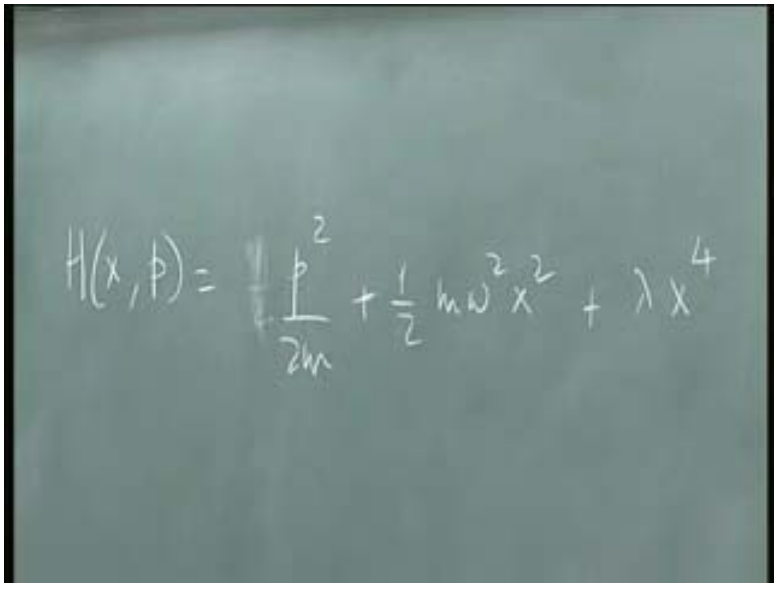

H (x) and p = p squared over 2 m + one/2 m omega squared x squared. That's of course integrable classically. Quantum mechanically we will solve this problem and show that its energy levels are actually computable analytically. But if you add to this, some lambda x to the power four for instance; make it an anharmonic oscillator with some positive constant lambda, and then classically the problem is integrable. This is because every1degree of freedom of system is actually integrable. The Hamiltonian = constant e is in fact this equation to the phase curves in the phase trajectories. But quantum mechanically this problem is not solvable in closed form. You can't find the energy levels of this system exactly. You can of course find them to arbitrary accuracy by good perturbation methods but you can't find them exactly. So in fact you see that quantum mechanics in that sense is more difficult than classical mechanics. Even the few integrable problems in classical mechanics are not necessarily integrable in quantum mechanics.

It's immediately related to the non-commutativity of x and p. that's what makes it immediately more difficult to solve. So we talked a little yesterday about the problem of a particle in a box and then in 2 dimensions and then in 3 dimensions and so on. It gets progressively harder to impose these boundary conditions as the shape of the box becomes more and more complicated. But1important lesson we learnt was that the movement you go to higher dimensions, it's possible to have degeneracies in the spectrum. It may not always be the case, like we saw in the case of a rectangular box in which the ratio of the lengths of 2 sides is incommensurate but under suitable conditions, if there is suitable symmetry in the problem then the levels can become degenerate. so the lesson I want you to remember right now is symmetry implies degeneracy in quantum mechanics. And we will exploit this fact as we go along and see how what important and how important a role it plays.

One aspect I want to mention right now and which we will return to later on has to do with nature of symmetry in quantum mechanics as opposed to symmetry in classical mechanics. It's a very profound implication but let me mention this right now and then we will return to this when we do 3 dimension problems. Let me do this by the way of a simple example. In classical mechanics, if you look at a particle executing a circular orbit around an attracting center, you have a situation where the hydrogen atom for example of the Kepler problem.

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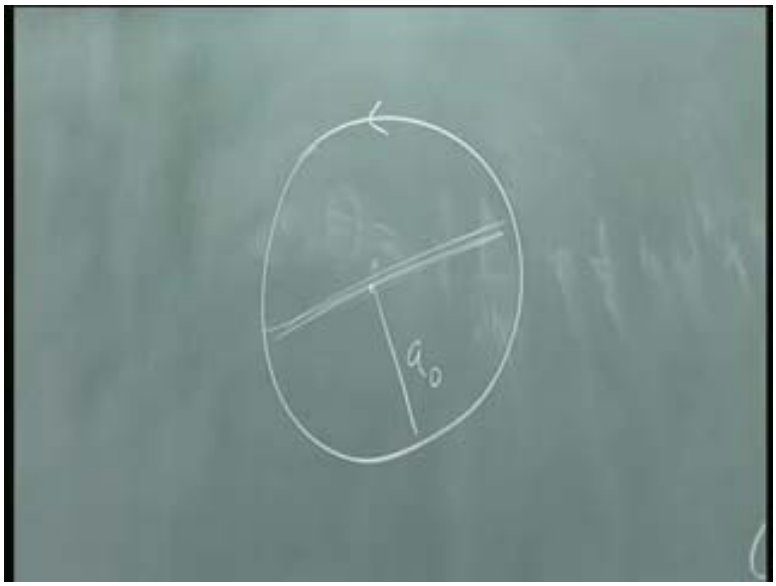

You have a particle going around in an orbit in this (Refer Slide Time: 05:48) fashion. Let's assume for simplicity it's a circular orbit. Then we know that the angular momentum of this particle is constant under one over r four or any central force and we also know that the angular momentum is not 0 because it's = m v times the distance in magnitude and that's certainly not = 0. On the other hand when you do the Bohr's theory of the electron in a hydrogen, you're advised that the angular momentum mvr is nh.

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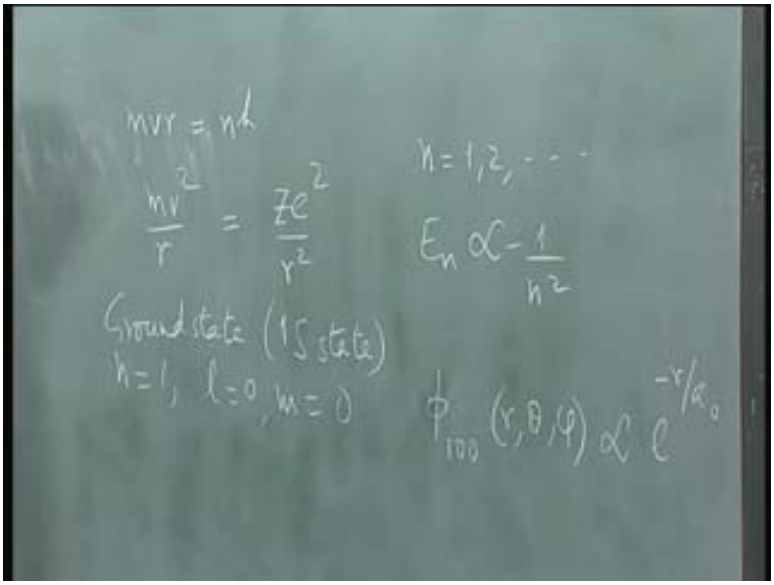

This is one of the equations you write down in the Bohr's theory saying the magnitude of the angular momentum in an orbit is an integer multiple of Planck's constant. That is the first input. And the next input is to say that the force is an electrostatic force. so you write down the centripetal acceleration which is mv squared over r. this is the magnitude of the inward acceleration due to the circular motion and this is = the centripetal force, the attractive force due to the nucleus. That's = e squared or z e squared over r squared. Then you take these 2 equations and we eliminate and find v and r. this is how you normally do the Bohr atom. After that you write n = one, 2, 3, etc and you discover E_n is quantized and is proportional to 1 over n squared.

