Quantum Physics

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Lecture No. # 11

In one dimensional problems, there is an interesting theorem which essentially says that the ground state has no node, the first excited state as one node, the second excited state as 2 nodes and so on. So the question is why does the number of nodes increase as the energy increases and a very crude answer is the following.

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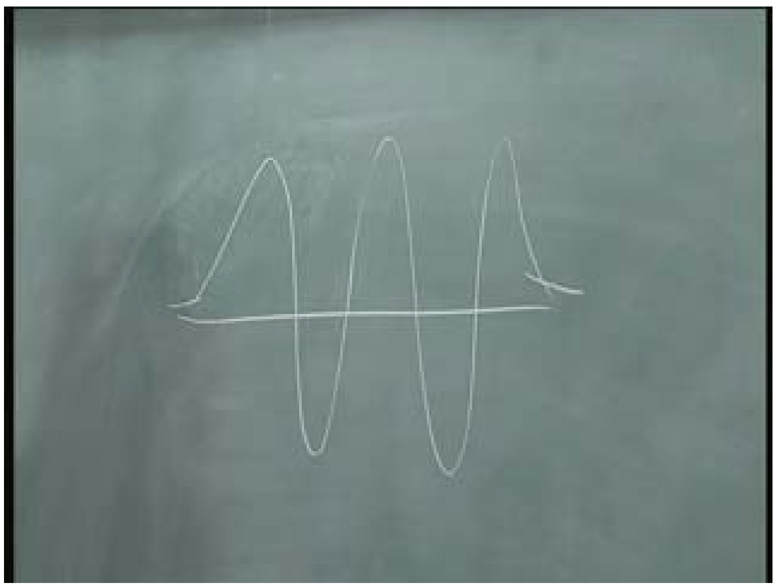

Although one can make this formal, it's called the ordering theorem, it's because on the x axis, you would like to have a wave function that's normalizable; that means it must go to zero at both ends. So it starts off with zero and then it must end at zero on this (Refer Slide Time: 01:41) side. In between whenever it goes up it has to come down. So if it goes up and comes down a repeated number of times, you can see the curvature keeps changing up and down. So the second derivative term contributes significantly and the larger the number of nodes, the more the contribution and therefore the larger the energy on the right hand side.

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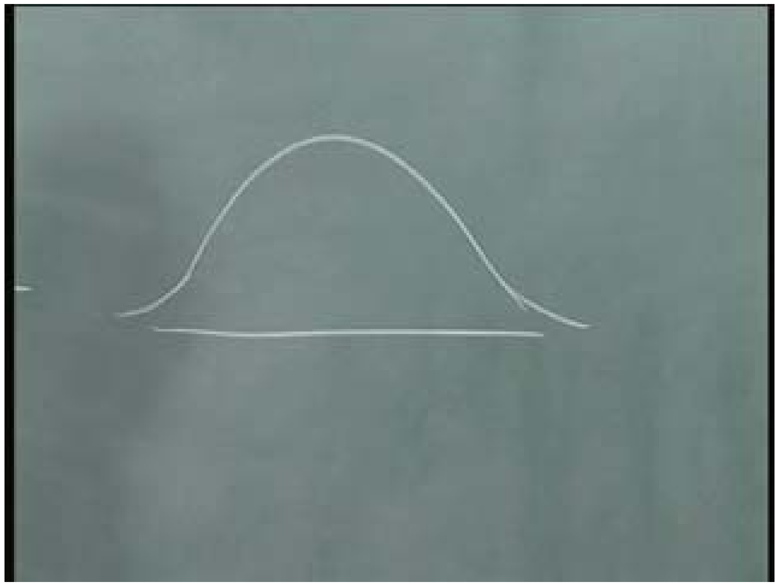

So in a very rough sense, you would expect that the ground state of the system would be something where these gradient terms don't contribute at all; something which goes up and has to come down. So the simplest way for it to do is in this (Refer Slide Time: 02:18) fashion. Therefore there are no nodes at all. Every time there is a node it means there is a maximum and the curvature terms contribute more and more. So that's a rough idea of why as the energy eigenvalue increases, the number of nodes in the wave function also increases. Now we can prove some fairly general theorems on what the wave functions look like in a one dimensional potential problem. I will make some statements and later on we will see how to substantiate this.

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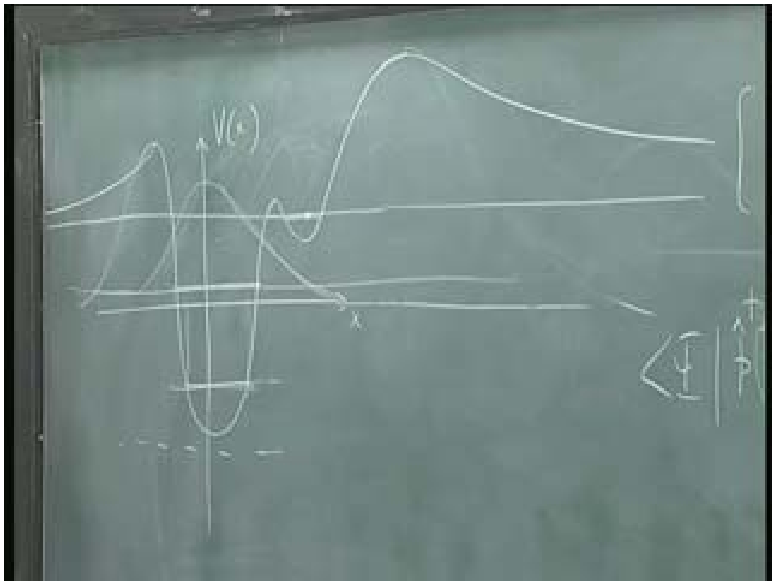

If you have a potential V (x) which is perhaps something which goes to zero at the ends and then it goes up and comes down with a well and goes about in this fashion (Refer Slide Time: 03:15). In such a potential, one could ask what the Hamiltonians look like. First of all, if it's a bound state, it must be normalizable. This means a wave function must vanish at the end sufficiently fast. Now clearly you could not have an energy level below the least value that the potential takes.

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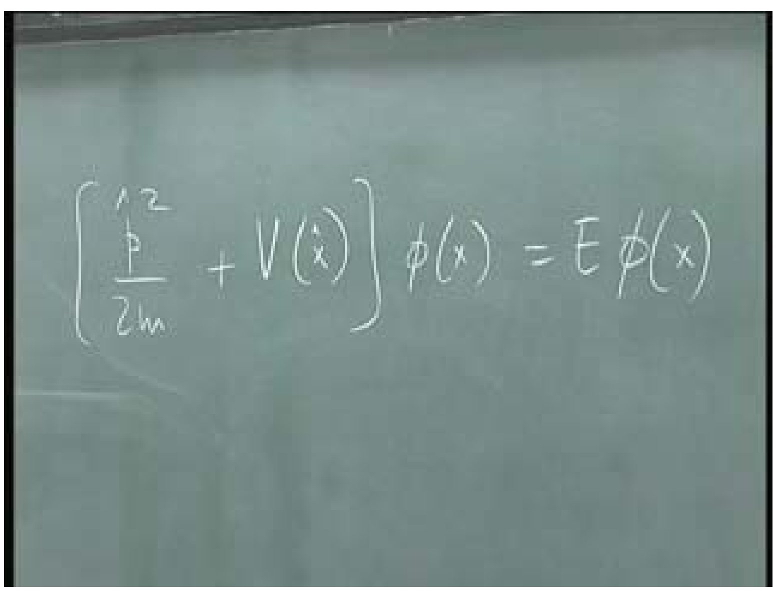

That's not very hard to establish because after all, the equation that you write down looks like p squared over 2 m operator + V (x) operator acting on phi of x or a state vector is E phi of x. where in the x spaces V (x) operator is just multiplication by V (x) and this stands for the second derivative if you like. Now that's the eigenvalue equation that you have to solve. In general, the kinetic energy does not commute with the potential energy because x and p don't commute with each other.

Therefore this particle cannot have a definite value of its kinetic energy simultaneously or in the same state as the one in which it has a definite value of its potential energy. In general, the Eigenstates of the Hamiltonian are not Eigenstates of the kinetic energy or the potential energy separately. That's crucial to remember. That's completely different from classical physics where you can actually take the total energy and say how much kinetic and potential energy are. Although the Hamiltonian is the sum of the potential and kinetic energy terms, please remember in a stationary state of the system, the particle does not have a definite value of either its kinetic energy or its potential energy but only of the sum of the two. That is simply because x and p don't commute with each other. However we can say that no matter what state you are in, this contribution can't be negative even in the quantum mechanical case.

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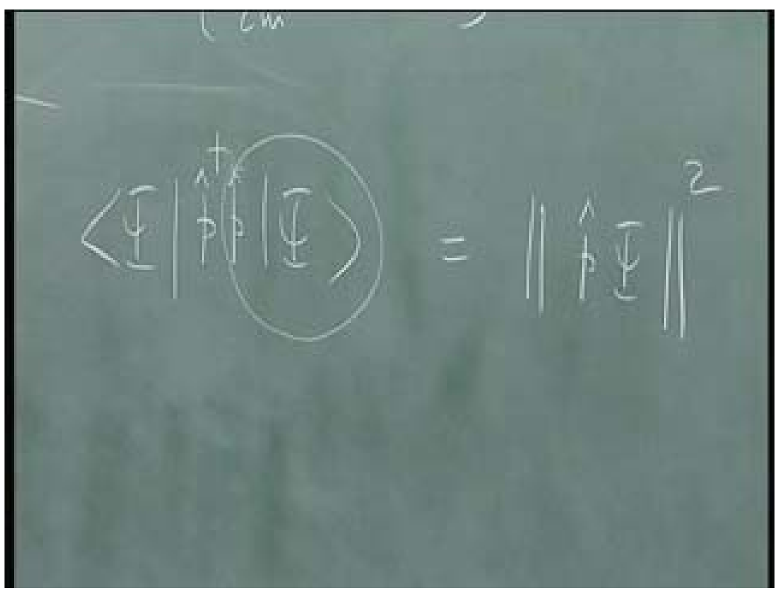

That is because in any arbitrary state psi, I take p squared psi; in any normalized state, this (Refer Slide Time: 05:40) is the expectation value of p squared by 2 m and you get the expectation value of the kinetic energy. But this is equal to the norm of the state that you obtain by doing this (Refer Slide Time: 05:57). This is because; remember that p is a Hermitian operator. Therefore you can write p squared as p dagger p and it's just the scalar product of this state vector with its adjoint. Therefore, it's a square of the norm of that state vector. And you know that norm square of the norm of a state vector cannot be negative. It’s zero if and only if the state vector is the null vector in the vector space. So this proves that the expectation value of the kinetic energy is always positive. And it’s a trivial matter to prove that you cannot have an energy of this kind because this would imply that the expectation value of the kinetic energy is negative. The other classical idea you must get rid of is to ask when the particle is at a position, what’s its energy. Such a statement has no meaning at all because the position operator does not commute with the Hamiltonian and therefore the question of the particle having a definite energy when it is in a particular place doesn’t exist. The particle is actually local everywhere. There is a probability amplitude for the particle to be anywhere on the x axis. And all you can ask is what’s the probability if the particle in a certain energy Eigenstate lies between two points. but you must get out of this classical way of thinking which says that with the particle you can associate a trajectory so that at every instant of time, you can associate both the position and momentum with it nor should you think that the particle when it’s in an Eigenstate of the total Hamiltonian has so much kinetic energy and so much potential energy. That’s not true either nor should you think that the particle has so much energy and momentum when it’s at this point. Those ideas are classical and they are completely invalid in quantum mechanics. Once you appreciate that, then it becomes much easier to understand. So my point was that because the expectation value of the kinetic energy cannot be negative in any state of the system, simply because the kinetic energy is the square of a Hermitian operator, it’s of the form p dagger p if you like and its expectation value cannot be negative. It implies that there can be no energy levels lying below the least value of the potential.