And if you use the fact that when the electron and proton infinity separated the energy is 0 the potential energy is 0, then bound state energies are all negative and they are labeled according to n and it's an infinite sequence of such bound state energies. This much we know from the Bohr's theory. And the values of n are 1, 2, 3, 4, etc. but there is a little bit of cheating that's being done here.

This n comes about by quantizing the orbital angular momentum. mvr is the orbital angular momentum but we also know that when we solve the Schrödinger equation, the ground state of the system has n = one, also called 1S state has l = 0 and m= 0. This m is a magnetic quantum number. The ground state is spherically symmetric. The wave function in fact can be written as phi $_{100}$ (r theta phi) in spherical polar coordinates is proportional to e to the - r over a $_0$; a_0 is the Bohr radius and there is no angular dependence. The ground state is spherically symmetrical but the orbital angular momentum is 0. How does that tally with this fact that this electron as suppose to be going around in a Bohr orbit in which case it's angular momentum is distinctly not 0.

How do these pictures match? Forget this spin. This is independent of this spin of the electron. we see the difficulty of the problem is, classically if you have a particle orbiting at a distance a $_0$ from the center, the angular momentum is not 0. Quantum mechanically, the correct ground state energy E is proportional to -1 in Rydberg units, the ground state is characterized by principle quantum number, 1 orbital angular momentum 0 and therefore the projection quantum number 0. But l = 0 implies that the angular momentum is actually 0. Now how could it possibly be 0 when it's orbiting at a distance a_0?

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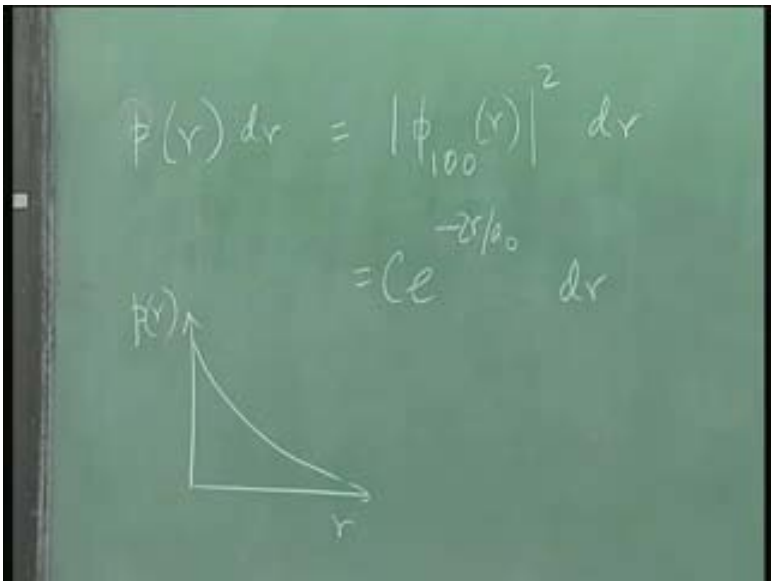

Of course you would say the answer it's not orbiting at a distance a_0. there is only a probability density or probability amplitude and indeed the angular momentum is not an eccentric trajectory and if I plot the probability that electron is at a distance r between r and (r + dr) from the nucleus what's that = in the ground state what's that = that's the probability density. So you must find it from the wave function. So this is = mod phi10 0 of r. let me drop the theta and phi because there is no theta phi dependence. If this were true, apart from some constant, this will be e to the - 2 r over a_0 dr and we I sketch this as a function of p (r) versus r, this is a damped exponential. So it says, in fact that the probability of finding the electron at the nucleus is much larger than that of finding it anywhere else. There is an r squared as well.

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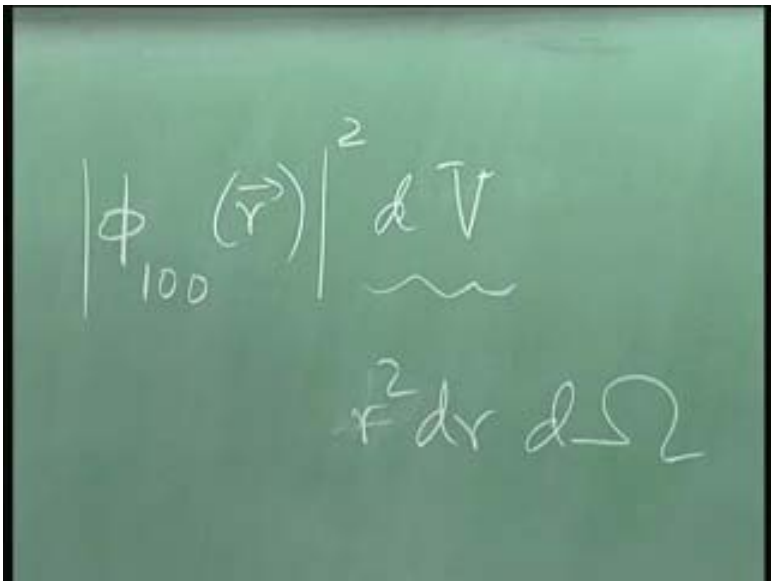

So we have to argue is that the actual probability is the wave function of this electron in this state as a function of r mod squared dV. This is the probability of finding the electron in any volume element dV. and now if you say the probability of finding it at a distance r, you must integrated over the angles but this dV has its r squared dr d omega, where d omega is the solid angle element and when we integrate over d omega, you get a famous four pi factor.

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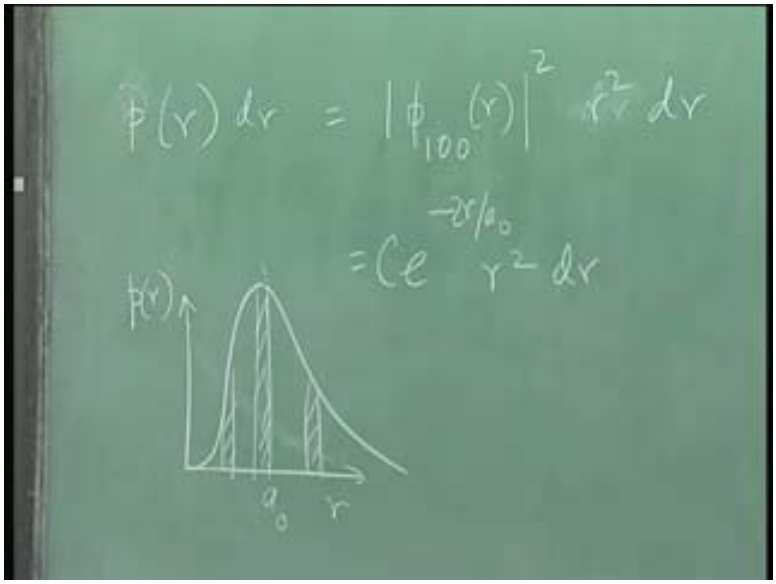

And once you put that in, there is an extra r squared factor and this whole thing changes. This is no longer the probability density. The right one is with an r squared. this r square is an increasing function of r and e to the - 2 r is a decreasing function of r. the product of a 2 of course will be something which is parabolic there and then dies down exponentially. And it's not hard to check that this is near a_0. So the maximum radial probability density peaks at r_0. So the probability of finding this electron in a small interval about a_0 is much larger than that of finding it in an interval dr anywhere else. That's certainly true. Still it doesn't answer this question of how does the angular momentum become 0. Because, classically, the angular momentum can be zero only if the electron passes through the origin. You know if this goes back and forth, then it is passing through the origin and the distance of closest approach is 0 and therefore the angular momentum is 0 about that point. But if it's most of the time at a distance a_0 and is orbiting around, the angular momentum can't be 0. And yet you are told that is the exact solution. It says the angular momentum is 0 but it matches in all other ways. The energy level is actually right; whatever we get from the Bohr Theory is actually right. The conclusion that the electron is exactly at a_0 distance is wrong but it's predominantly at a_0 distance.

How is it that an electron which is predominantly at a distance a_0 has 0 angular momentum? Well, you shouldn't think of it as going through a trajectory. That's the first mistake. Quantum mechanically the particle doesn't have a trajectory at all. If you did, then you know its position and momentum instantaneously. But in spite of that how is it that you end up with a 0 angular momentum, quantum mechanically? What fixes the direction of the angular momentum classically? The initial conditions fix the plane in which the particle moves. Once you tell me r_0 and p_0, r cross p is constant and it fixes it. So classically, the symmetry of this central force implies that any initial condition that you impose will forever fix the direction of the orbit. That's what conservation of angular momentum means. And what does rotational symmetry physically mean? It means that if an orbit is permitted in this plane, it is permitted in the other planes as well because these planes are all related to each other by a rotation of the coordinate axis. What you call the xy plane, I may call the yz plane because I simply chose another coordinate system. The physics doesn't change between yours and mine.

Classically different solutions which differ in the direction of the angular momentum are related by rotation transformations. You can go from my solution with says that it's orbiting in the xy plane to his solution which says it's orbiting in the yz plane by a rotation of the coordinate axis. So the group of transformations under which the Hamiltonian is in variant namely the rotation group each element of that group of rotations takes you from one possible solution to another possible solution. What you call initial position momentum I would call it slightly differently in my coordinate system. But the 2 of us are related by a coordinate transformation. Once you fix a coordinate system and once you specify the initial conditions the orbit is fixed. This is the meaning of symmetry in classical mechanics.

Now quantum mechanics however says super position is valid. Therefore any solution is a super position of all possible solutions. That's the crucial role of symmetry in quantum mechanics. It says if 2 solutions are related to each other by a symmetry transformation the general solution is a super position of these 2 solutions. You don't have to superpose it nature superposes. And then of course it is easy to see if you took this orbit and put it in all possible planes and added up all the angular momentum, the net angular momentum be 0.

So that's the reason why in quantum mechanics, you can still sustain a 0 angular momentum solution even though the electron has overwhelming probability to be at a non-zero distance from the origin. This is the very profound and deep aspect of symmetry in quantum mechanics. It is totally different from what you in classical mechanics and that's the power of the super position principle. If you have understood that then a great deal of understanding is gained on what symmetry really does in quantum mechanics. So you can see that symmetry in quantum mechanics is actually much more powerful statement than it is in classical mechanics because of this possibility of super position.

So we will exploit this now. We shouldn't use the word most of the time because there is no time involved here. These are stationary states. So I would say it's the most probable value. This is now leading as in very deep orders about quantum ergodicity. So there is no concept of a phase space and a point in phase space in quantum physics. So this question of is it ergodic in this sense is not a very meaningful one.

The time dependence of these states is just an exponential in time. Just sinusoidal completely. So that varies but that's not going to affect probability densities because it's a pure phase factor. So when you take mod psi squared, the time dependence goes off completely. So it's not as if probabilities are changing in time. we will look at examples where we have an atom in 2 possible states and is flipping between the up state and the down state or a spin flipping between up and down, then the probabilities could change in a time dependent way. And that is indeed what happens in real physical systems.

Now that we did the particle in a box, let's get our hand in by doing one more problem and then we will go on to a harmonic oscillator. And this is the problem of a particle in a potential. We looked at it as a free particle inside a box but now let's put in a potential and see what happens.

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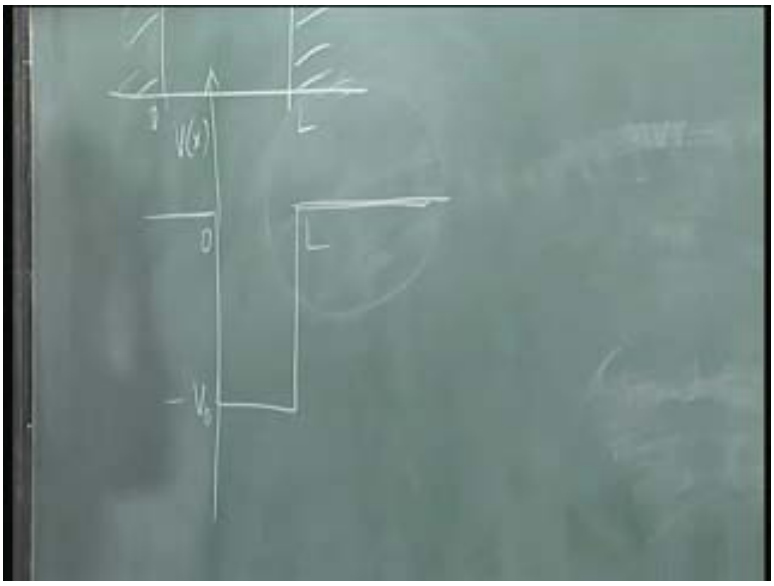

Now one way of doing this is to say there is a box of size L and it's got infinite potential here. So this really like saying there is an infinite barrier on this side and infinite barrier on this side and the particle is inside this box because I put V to be infinite outside and 0 inside. So the infinite well its deep inside this well. One could ask what about the problem of a particle inside a finite well. So that's my potential. If I draw the potential energy V (x) and is 0 here and L here (Refer Slide Time: 22:06) and it is 0 outside this distance L and it's a - V_0 in the particles inside (Refer Slide Time: 22:15). if V_0 tends to infinity, then of course I have the problem of a particle in a box. And the question asked is what the energy levels of this particle are. Now it will turn out that the ground state which earlier was strictly like this (Refer Slide Time: 22:33) from 0 to L and then vanished at the end can no longer be so.