You could have an energy level here (Refer Slide Time: 08:43) at this value, but the wave function of the particle in general would not be confined to this region. It would in general be an extended wave function. There is a probability to find it outside; a finite probability, but that is a completely non-classical region. Classically, of course if you tell me this is the total energy of the particle, you would simply say it oscillates back and forth in this potential well between these amplitudes or turning points. That’s no longer true quantum mechanically.

If I plot the wave function corresponding to this (Refer Slide Time: 09:20) energy value, it would be something localized like this in this fashion and dies off sufficiently rapidly and definitely with overwhelming probability it would be inside the well. But there is a finite nonzero probability for it to be outside its classical amplitude as well. Could you have an energy level of this (Refer Slide Time: 09:47) kind somewhere here? Or could you have some Eigenstate like this (Refer Slide Time: 09:58)?

The answer is it cannot be stationary states. Because what would happen if you had an energy value here is that there is a classical potential barrier in this (Refer Slide Time: 10:16) region of finite width and finite height and there is a probability for the particle to tunnel through from here to there. If you start with an initial state here and wait long enough you would have a nonzero probability of finding the particle there. So there cannot be a strict bound state once you have a escape possible by tunneling. Exactly similarly you couldn’t have a particle localized at this (Refer Slide Time: 10:45) point.

If you start by putting the classical quantum in a small range about this point initially, as time goes along, this state would evolve under this Hamiltonian such that you end with a finite probability of finding it in this well. so it has tunneled through this (Refer Slide Time : 11:04) well and it would tunnel through here and then of course it can reach all the way up to infinity which means the wave function cannot be normalized anymore and ditto on this (Refer Slide Time: 11:15) side.

However its possible for instance, if I find an energy value here and if I start with the particle here, if this barrier is long and high enough and similarly on the other side, then the tunneling probability could be exceeding low and you might find the particle inside the well for a very long time but eventually it is bound to escape and such a state is called a metastable state. So you have metastable states but then eventually things would tunnel through. Tunneling is something we may not have time to get to, but it’s a quantum phenomenon.

Had this barrier been infinite in height with a finite width, then there is no possibility of doing this. It then has to really overcome an infinite barrier. So the tunneling probability depends on the range, i.e. the width as well as the height of the barrier and it decreases exponentially in the height of the barrier. So if the height goes to infinity, the tunneling probability goes to zero. Suppose you had a delta function barrier, could it tunnel through? This would indeed because now even though the height goes to infinity, the width goes to zero and there is a tunneling probability across. But if the width is finite and the height is infinite, then it’s not possible for it to tunnel.

Similarly, if the width is infinite, of course if this potential goes like that and asymptotes to that value on that side and the same value on this side, then an energy level here is definitely possible. There is nothing for you to tunnel through. It’s an infinitely wide barrier on this side. So those are the sort of rough guidelines which you must use, but I emphasize once again you have to get over the classical idea that the particle has a definite energy when it’s at a definite position. Now let’s do one more property of these wave functions and after that let’s solve the harmonic oscillator problem. And the property I had in mind was what happens if the potential has a certain symmetry, how is it reflected in the Eigenstates or the Eigenfunctions of the energy.

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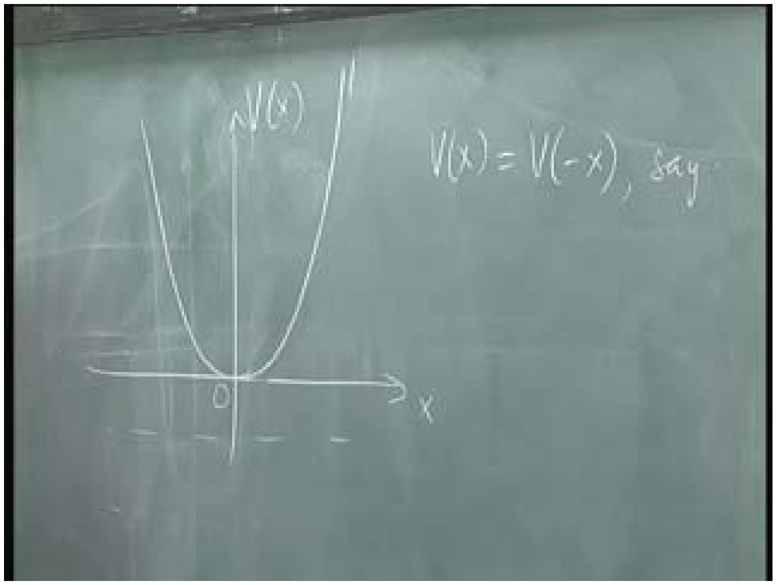

So let’s look at a situation where you have a potential and I won’t specify it at the moment, V (x) which has some symmetric shape, say x squared or x power 4 or a combination of x squared and x power 4 which is completely symmetric in shape. What you are given is V (x) = V (- x). This is a symmetric function about the origin. Now what kind of energy eigenvalues would you expect? By what I have said earlier, you couldn’t possibly have any energy eigenvalue. There are no negative values below the least value of the potential which I take it to be at the origin. So if I take this as a zero level of energy, you can’t have negative energy levels in this problem. You could have positive energy values. You could have all sorts of energy levels here and in general, because the particle is confined, you would end up with a discrete spectrum.

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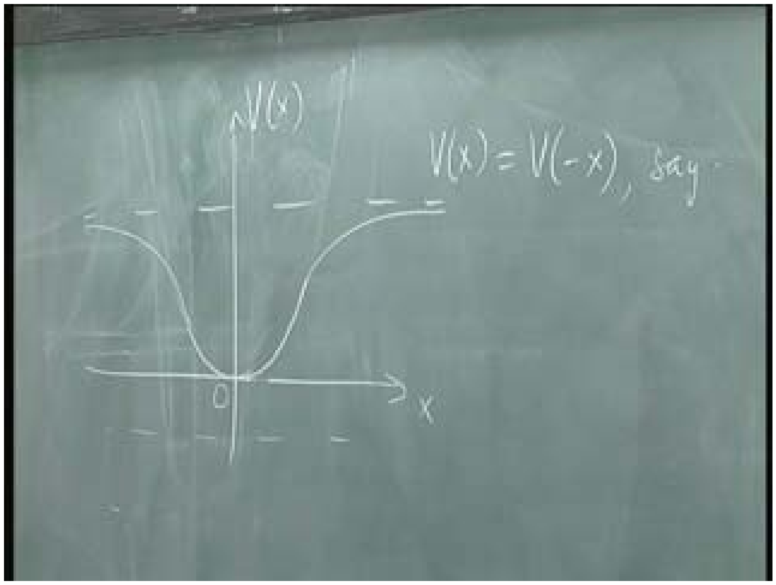

Suppose this potential well had asymptoted to some level, what kind of eigenvalues would you have? You would have a discrete spectrum here certainly, but then you could also have a continuous spectrum up there (Refer Slide Time: 15:28). Beyond that, it's not bound anymore. Then the particle could have non-normalizable wave functions which would correspond to a free particle zipping from left to right. but as it zips across for instance if you shoot a particle from the left as it zips across it is really as if its entering a medium of different refractive index because out here you could say the potential is essentially zero or a constant and therefore it's like a free particle But once it comes here, there is a certain potential and therefore the effective k squared changes and which means that the wave number changes, which means that the particle propagates as if it's going through a different medium to the other side.

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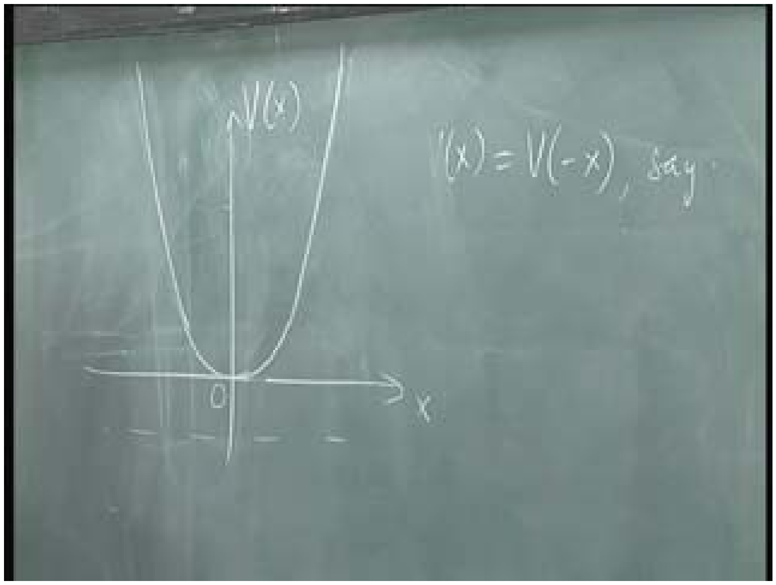

But let’s look at simple cases such as only bound states. So it goes off to infinity on both sides. One is guaranteed that all the Eigenfunctions of the Hamiltonian are in fact normalizable. They all correspond to bound states and you have a pure discrete spectrum. Now I add the condition that V (x) is V (- x).