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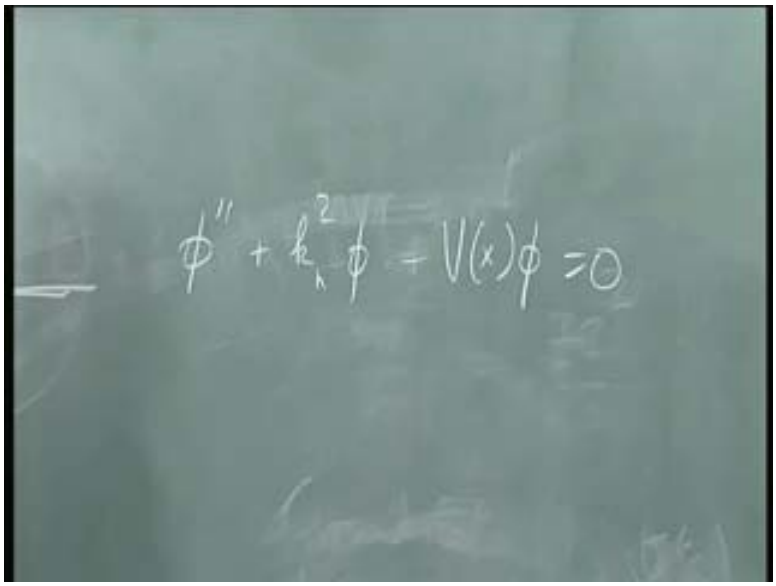

And that is immediately clear because if you recall our equation, it was of the form phi double prime + k_n squared phi - V (x) phi = 0. This kn here was proportional to the energy at these points there is a finite discontinuity in the potential. So this term has a finite discontinuity. Phi itself is continuous but V of x is a finite discontinuity that was we cancelled by the finite discontinuity here. So the second derivative has a finite discontinuity. For the first derivative, what do you think would happen at the ends? It's certainly not a delta function. It is not infinite like it was earlier. so this is going to be much milder and is not hard to see that in this problem, the wave function will in fact spill over because remember we have to solve the problem from - infinity to infinity. in this problem, the wave functions spill over and has something like that (Refer Slide Time: 24:10). So there is a finite probability for the particle to actually tunnel into the other region but not very far.

It would damp out. Let's simplify this problem and solve an even simpler problem. That is, I assume that the width of this well goes to 0 and that simultaneously the depth goes to infinity such that product is finite. What would we get in the limit? We would get a delta function and I would like to have a bound state. I would like to see if the potential can attract this particle and retain it in a localized form. So let's assume that this is a negative delta function. If its positive, it's a repulsive barrier. Then of course there is no possibility of any bound states. So let us do that problem and see what happens.

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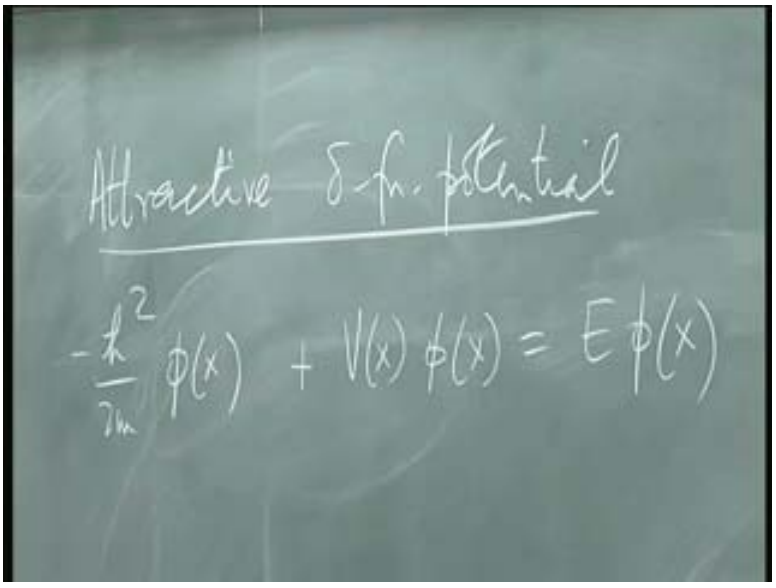

It's an attractive delta function attractive potential. Now without further ado, let's just write down the Schrödinger equation for this particle. - h cross squared over 2 m phi double prime (x) + V of x phi of x = E phi of x. this is the time independent Schrödinger equation and I am trying to find out if their eigen values e and non trivial eigen functions phi for which this equation is satisfied.

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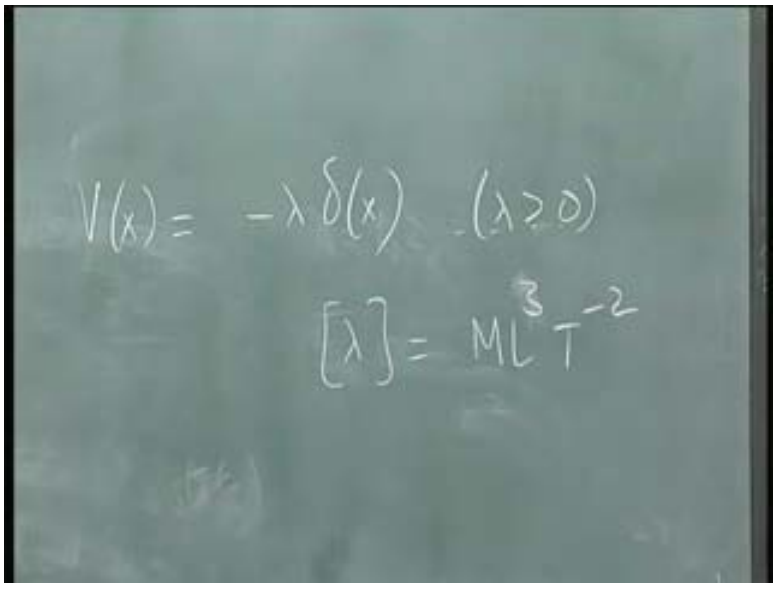

Let’s put the delta function to be anywhere on the axis it doesn’t matter since it’s an infinite axis. Let’s just put it at x = 0. So V of x = - lambda delta (x); lambda greater than 0.

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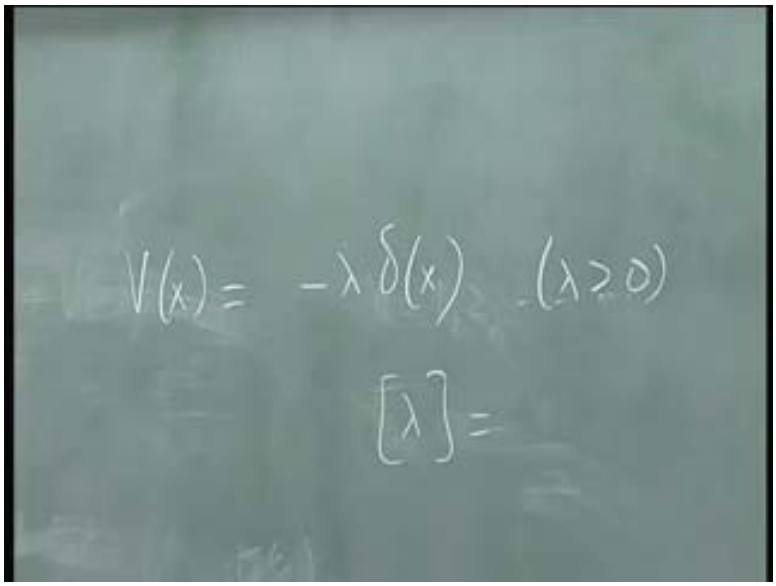

What are the physical dimensions of lambda? Well, this is potential energy. So it is equal to ML squared. That’s T to the – 2 and that’s energy but this delta function has dimensions 1 over length. So when I take it to the other side, its ML cubed. So this is the problem we are going to solve. By the by if there is nontrivial E; we are trying to find out if there is one or more eigenvalues, what can it depend?

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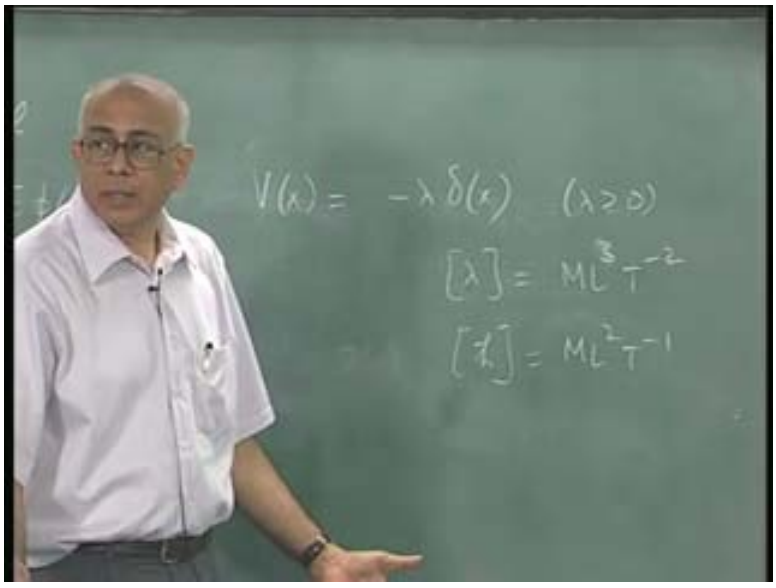

It could depend on lambda, m and Planck's constant. It cannot depend on the length scale in the problem because it has 0 widths. This problem has a potential which looks like this (Refer Slide Time: 27:47). At 0, there is a negative delta function. so it must depend on lambda, h cross and m. can you find a quantity of physical dimensions energy with respect with these 3 quantities? If you can't, then the problem is a non-starter. It's reasonable to expect that the answer would be proportional to lambda. The deeper it is, the deeper the energy would be. But there is a - 2 there and you got to cancel the T's. So what should I get?

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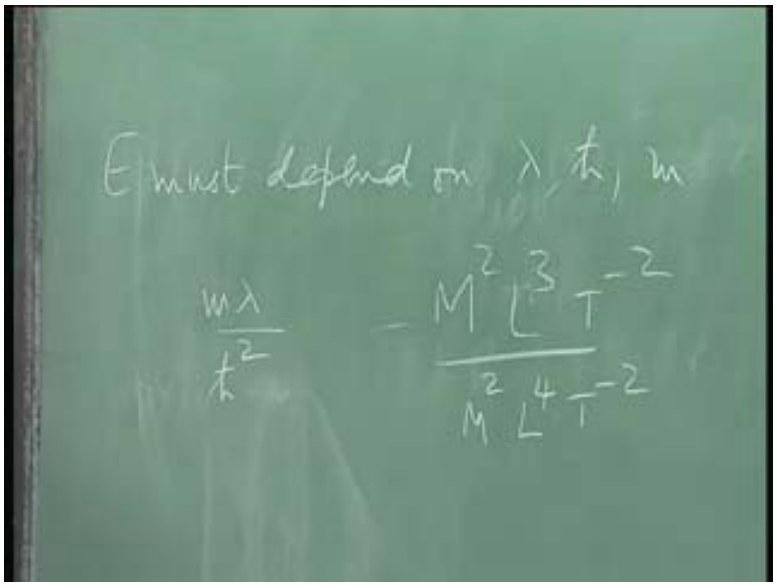

So E is proportional to m lambda squared over h cross squared. That's the first guess. Clearly when lambda goes to 0, there can't be a bound state. So it must in the numerator. So armed with that, lets try to solve the problem here. Now the way to do this is it is a delta function out here. So it's obvious that you must try to solve it by first looking at what happens when x is not 0 and then asking what happens at the boundary when x = 0.

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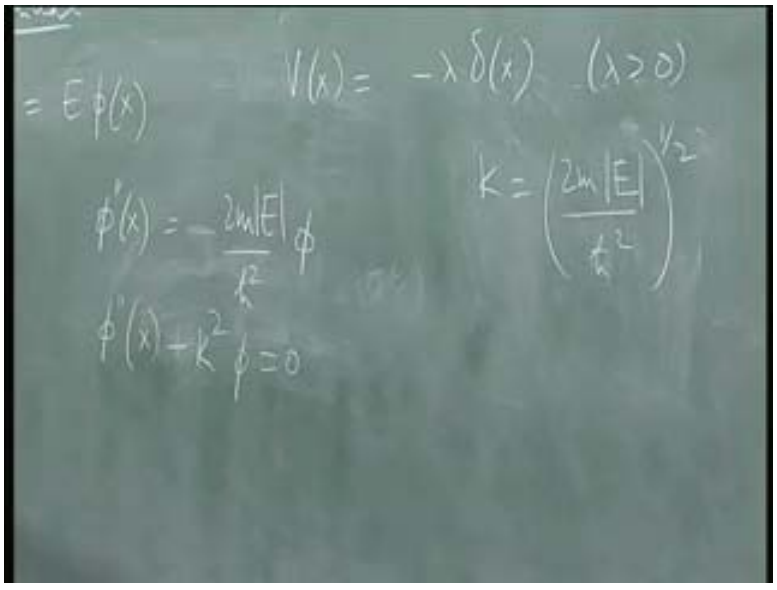

So for x greater than 0, it says phi double prime of x = 2 mE over h cross square phi with a minus sign. Now please notice that the energy levels must be negative. If it's positive, there is no potential at all. It's a scattering solution. So E must be negative if it's a bound state energy because it's relative to what happens at infinite distance when there is 0 potential. So let's write this as 2 m modulus E and put a plus sign. So the equation is phi double prime x - k squared phi = 0 where k = 2 m mod E over h cross squared the whole half. That's the first equation. What are the solutions?