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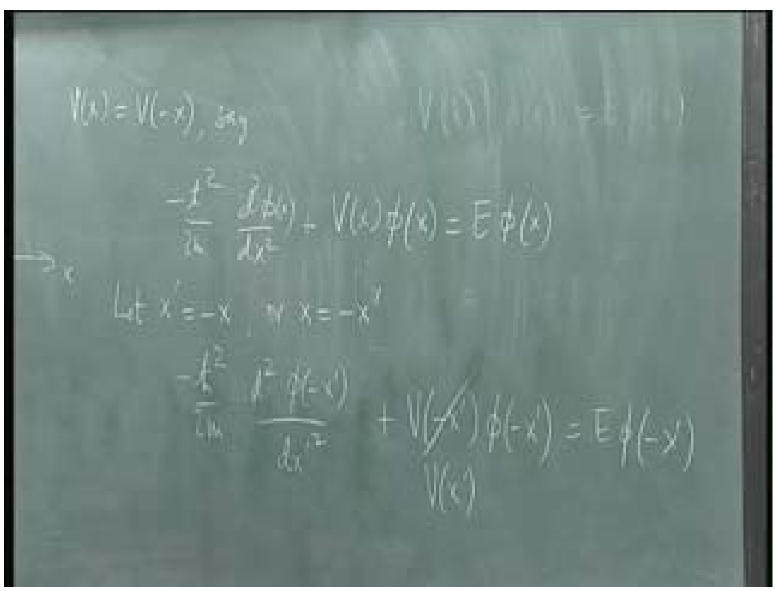

Well please remember that each Eigenfunction must obey this, - h cross over 2 m d 2 phi dx 2 + V (x) phi of x = E phi of x. and now let me make a change of variables. Let me make a transformation of variables from x to x prime. So let x prime = - x. so it proceeds in 2 steps. One has to be careful in this argument. Let's see what happens to this equation. It becomes - h squared h cross squared over 2 m d 2 phi of - x prime because x is - x prime, over dx prime 2 ; its a second derivative and therefore it doesn't change sign + V of - x prime phi of - x prime is E phi of - x prime. I have merely rewritten the same Schrodinger equation for the Eigenfunction phi of x and the eigenvalue E in different coordinates. But V of - x prime is V (x) prime by symmetry. So here I can replace this by V (x) prime and I can drop the prime and you could call it anything. It's exactly the same Schrodinger equation as before. So it says if phi of x is a solution of this equation corresponding to eigenvalue E, so is phi of - x. If the system is not degenerate, what does that imply? There is no degeneracy in one dimension. Therefore every eigenvalue must have a unique Eigenfunction. But now I just proved that phi of x is an Eigenfunction with eigenvalue E, so is phi of - x. therefore it implies that phi of - x must be linearly dependent on phi of x.

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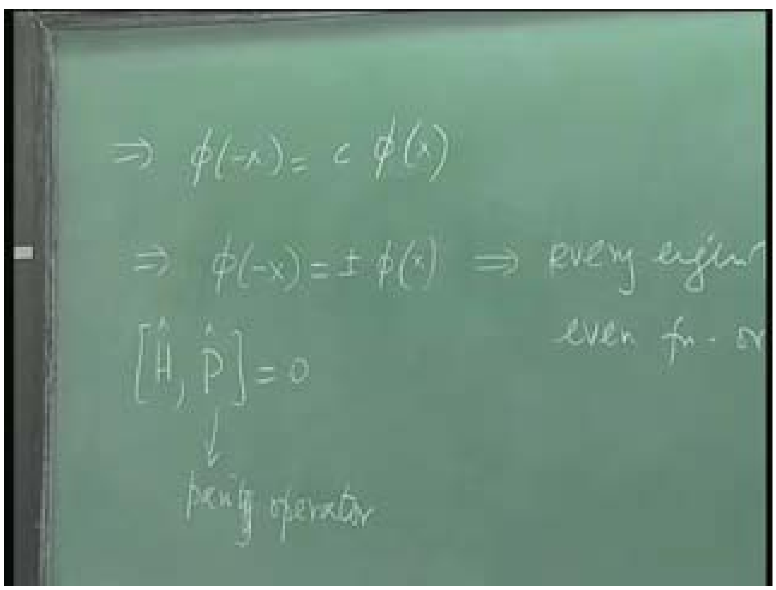

So this implies phi of - x = some constant times phi of x. There is no other alternative. That immediately implies that c squared is one. Because I can now go from - x back to x once again and therefore C is + or - 1. + implies phi of x is an even function and the - sign implies it's an odd function. So this proves that if the potential has reflection symmetry or parity symmetry invariance, then the solutions have definite parity. So I am saying that if the potential is an even function, the wave function must be even or odd but it can't be a mixed function.

So the Hamiltonian commutes with the parity operator and H P is zero. That’s the statement that we just made. The Hamiltonian commutes with the parity operator. This implies that the Eigenfunctions of the Hamiltonian are also Eigenfunctions of the parity operator. Every Eigenfunction of the Hamiltonian is either an even function or an odd function and therefore they can be classified into even and odd functions.

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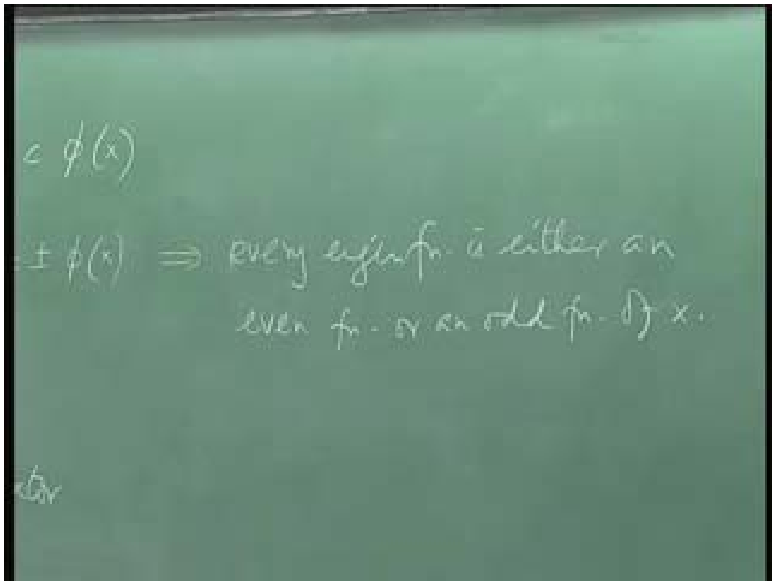

What would the ground state be? We can make a statement about the ground state immediately. Would that be even or odd? It would be even because the wave function has to be continuous and if it’s continuous and an odd function, then at x = zero it must be zero, which means it has a node. But the ground state doesn’t have nodes. So the only possibility is that the ground state is in an even function.

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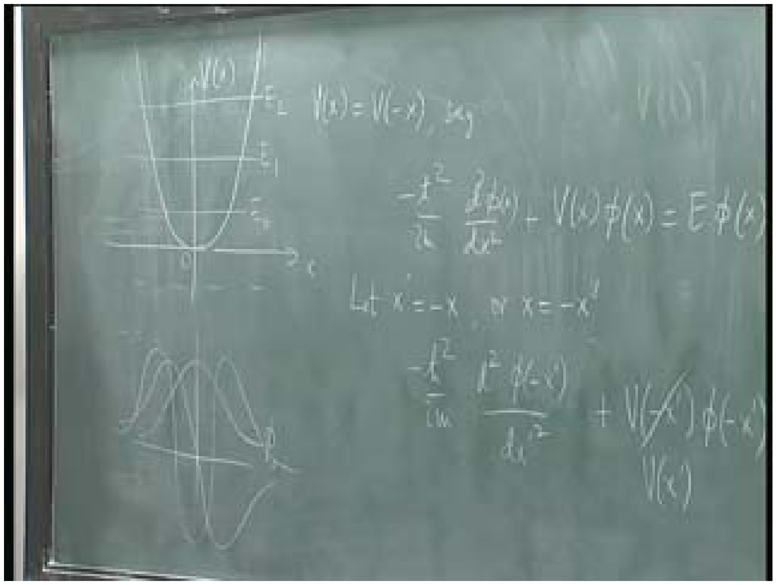

So you would in general have an Eigenstate like that (Refer Slide Time: 22:53), an eigenvalue like that corresponding to an Eigenfunction like this would be the ground state. So if I call this level E_0, this would be phi $_0$ of x (Refer Slide Time: 23:01). In general, there will be some level E_1 here (Refer Slide Time: 23:06) and that would be an odd function. That will have one node. And then a level E 2; it doesn't have to be equally spaced and it would be an even function. It will perhaps do something like this (Refer Slide Time: 23:26) and that would have two nodes but an even function. So under fairly general considerations, simply by using the symmetry of the potential, one can come to a conclusion that the Eigenfunctions would be odd, even, odd, even, odd and so on.

Now here is an instance where two operators commute with each other and we are finding a complete set of common Eigenstates. But all even functions are not Eigenfunctions of the Hamiltonian but all Eigenfunctions of the Hamiltonian are Eigenfunctions of the parity operator simultaneously. The class of Eigenfunctions of this operator is much greater than the class of Eigenfunctions of a subset of this (Refer Slide Time: 24:18). So having seen this, let's see whether we can actually substantiate this by solving the Schrodinger equation in the simplest case. The simplest even potential which is smooth and so on which we can think of is x squared. We put that in and that's the harmonic oscillator. But even before I do that, let's look around this in one more direction and ask what kind of Eigenvalues I expect. It's important to try to guess the answer.

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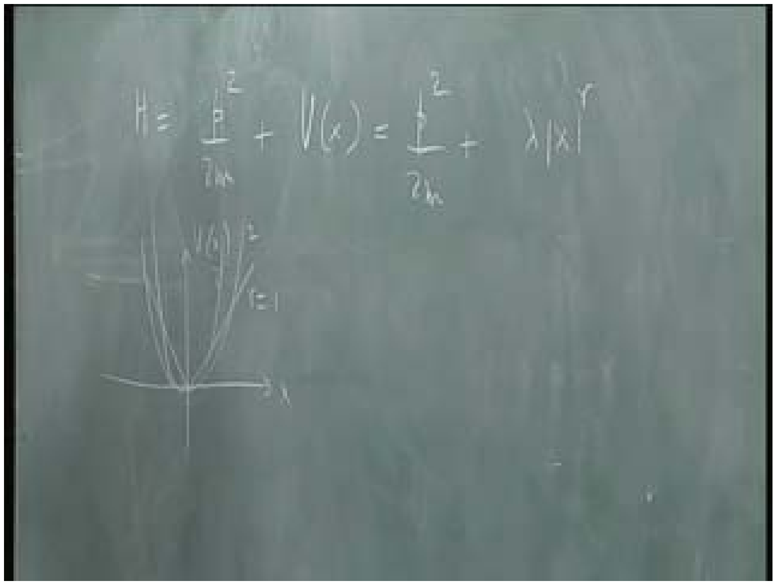

So we have this classical problem of a Hamiltonian which is p squared over 2 m + V (x), I am going to take V (x) to be just an even power of x say. So let me take this as some lambda; which is a constant, x to the power r and to make it more general let's take this to be an even function. This can be any power r and let's make this modulus. Of course, you immediately see that at the origin, it would have a cusp if r is = 1 for instance, but that's not serious. What does the potential look like for r = 1? It will just be a thing like this (Refer Slide Time: 25:57). For r = 2, it will be a parabola. For r = 3, it would be steeper. Remember there are no singularities here. So it would be even flatter. How about r = 1/2?

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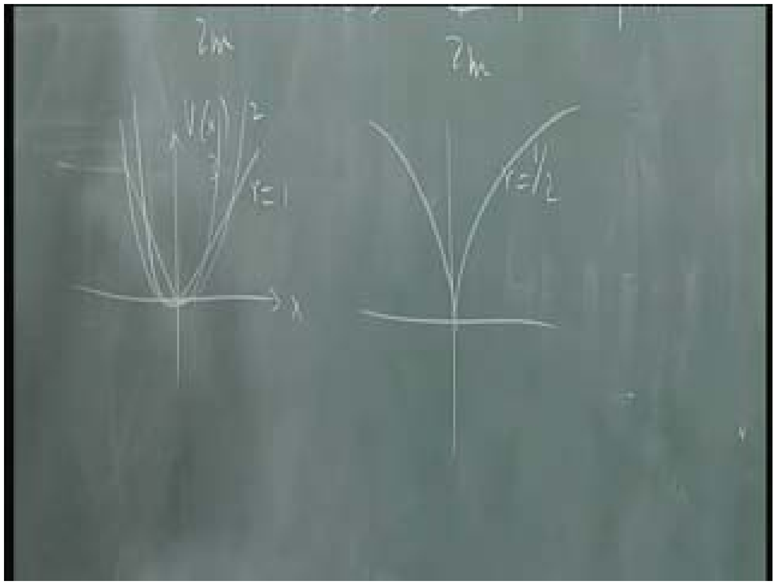

Well, we need to still do something like this (Refer Slide Time: 26:33). In all these potentials you would expect a set of bound states or discrete levels. What does the particle do classically? What would the phase trajectories be?

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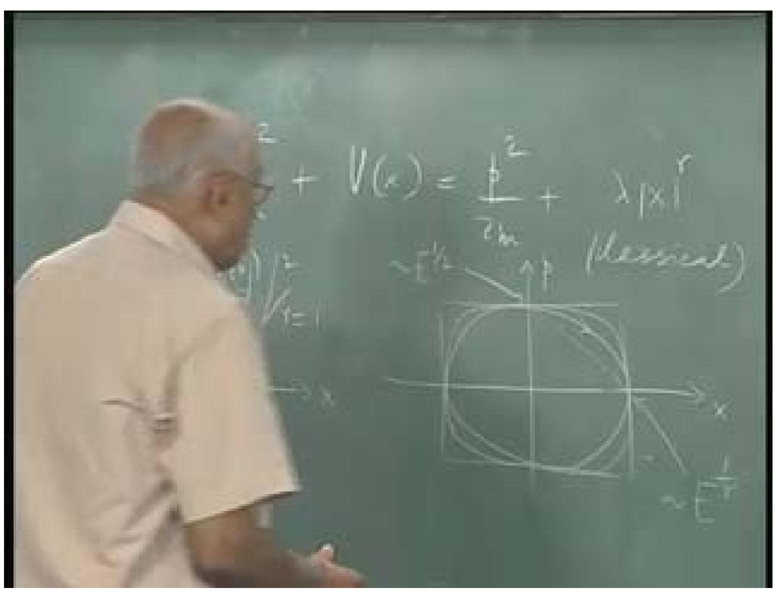

Well, the phase trajectories of this particle if I plot x versus p; this is classical, they will be close curves but won't be ellipses unless r = 2. So you have some kind of amplitude for a given energy and then the particle would execute something like this (Refer Slide Time: 27:28). If r = 2, it would be an ellipse. But if r = 4 for instance, then it will be a sort of a flat oval for and r = 1, there will be all kinds of curves. What we would like to do is to find out semi-classically, what's integral pdx.

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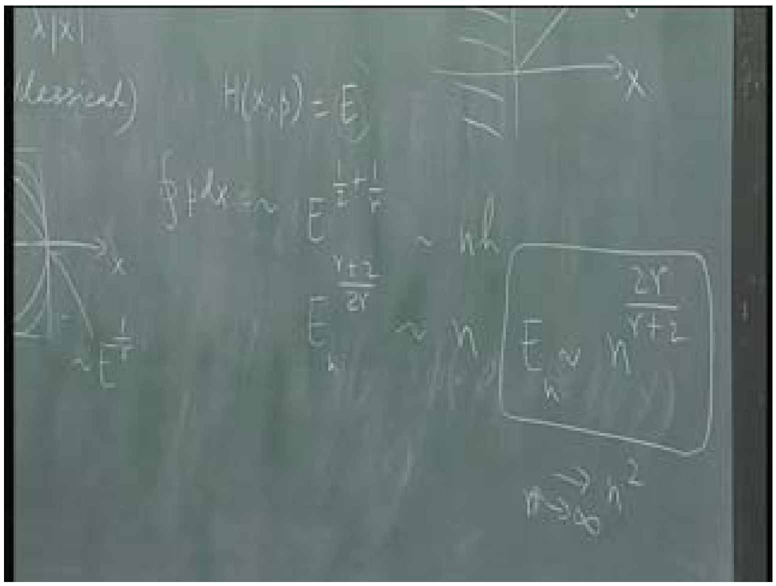

So when the particle is executing these trajectories, what's integral pdx? And then we apply Bohr quantization. Integral pdx is the area of this curve. And how do we estimate it as a function of the energy? So classically what you would say is, for a given set of initial conditions you find the Hamiltonian H of xp, you say this is equal to E and this is given to you as the total energy of the system. And then it swings back and forth, exchanging kinetic and potential energy and we want to know what the area under the curve is. Now it's clear that at these points, the potential energy is zero by construction and the energy is completely kinetic classically. The intercept is equal to square root of 2 m e because all the energy is kinetic energy.

So this (Refer Slide Time: 29:12) intercept goes like E to the power half apart from the root 2 m e and what does this (Refer Slide Time: 29:15) intercept go like? Well, the energy is completely potential at this point and there is no kinetic energy. So it's clear that this goes away and you get x to the power r which is E. therefore this amplitude goes like E to the power one over r. therefore what does the area go like? I would be just a product of the 2. I mean apart from numerical factors this area whatever it is bigger than this triangle and is smaller than the rectangle. And the area of the triangle is half base times height.

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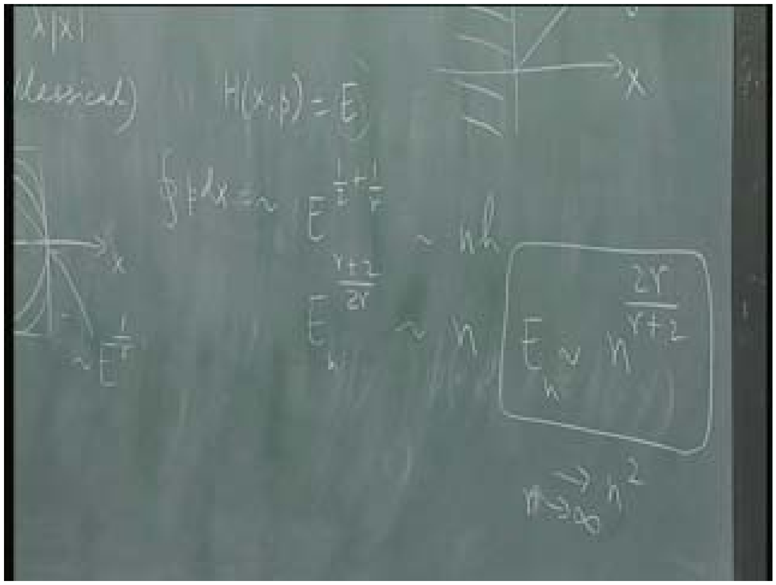

So as far as the energy dependence is goes, this (Refer Slide Time: 30:09) thing here is proportional to e to the power half + 1 over r. It’s guaranteed that that’s true apart from numerical factors but this we are advised is n times Planck's constant. When you do Bohr quantization, it says these orbits are quantized in such a way that integral p dx is n times Planck’s constant. This says that E_n, the energy level to the power (r +2) over 2r goes like n En which is proportional to n to the power 2 r over (r + 2). So it says that at sufficiently large values of the quantum number n, when you expect the semi classical argument to be valid, the energy levels En must change with the quantum number n according to that law. We are not saying what’s going to happen in the ground state or the first excited state. That requires detail calculation but for sufficiently large n, this is going to be true. It becomes proportional to n.

So I expect that in the simple harmonic oscillator problem, the energy levels sufficiently far away when n is much bigger than one, I expect the energy levels are going to be proportional to n itself and to the first power. What happens when r is = 1, 2/3, etc? It says it’s sub-linear and doesn’t increase as fast as n less than n to the first power. The energy levels do go up all the way to infinity but increases sub-linearly. This means if we took a ball, a potential which is constant; mod x is essentially a constant for a linear potential that’s like mgh.

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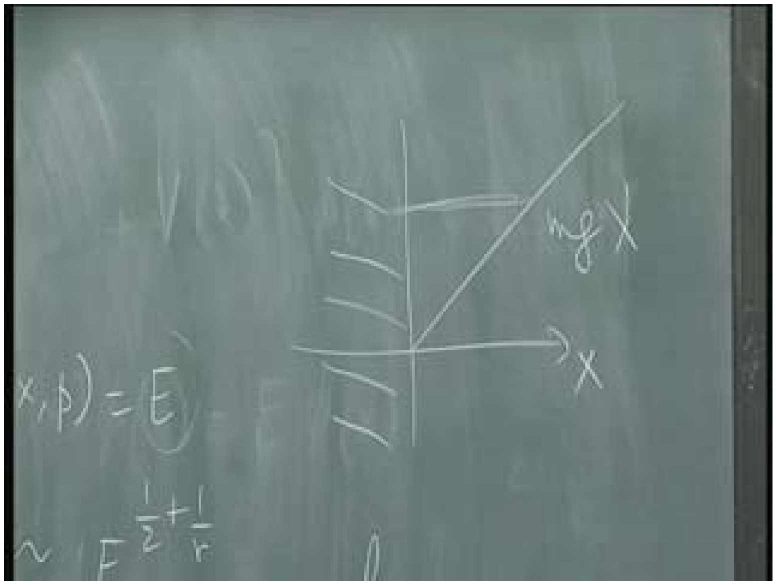

So for example, if you bounced the quantum ball up and down on the ground, then the potential hits the ground and it cannot go below that. but this is linear mgx, if this is x,and then the particle would bounce back and forth classically but quantum mechanically the energy levels in this potential here are guaranteed to increase like n to the power 2 thirds, n to power 2 thirds less then proportional to n. what happens when r is = 4; quadric potential? It increases faster than n. what's the maximum it could increase up to? It can only go up to 2 because as you increase the power, this potential gets flatter and flatter.

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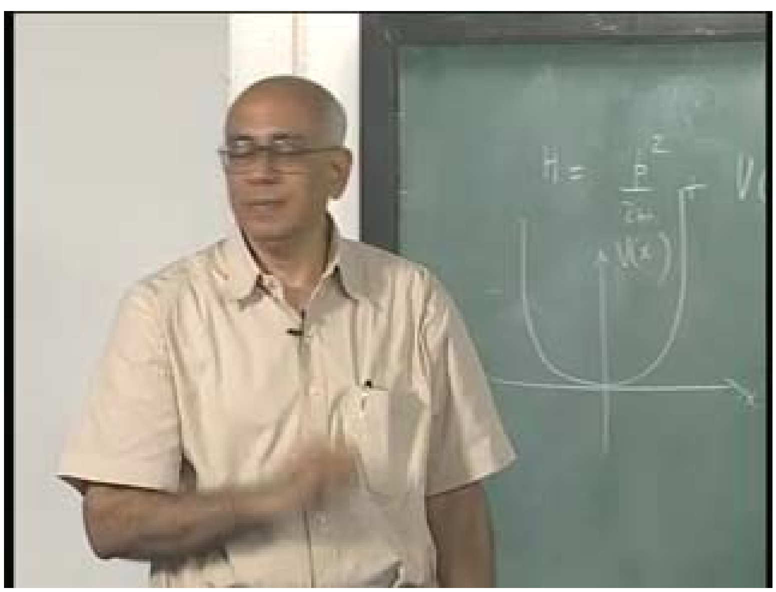

So x is along the x direction and V (x) is along the y direction, you end up with potential with slope like this (Refer Slide Time: 33:37) which has very high power and then as r tends to infinity, it goes like n squared. That's the worst it can do and what does the particle in a box do? It goes like n squared. Now, you see why the particle in a box went like n squared. It was like taking and putting it in the potential and then making the potential infinitely high. The slope becomes infinite and then it ended up with n squared. now you could say well, I have taken problems in which the power was x to the power r and I kept on increasing r such that finally it reached a vertical line, like a rigid box but more than a power, you could have an exponential. What would happen if the potential goes like e to the power x? We would like it to be symmetric. So let's make it e to the power mod x or cosh x.