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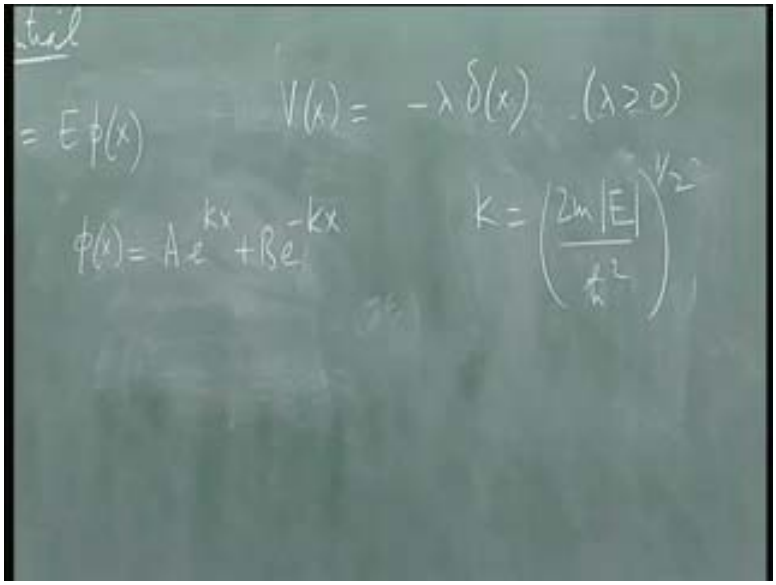

So for x greater than 0, the solutions are phi of x = A e to the kx + B e to the – kx. Now you want this to be a normalizable solution. Therefore mod squared of phi must be finite. phi must go to 0 as k tends as x tends to + infinity. Therefore this (Refer Slide Time: 32:36) is not permitted because it's not normalizable. The solution therefore is of this (Refer Slide Time: 32:44) form. Notice we put in the condition of normalizablility. The boundary condition at infinity has been put in. and for x less than 0 what is the solution? Again the delta function vanishes. So it's a same equation has before except its = Ce to the kx + D e to the – kx.

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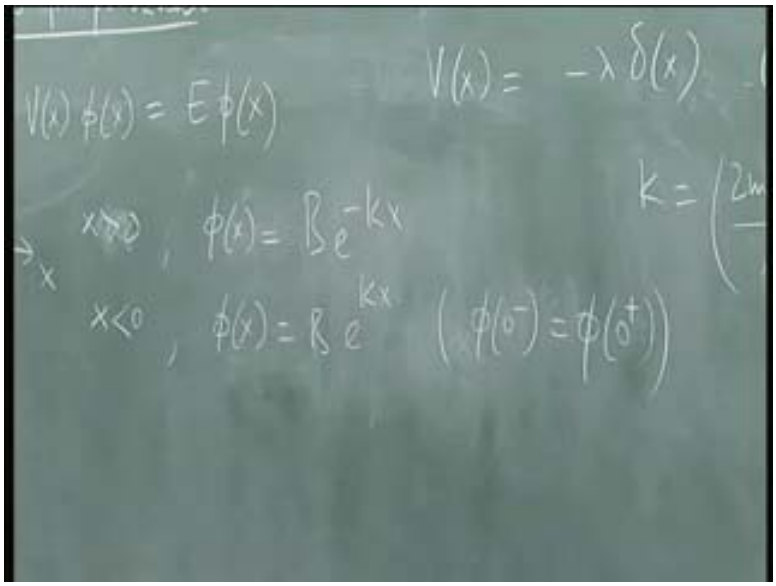

You want normalizability and time x tends to – infinity. So D must be 0 so this (Refer Slide Time: 33:41) is the solution. So that is for x less than 0 and you want the wave function to be continuous at the origin. So this implies that B = C.

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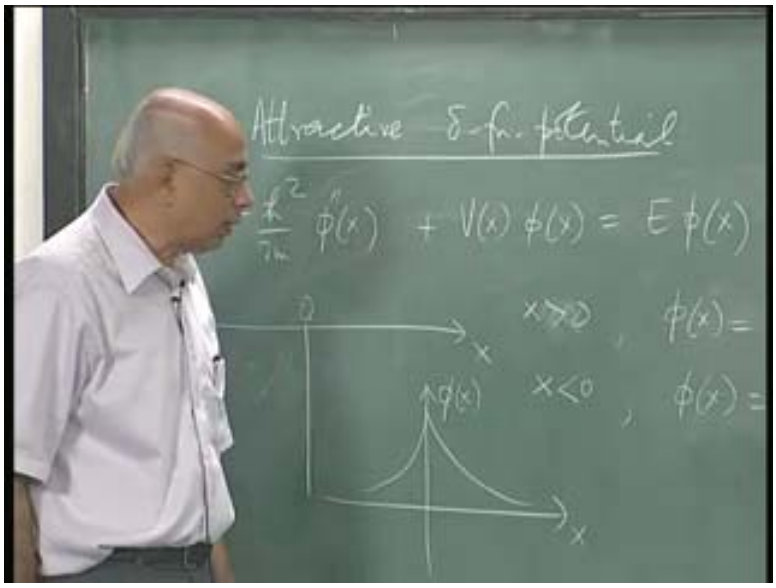

So continuity implies that as you come from the left and as you go the right, these (Refer Slide Time: 34:02) two must be the same. B and k are unknown here. If you know k then you found what energy is possible. What is the shape of the wave function? It's the

double exponential. So if I plot the shape of the wave function, assuming that B is real, it something like this and something like this (Refer Slide Time: 34:41). There is a slope differences cusp at the origin but it's continuous. Now because there is a cusp at the origin the slopes are different. Phi prime of x is a discontinuity at the origin. Therefore phi double prime has an infinite discontinuity. And indeed it does because phi double prime has a delta function sitting there at the origin. so it becomes worse and this is a real discontinuity. Now how would I find B? I just say the whole of mod phi squared from - infinity to infinity should be equal to 1. That fixes B in terms of k. How do I find k? I haven't put in the information of the potential at all. How do I do that? So that's my solution and let's write the Schrodinger equation down properly.