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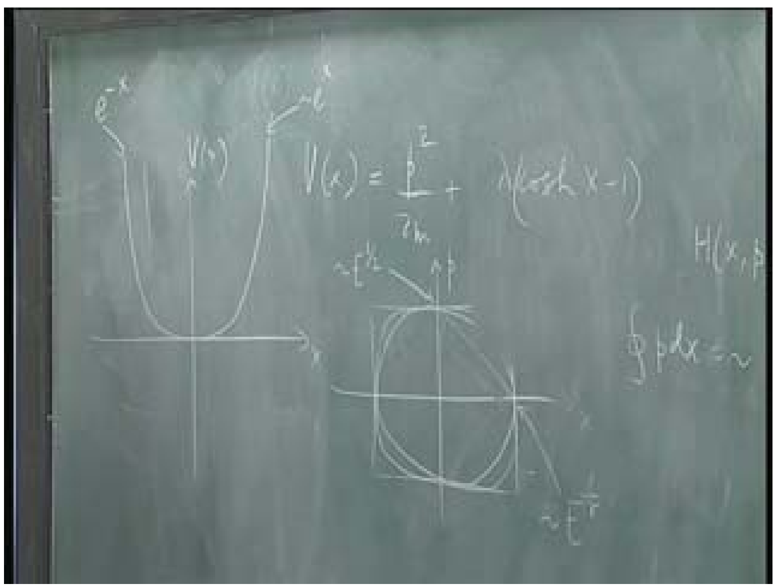

So what would be the energy levels like? So here is x and let's make it (cos x - 1) by adding a constant so that the potential looks like this (Refer Slide Time: 35:08). This is the cosh function. It's symmetric and cuts the axis at 1. It goes exponentially fast. So this curve here is e to the power x and e to - x in the other direction because e to - x is negligible here (Refer Slide Time: 35: 25) and e to the + x is negligible here. So it goes like this exponentially fast, faster than powers, what would the energy levels look like? They can't go bigger the faster then n square they can't increase with n and faster than n. squared because that's already for an infinitely high wall. Rigid wall but at the same time it can't be a power less than 2 because then that would be infinite. So let me let me write this out.

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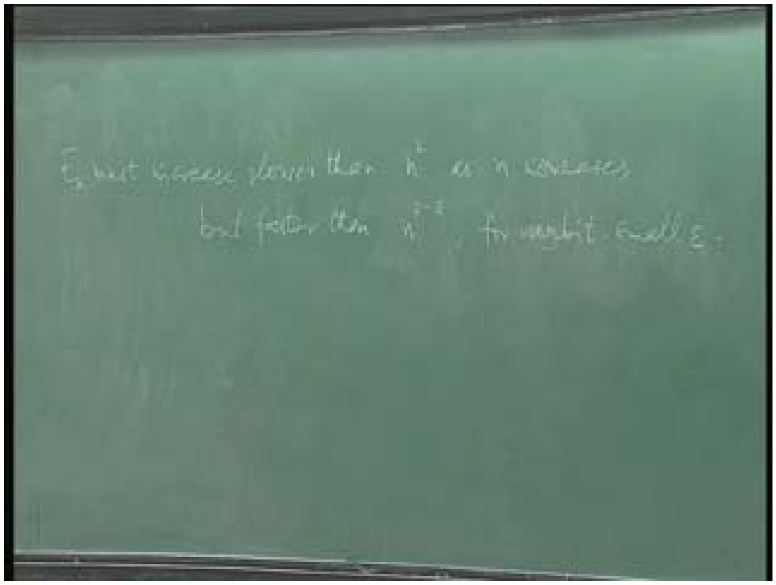

En must increase slower then n squared as n increases but faster than n to the (2 – epsilon) for arbitrarily small epsilon. It can’t go like n to the power 1.999. That’s not allowed nor can it go like n squared. It must be slower than that. (Conversation between Student and Professor) Then what it would do? n squared by log ? Where did the log come from? n squared by log what? It can’t be a power less than 2. It can’t be 2. What would I do? He is suggesting n squared divided by log. Does n squared over log n sound reasonable to you? Why not log n? Does the idea of logarithm sound upsetting to you? It is a very good intuition. That’s exactly what it does. There is a logarithmic correction and that’s the one less weaker than the power. Let’s see what it does. Once again it involves a very simple calculation.

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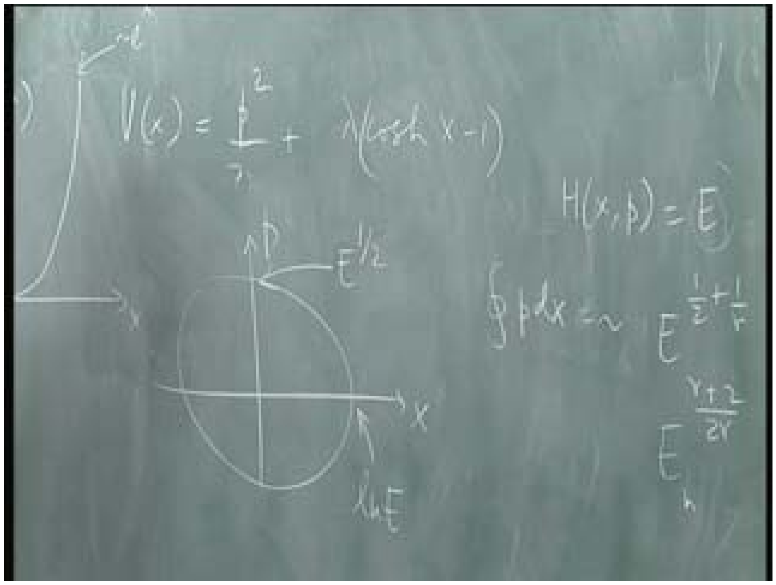

Once again in x and p, these are some kind of ovals but this amplitude here (Refer Slide Time: 38:25) is E to the half because that’s the kinetic energy and look at what the potential energy would do? What about this p? You see if you say this is equal the energy E and p is zero on this axis, then it says cosh x is like E. but cosh x is dominated by E to the x for large values on this side. So E to x is like E and x is like log E (Refer Slide Time: 38:52).

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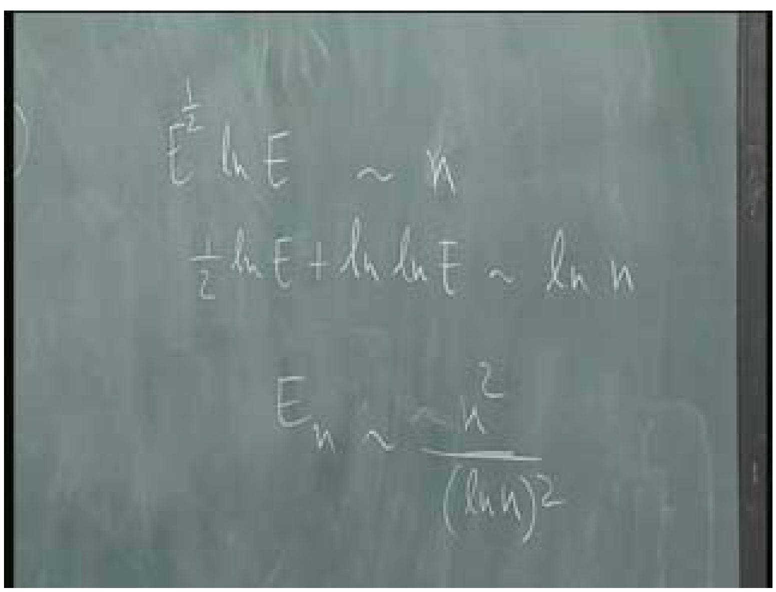

Now the area inside the curve is E to the power half log E. that's the product of p times x and this is n. you got to solve this equation and that's not easy to solve because it's a transcendental equation; there is both a power and a log but you solve it by iteration. To leading order, E doesn't vary much. So to leading order, it's clear that E goes like n squared. So you put that in here (Refer Slide Time: 39: 31) and then do an iteration. Or better still, take logs on both sides. so we get ½ log E + log E which is like log n. log log E is much smaller than ½ log E. so it immediately says log E to first approximation is like 2 log n or E is like n squared. Substitute that in this (Refer Slide Time: 40:02). So it says E to the 1/2 log n squared is like n. but log n squared is just 2 log n. so E to the 1/2 is like n or En is like n squared over log n squared. So the guess was almost right. Although you can't solve this problem, it's a very difficult differential equation to solve with this cosh you can't solve it explicitly. You still can estimate what's going to happen to the energy levels for very large values of n. there is a logarithmic correction to the power law.

Now let's back to our simply harmonic oscillator problem. We have enough machinery now to ask if this is solvable exactly. We would like to explicitly solve it. There are many ways of doing this and it's the most fundamental problem in quantum mechanics at this level for very deep reasons and it appears over and over again all the time. Because of this single property which we will now see explicitly, the energy levels are going to be equally spaced as you all know. And this is the reason why it makes an appearance once again in the quantum field theory. Because in a nutshell, when you take many particles you include relativity, the possibility of interactions etc and you put all these particles together. Then, when you want to describe a set of free particles or non-mutually interacting particles and you want to quantize it, every time you add one more quantum in the field, you are adding the rest energy of this particle of this quantum. Therefore addition of one more particle is addition of a constant amount of energy to the total energy. Therefore it's natural that what appears in this problem is precisely the harmonic oscillator solution in the disguised form because this has exactly discrete energy levels which are equally spaced. I have to say right away that the harmonic oscillator is not the only potential which has equally spaced levels. There is an infinite family of potentials called isospectral oscillators, all of which have equally space levels but this is a first member of the lot in the simplest of them. Now our task is to solve the linear harmonic oscillator.

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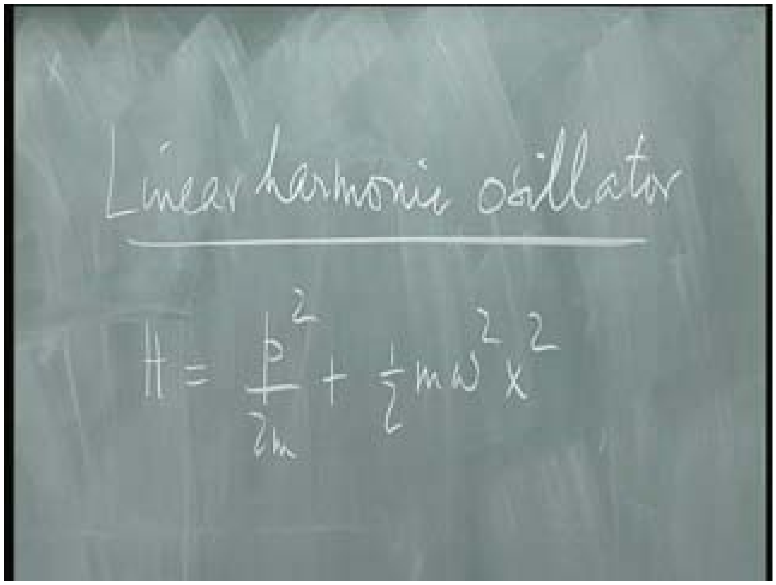

The Hamiltonian operator is given by p squared over 2 m + 1/2 m omega squared x squared. And just as classically, we are given the fact that x and p obey Poisson bracket relations. Quantum mechanically you have the fact that x commutator p = ih cross times the unit operator. As a first thing, you got to realize that in the position basis, p is a differential operator; - ih cross d over dx. But that's only in the position basis. The energy eigenvalues would be independent of what basis you choose to describe the problem. That's just one way of describing the state vector in the position basis.

So it's like choosing a particular coordinate system to describe an abstract vector but the eigenvalues and the state vectors corresponding to these eigenvalues are independent of what basis you choose to solve the problem in. you could solve it in any basis and transform to whatever basis you like. And this is what Dirac did he found an operator method of solving these equations. now of course a operators suggest immediately there is an algebra matrices appears somewhere and so on but I would like to disabuse you immediately of the notion that you can do this with finite dimensional matrices because this commutation relation precludes the possibility of being able to represent this system in terms of a finite dimensional space. The Hilbert space is infinite dimensional.

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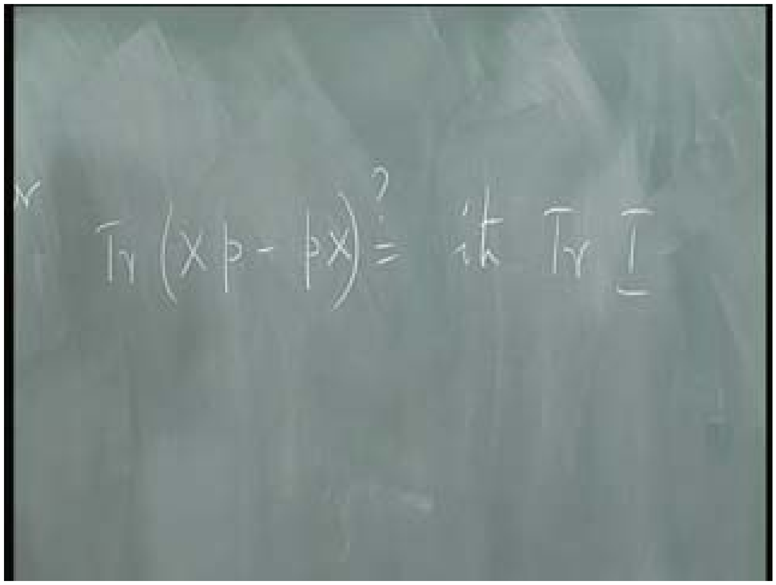

You cannot express these operators as finite dimensional matrices and that's immediately true because the moment you write xp - px = ih cross times the unit operator or the unit matrix, if you write it as matrix representation and take trace on both sides; we know that trace ab = trace ba even if nb don't commute as long as a and b are finite dimension matrices. So the left hand side would give your zero. If it is finite dimensional, the trace of the unit operator is just the dimensionality of the space. That's finite and this is zero so this is a contradiction. It's not possible to write x and p in terms of finite dimensional matrices. So this identity is no longer true and you can't make such a representation. We will see that you need finite dimensional matrices if you choose to use a matrix representation. But if you use the differential operator representation, then there is no question of matrices anyway. We would like to solve for the eigenvalues and Eigenfunctions.

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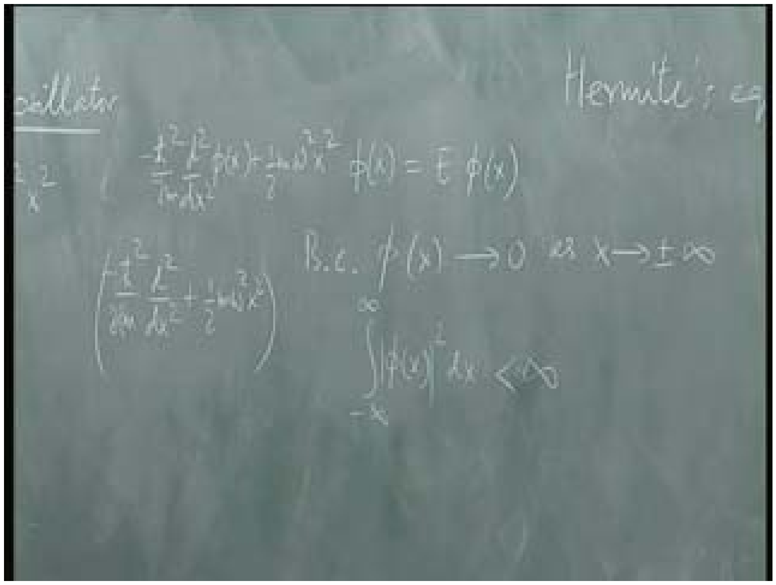

If there is an eigenvalue E and an Eigenfunction phi of x, then this must be = - h cross square over 2 m d 2 over dx 2 phi of x + 1/2 m omega square x square phi of x is = E phi of x. when one tries to solve this, we know from the shape of the potential already that E must be some non-negative number. So we already know that E is a real number and a non-negative number because the potential has an absolute minimum at x = 0. And then the question is, does this equation have solutions? You need to put boundary conditions and what are the boundary conditions? You would like it to be a bound state you and should be normalizable.

So the natural boundary conditions would be phi of x goes to 0 as x tends to + or - infinity. Both sides it must vanish, after that we would like to normalize this wave function. It's some number if you find it to be 6 for instance. Then you redefine your phi as 1 over square root of 6 times the original phi in which case, you have normalized it to unity. So this is the strategy. What sort of differential equation is this (Refer Slide Time: 47:30)? It's an ordinary second order differential equation but there is a slight complication here this (Refer Slide Time: 47:38) coefficient is not a constant.

It's a function of x which means that you can't solve it simply as a superposition of 2 exponentials. The original trial method of trying exponential doesn't work because the coefficients are not constantans. this is an example of what's called Hermite's equation, n not quite directly but it can be transformed into that and then the solution appears as the product of an exponential factor; e to the - x squared multiplied by some constant times a polynomial in x. these are called the Hermite polynomials. So you need to use a more sophisticated method to solve this equation. You need to use this method of series, the Frobenius method.

So we need to use that to solve this equation here. But what we will do is follow Dirac and solve this equation by an operator method which gives us the solution explicitly without going through this relatively difficult boundary value problem. The hard part is that it's a second order equation. Had this been a first order equation, you could write down the solution by a very simply formula. So Dirac string actually reduces to saying that this becomes a first order equation. This is a second order differential operator. so it's - h cross squared over d over 2 m d 2 over dx 2 + 1/2 m omega squared x squared acting on the wave function. And what Dirac did was to break this up into 2 first order factors. once you do that, then a solution of this equation implies that each of these 2 factors; if they commute with each other acting on the wave function must give you E times phi. So just factors the second order differential operator into 2 first order factors and then the answer is a more or less obvious immediately. Another way of saying is I have x squared + p squared, if I want to write it as a product of 2 factors, what should I do? The first step is to get rid of the ih cross factor and we would like to make it simpler. There is a length scale in the problem. The parameters in this problem are m, omega and h cross.

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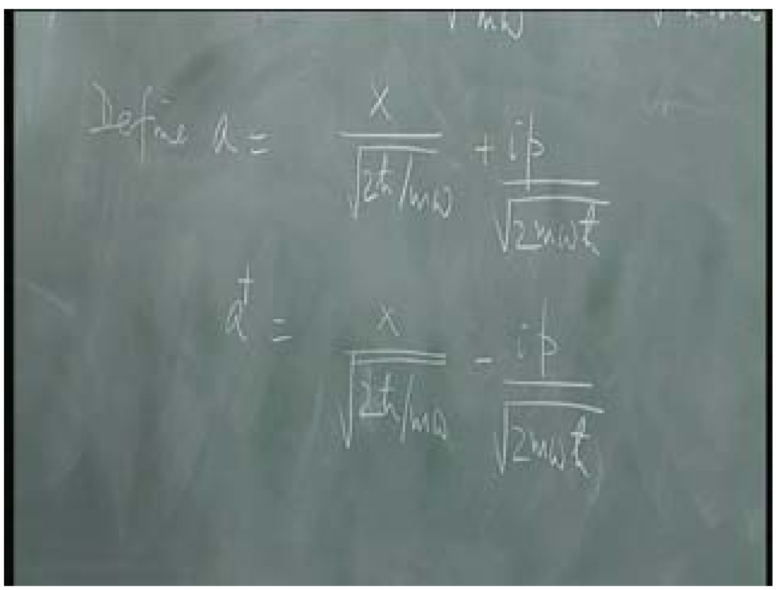

So out of these parameters, you can construct a quantity of dimension x and dimension p and what's the quantity of dimension length? The length that you can construct = M L squared T to power -1. MT inverse is omega. So I could construct h cross by m omega square root is the length and what's the momentum? Momentum is mass times velocities, MLT inverse. So if I took m omega h cross, this is MT inverse and then M L squared T inverse and I took the square root of that, I get MLT inverse. So this suggest that square root of h cross m omega has dimensions of momentum. So when I construct new operators which are linear combinations of x and p, I may as well get rid of these dimensional quantities.

So let’s define an operator a = x divided by this quantity here (Refer Slide Time: 52:24). So it’s dimensionless + i p divided by m omega h cross. And a dagger is not Hermitian. These (Refer Slide Time: 52:47) are Hermitian but this operator is not Hermitian because I have got an i sitting there and that operator is x over square root of h cross over m omega - i p over square root of m omega h cross. so I am writing x + i p and x - i p but when I multiply the two, I get x squared + p squared and I have got this factor 1/2 sitting here. I’d like to get rid of that (Refer Slide Time: 53:23) 2. So let’s make this a 2 here (Refer Slide Time: 53:25). This will make the Hamiltonian look very simple because I got rid of that and when I multiply the 2; I get 1 over root 2 and 1 over root 2. That gives me a half and that will exactly match this here. First thing I got to ask is are these operators, a and a dagger Hermitian? They are not Hermitian. So these are directly not physical observables. They are combination of these operators here and there is this important i factor. What is a with a dagger equal to? x commutes with itself, p commutes with itself. So I got to take the commutator of this with that (Refer Slide Time: 54:15) and add it to the commutator of that with this (Refer Slide Time: 54:19).