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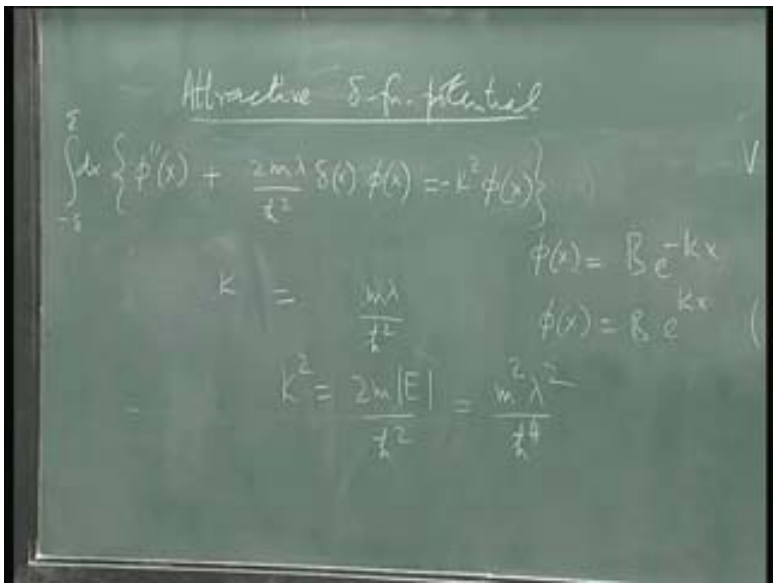

It's phi double prime of x - 2 m lambda by h cross squared delta of x phi of x is = - 2 m E by h cross squared phi of x, that is k squared phi of x. that is the equation and we solved it for x less than 0 and x greater than 0 in which case for delta of x didn't play any role at all. Now I need to find what this discontinuity of the slope is. So I would integrate on both sides. Well, if I integrate from - infinity to infinity, I am not going to focus on what happens at the origin. We are not going to get anything. So we would integrate from some - epsilon to + epsilon. I integrate on both sides and then let epsilon go to 0. So integrate - epsilon to epsilon dx on both sides of the equation and then let epsilon go to 0. What does this (Refer Slide Time: 37:13) give you? Well, it is second derivative. So when I integrate I get the first derivative at epsilon and then – epsilon. so this says d phi over dx x tends to 0 +; from the positive side when I let epsilon go to 0, - d phi over dx, x tends to 0 -. So what we are doing is finding this slope and this (Refer Slide Time: 37:47) slope and taking the difference of the 2 slopes. And - 2 m lambda by h cross squared.

What does this (Refer Slide Time: 37:58) give you? It would be phi 0 and that's a finite number. In fact phi of 0 is B and that is equal to 0 because it's the area under the curve and is finite as epsilon goes to 0. and what is this number d phi over dx as x goes to 0? All you have to do is solve, take the slope here and put x = 0. That's - kB and then subtract from another kB. So you get - 2 kB. That is the equation. B is not 0 because if it were 0, there would be no wave function at all. The 2 goes away and you get k = m lambda over h cross squared.

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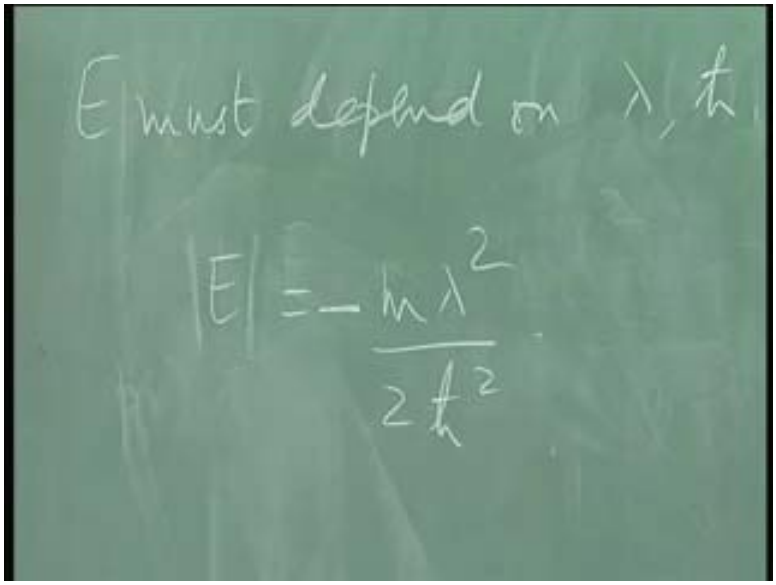

So k squared = 2 m mod E by h cross squared = m squared lambda squared by h cross to the four. This implies mod E = - m lambda squared over 2 h cross squared. And there is a single bound state. Its energy is given as we expected from the dimension arguments. So the only new thing is that the exact answer was half of this combination m lambda squared over h cross squared. And this tells you that no matter how small lambda is, this system supports a bound state which is normalizable. The wave function dies exponentially fast as you away to x from + or - infinity and that's the single bound state that you have. when you have a finite well, then more bound states could happen and depending on the product of the range of this potential a times the depth V_0, there is a combination V_0 a squared; the quantity of dimensions V_0 a squared which plays a fundamental role, you get one or more bound states of course if you put the particle in a finite. Then you have an infinite number of bound states of some finite width.

So its clear that as the depth goes higher and, higher more and more bound states get supported. and they are always scattering states but we would be not concerned with that at the moment. I want to you notice that even a single delta function where the potential goes to - infinity and that supports a bound state. What would happen if you had 2 delta functions?

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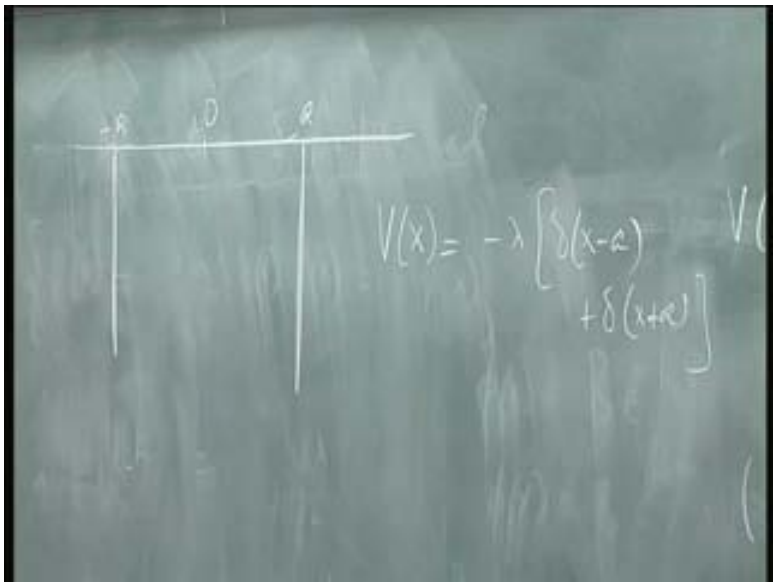

So let's suppose you have a, this is origin and you have a delta function here and a symmetric delta function here (Refer Slide Time: 42:45). So V of x = - lambda delta of (x – a) + delta of (x + a). What you think would happen? How would how would superposition work in this case origin? The reason I do this is because it teaches us something very deep about quantum mechanical energy levels. So imagine what would happen if you took one potential very far to the left the other one very far to the right. Each of them would have a bound state of some kind. So the wave function would look like this (Refer Slide Time: 44:04). Both these energy levels would be degenerate. So this is an energy level here (Refer Slide Time: 44:12) and an energy here and they have exactly the same values. it was found to be - m lambda squared over 2 h cross squared. Now you bring both the wave functions closer. Tunneling is possible here. These wave functions would overlap and what would the situation be? Let's look at it in terms of vector spaces. If you have 2 independent states which are not connected to each other, then the Hamiltonian in this 2 dimensional vector space would really look like this.