This with that (Refer Slide Time: 54:22), you can see what’s going to happen. It’s a half sitting in the denominator because of these 2 things here (Refer Slide Time: 54:29) and then there is an h cross. So there is h cross in the denominator. The m omega factor cancels because it’s in the denominator here and in the numerator there. And then x with p is = i h cross and the i with - i gives you + 1 and an h cross. But the h cross cancels with whatever was in the denominator. But the half remains and then in the other term, this (Refer Slide Time: 54:55) with that is exactly the same thing except now you get a - sign. You get a - i. but there is a +i here, so that again gives you a half. So it’s immediately obvious that this is equal to exactly 1. It has been normalized in a such a way the that it is exactly 1.

And remember a and a dagger themselves are dimensionless. The physical dimensions are M to the 0, L to the 0 and T to the 0. so it’s a great advantage to be able to write the Hamiltonian in these dimensionless variables. And what happens to the Hamiltonian itself? Now we can see all we have done is to factor this Hamiltonians with that h cross an omega put in.

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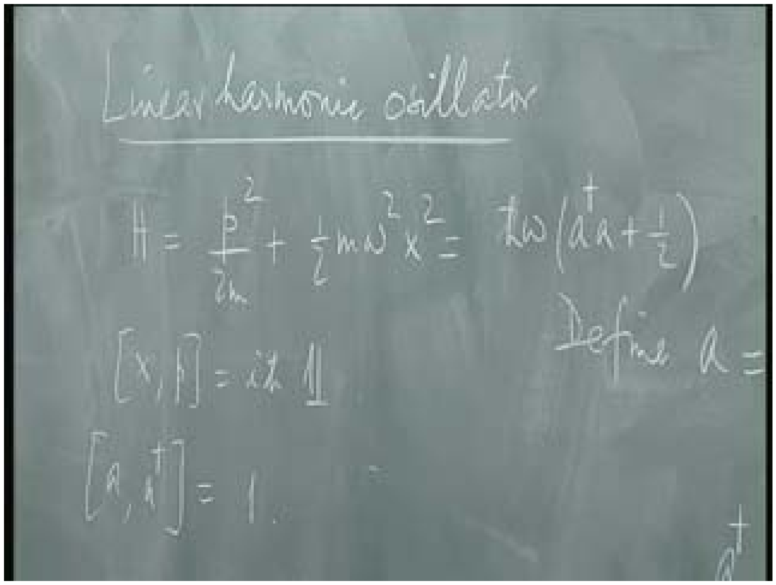

So we get h cross omega, a dagger a + ½. I leave you to verify that you get this extra term there. This is the well known oscillator Hamiltonian written in terms of a and a dagger. These operators are called ladder operators or raising and lowering operators for a reason which will become clear. They are also called creation and annihilation operators in quantum field theory. This is starting point of quantum mechanics in some sense. so our job know is to find the eigenvalues of this (Refer Slide Time: 56:35) operators; this is half times unit operator incidentally. We have to find the Eigenvalues of this operator given this commutation relation; a with a dagger. This should be the unit operator incidentally but I am just going to write it as a dagger = 1. Incidentally that again shows that it cannot be finite dimensional because trace a dagger is trace a dagger a but that’s zero and can’t be the trace of the unit operator for any finite unit operator. Now Dirac’s solution was the following and this method is due to him.

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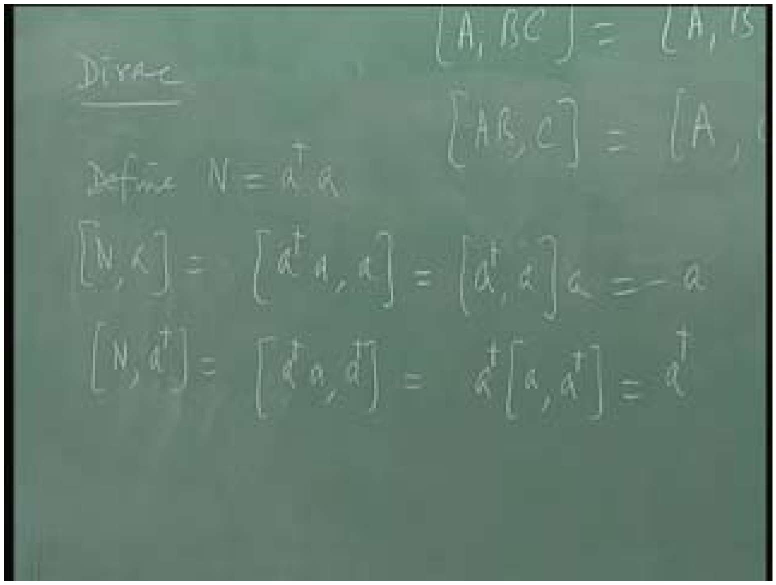

P. A. M. Dirac was one of the founders of quantum mechanics as you know and he is the one who proved the equivalence of the Schrodinger and Heisenberg pictures. He gave the operator formalism of quantum mechanics that was in fact is PhD thesis and he is possibly the only person in the world who could ever have a PhD thesis whose title was quantum mechanics. He was very young when he did this. A few years later he got the Nobel Prize and when he walked into the High Table at Cambridge in his college, there was a round of applause. Lord Rutherford was presiding over the table. He had already got the Nobel Prize and there were several other people who got it already. When the applause went on for a little longer, Rutherford sort of growled and said, “That’s enough of that. This is not the first time the prize is coming around this way.” Dirac was one of the greatest physicists of all time and his idea was to introduce these operators, which has now become a very standard fare in quantum mechanics. He is the one who first introduced the bra and ket notation to start with. He also called it transformation theory because the whole thing was just going from one basis to another and how to write things in different bases and so on. He essentially laid the foundations of the modern way of looking at the subject.

Now the problem is, define N = a dagger a. I will call this operator as capital N. it's called the number operator, the reason being that N's eigenvalues turns out to be 0,1, 2, 3, and so on. They will be all natural numbers. Now what's the commutator of N with a?

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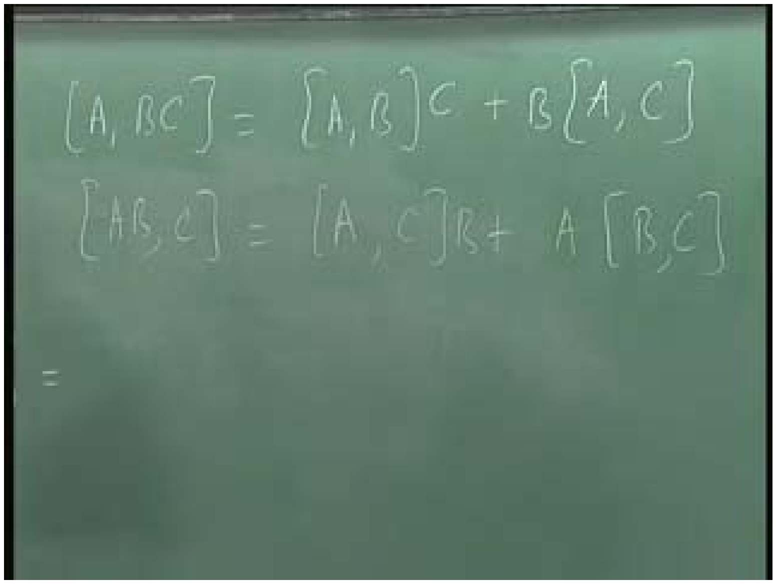

By our rule for commutators which follows from the rule for Poisson brackets, we know that A with BC is A with B with C on the right hand side and A with C with B on the left hand side. Never change the order of the operators. B appears in the left C appears on the right. Similarly, AB with C is A with C with B on the right hand side + A on the left and B with C. It is a fundamental rule for commutators and all we have to do is to apply that here. a commutes with itself. So that is zero and all you have is a dagger with a, with a on the right hand side. This a (Refer Slide Time: 01:00:47) goes out and that's on the right hand side. But a dagger with a is - a with a dagger. So this is equal to – a. and similarly N with a dagger is very simple. It's a dagger a, with a dagger and that is equal to a dagger on the left hand side, a with a dagger and that is a dagger. So there is a little algebra that is formed here. The original algebra was a with a is zero, a dagger with a dagger is zero, a with the unit operator is zero, a dagger with the unit operator is zero and a with a dagger is one, the unit operator. That formed an algebra called the Heisenberg algebra. And once you add N to it, you can see there is a kind of closed algebra. The commutator of any two of these quantities is a linear combination of the same set of operators.

Now suppose our job is to find Eigenstates of this quantity (Refer Slide Time: 01:01:58), this (Refer Slide Time: 01:02:00) is trivial because this is a unit operator. Anything is in the Eigenstate. So let us suppose there exists an Eigenstate.

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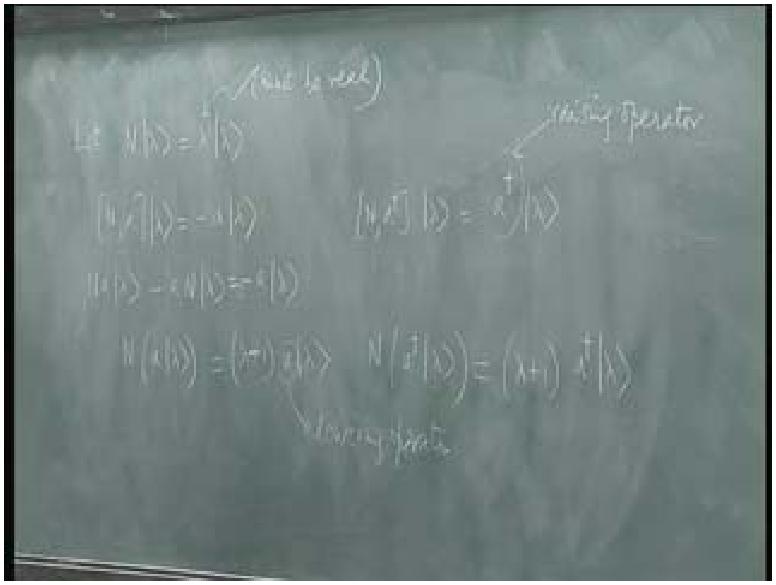

Let lambda be an eigenvalue and let's suppose N operator acting on Eigenstate lambda gives the eigenvalue lambda in the Eigenstate lambda. I should really write psi with a subscript lambda to show it's an Eigenstate with eigenvalue lambda but let's abbreviate notation and just put lambda inside the ket. What do we know of lambda? Can it be any arbitrary complex number? It must be real because a dagger a is Hermitian. You take the Hermitain conjugate of a dagger a, you get a dagger a once again. So after all, it's the Hamiltonian apart from a constant. So lambda must be real. Then take that statement N with a = a and apply it to an Eigenstate lambda. So I have this operator identity and I apply each side of this identity to the same state, lambda. This implies N a lambda - a N lambda = - a. so it says N acting on a acting on lambda; this is already some ket vector and N acts on it. What is N on lambda by definition? That is lambda on lambda, it's a number. Lambda is a number and so I move it to the right hand side and I get (lambda - 1) a on lambda. What conclusion do you draw from this?