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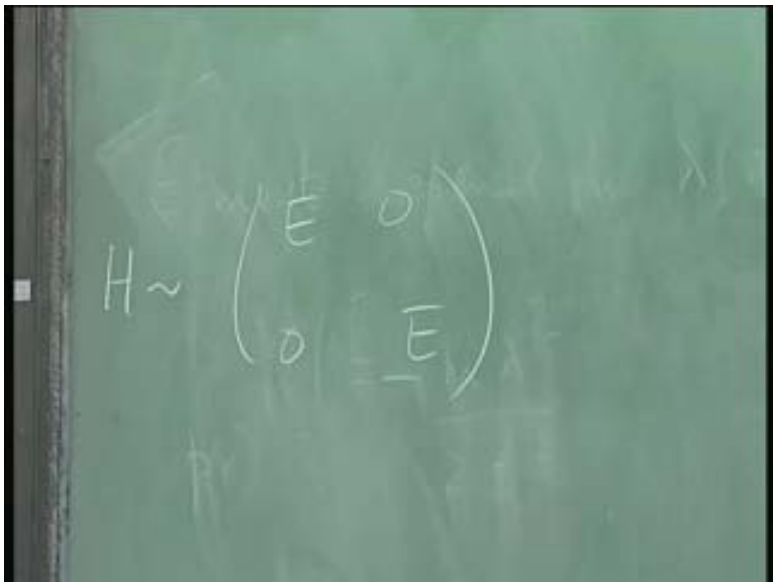

There would be an E, 0 and a 0; E. this is what the Hamiltonian would look like in that vector space. Now I switch on a coupling between the two because the particle is free to move from one potential well to the other. That would correspond to adding a little piece here (Refer Slide Time: 45:19) and a little piece there.

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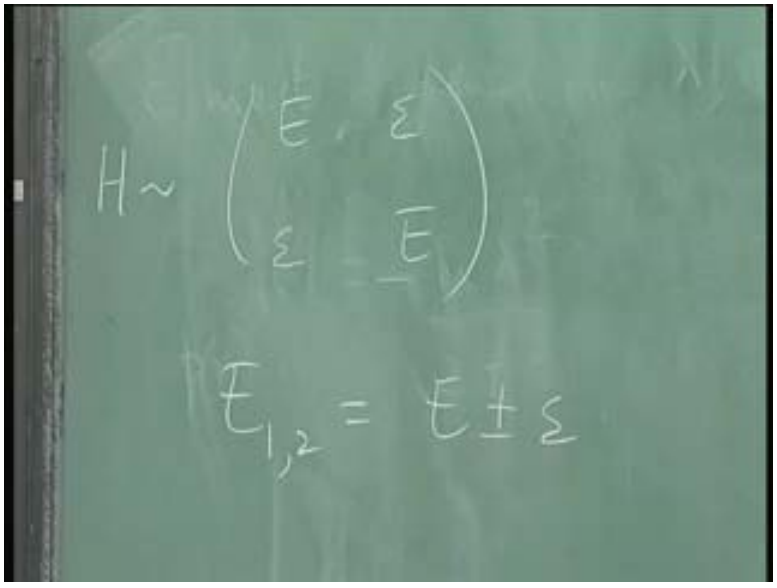

This is what the Hamiltonian looks like now. What happens when you diagonalized this Hamiltonian? it is just the eigenvalues of this Hamiltonian. That would be + or – epsilon. so it will turn out that in the 2 energy levels, one is slightly greater than E and the other is slightly less than E. so if you have 2 states sitting on top of each other, doubly degenerate and you switch on a coupling between the two, then what the system does automatically is split this degeneracy and go to an excited state and a ground state. That's E + epsilon and E – epsilon. That's what would happen here (Refer Slide Time: 46:26) because now you would solve the problem by imposing boundary conditions.

You would say its 0 on this (Refer Slide Time: 46:31) and 0 on the other side. so the solution on the left is e to the + Kappa x and the solution on the other side is e to the - Kappa x. the solution at the centre is a superposition of both because you can't rule out one or other exponential. Then you match both the wave functions and find their discontinuities. So you start by saying the solution on the left is A e to the Kappa x, B e to the - Kappa x + C e to the Kappa x at the centre and is D e to the - kappa x in this region on the right. you equate the values out here at x = - a and you equate the values out here at x equal + a. that gives you one condition between B, C and D. on the other you get one condition between A, B and C. then you find the discontinuity here (Refer Slide Time: 47:38) and the discontinuity there.

That gives you another set of equations between these unknowns. So you have four of these equations and a normalization condition. So we have five equations but now four equations are enough to determine four constants of integration but you also need to know what Kappa is. And that would fix the normalization constant. So there is just enough information to tell you what the possible values are and in accordance with that, it will turn out that you have 2 possible solutions or energy levels, one of which is lower and the other is higher. Now bring these wave functions closer and what would the wave function look like? Not surprisingly one wave function would look like this (Refer Slide Time: 48:48) and the other wave function would that look like that. One of them would be symmetric and the other would be anti-symmetric. Which do you think is going to be the symmetric solution and the anti symmetric solution?

The lower one is going to be symmetric because it costs more energy and you don't have a node here. In the anti symmetric one, there is a change of curvature and this is a node here. Therefore in the Schrödinger equation; remember this is a second derivative term the larger that is the more change of curvature there is, so that is going to contribute to the energy on the right hand side. Phi double prime + potential on phi is = the energy on phi. So roughly speaking when this phi double prime term becomes larger and contributes more definitely, you are going to get a larger energy.

So, the symmetric nodeless one is going to be the ground state and the one with the node going to be the excited state. You could do for an infinite array of delta function potentials. Remember by Fourier analysis, an infinite array of delta function potentials is equal to an infinity array of exponentials and that problem is called the Dirac Comb. And it's of great interest because we would like to find out either if there are potential dwells or barriers and the transmission coefficient. If I put in a beam of particles there, the amount of particles transmitted and reflected is given by the transmission coefficient. It's called the Dirac Comb and I will put that down as one of the problems you have to solve.

But in this lesson, we have learnt that the perturbation would lift degeneracy and it's a very general one and this is also a very important phenomenon because typically, a perturbation would lift degeneracies, in sense that crossing energy levels repel each other. This is called level repulsion and that is really what happens there (Refer Slide Time: 51:20). It's a very basic phenomenon and it's responsible for many things including the formation of forbidden gaps in energy bands in solids. And that's because of level repulsion ultimately.

Now that we have done two of these problems, I think I should stop here today. We are now ready to go on to solving the most important one of them which is the simple harmonic oscillator. But we wouldn't do this by solving differential equations because it involves special functions and it will indicate the solution. But I will show you a much cleverer method due to Dirac called the operator method which helps you to find eigenvalues and eigenfunctions without solving the Dirac second order differential equation. But it's completely equivalent.

Thank you!