If this (Refer Slide Time: 01:05:00) is an Eigenstate of N, so is this operator acting on lambda an Eigenstate of the same operator N but with an eigenvalue reduced by unity. In exactly the same way, you take N with a dagger on lambda = a dagger on lambda and use the factor its +a dagger there and it tells you that N acting on a dagger acting on lambda is = (lambda + 1) a dagger lambda. So it says if ket lambda is an Eigenstate of N, so is a dagger acting on ket lambda with an eigenvalue increased by 1. So a dagger is called the raising operator and a is called the lowering operator because these respectively raise and lower the eigenvalues of N.

Together of course you could call them ladder operators; they go up and down but we still don't know what lambda is. So if I start with some lambda, I apply a on it, I get another Eigenstate with eigenvalue (lambda - 1). I apply a once again, I get another eigenvalue with (lambda - 2) and so on. This will keep going down below. Eventually, since lambda is real, it will hit a negative value. But you cannot have a negative eigenvalue for a dagger a. why is that? N cannot have negative eigenvalues because in any state, what so ever, this operator a dagger a psi; that is the expectation value, for any arbitrary state. This is the expectation value of this operator and this is equal to the norm of a psi whole squared, exactly as I did for the kinetic energy. It says take this ket, vector take its bra vector and take the inner product. That's the square of the norm. No eigenvalue can be negative because in no state of the system can this have a negative expectation value. So what does that tell you? What is the only possibility lambda is real number? You start with some lambda, it is a real number but then if lambda is an eigenvalue (lambda- 1), (lambda- 2), (lambda - 3), etc. It's a negative value but it's not allowed to hit negative values. Lambda must be an integer. So you have no choice but to say that lambda must have been any positive integer and then you can keep going down till you hit zero but you can keep going up all the way to infinity. So that proves that lambda must be = N.

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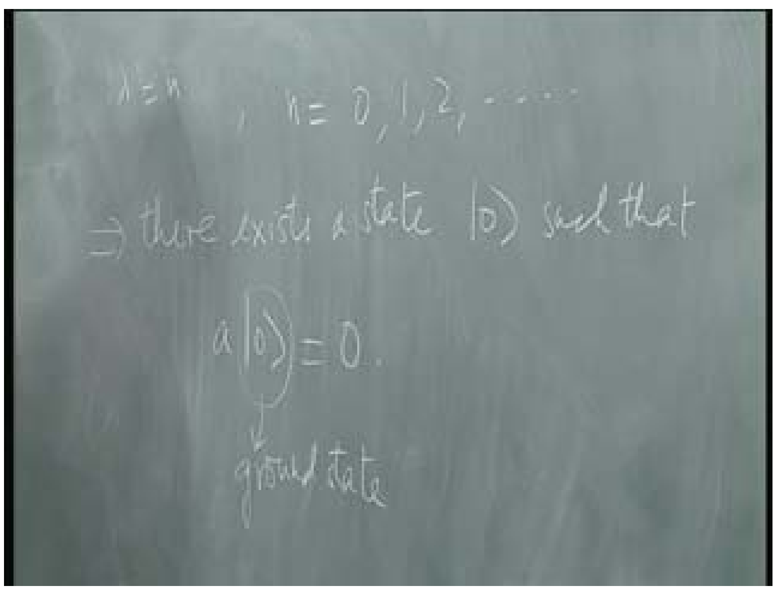

N is 0, 1, 2, etc. that's the least value it can have and it can't be negative. Suppose it's 1.1, then there is an eigenvalue 0.1. Then there is another eigenvalue (0.1 - 1) but that's not allowed. Student- (0 – 1) is also negative. Professor - No, there exists a state such that a acting on it must give you 0 and the eigenvalue has become zero. There is no way you can lower it after that. So it implies there exists a state zero such that a acting on zero is zero and then to go to - 1, you will have to act with a on that but it's already gone, its zero. So it can't be a fraction. If it were 1.5, then it will go to 0. 5 and then - 0. 5. So there must be a state with Eigenvalue zero such that a acting on that Eigenstate is zero and it annihilates it.

I should really call it phi subscript zero but I use this notation lambda. This state is the ground state. In field theory, it's called the vacuum and the annihilation operator a annihilates the vacuum. When it acts on it, it gives you a null vector. Zero is not the null vector in the linear vector space. This vector is not the null vector. This is zero times whatever vector you like. This vector here stands for phi subscript zero, just my notation that I use this zero here. Our job is to find out what are these states, what do they look like and so on.

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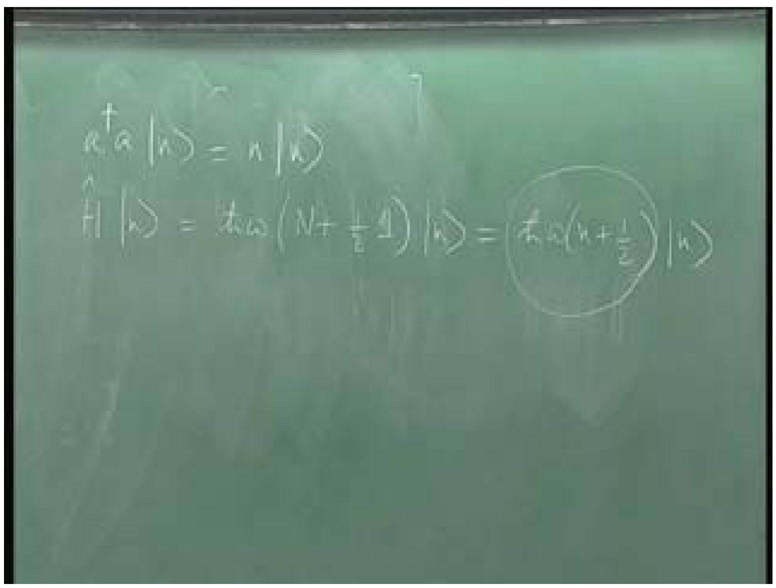

The next job is to find the Eigenstates n because we now know that a dagger a acting on n is n on n and incidentally the Hamiltonian acting on n is h cross omega N +1/2 unit operator acting on n. so these (Refer Slide Time: 01:12:30) are the energy levels. There is that extra half, it's called zero point energy and it says the lowest energy level in this harmonic oscillator is not zero but half h cross due to quantum fluctuations. We will see the significance of that.

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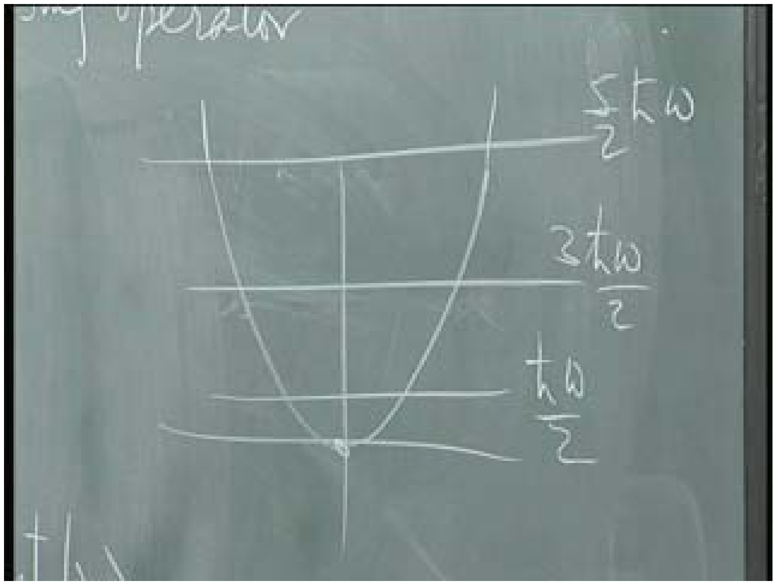

So it essentially says that in a potential like this (Refer Slide Time: 01:12:50), classically the equilibrium state is when the particle is sitting at the origin at rest; zero kinetic energy is zero potential energy. Quantum mechanically this is not is not possible because if you localize the particle at the origin, it's uncertainty in momentum becomes infinite. so you {cont} (01:13:12 min) can't have a state of absolute rest doesn't exist the ground state energy is here (Refer Slide Time: 01:13:19) at this point at half h cross omega and the first excited state is 3 h cross omega over 2 and then 5 half's h cross omega over 2 and so on. They are equispaced energy levels all the way to infinity. Now our job is to find the Eigenstates n and then to explicitly represent these Eigenstates. I need to find the wave functions I have to go back and find phi n of x for each of these quantities.

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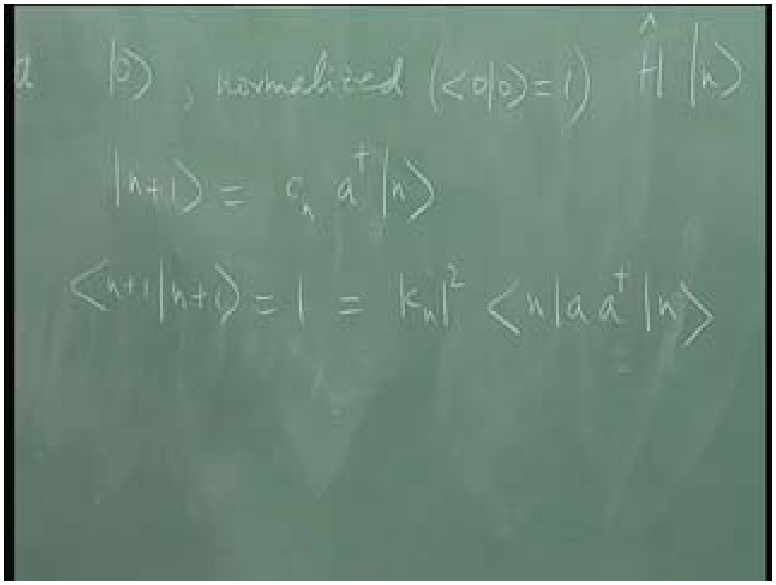

So let’s start by saying I have the ground state and I will normalize it. I will find its explicit representation later on but let’s say it is a normalized Eigenstate. Then I would like to find the first excited state. What is this equal to? It’s a dagger acting on this quantity. That’s what raises it up by 1. This corresponds to eigenvalue 1 of the number operator n, but I am not sure if it’s normalized or not. I need to normalize this. So I put some constant here. So it becomes constant times this quantity.

In general, if I start with this Eigenstate n and I apply a dagger on it, it’s going to go to n + 1. So in general, let’s write (n +1) as some constant which may depend on n a dagger on n. I raise with the a dagger and I lower with the a and I want this to be a normalized state. So the question is what is this cn equal to? Now what I would do is I take the bra vector on this side. So <n +1> <n +1> is 1, by construction all these Eigenstates are normalized, then this implies that mod cn whole squared n a a dagger on n is 1 because I take this (Refer Slide Time: 01:16:06) quantity and I take its bra. The bra of it is n bra and then an a on the left.

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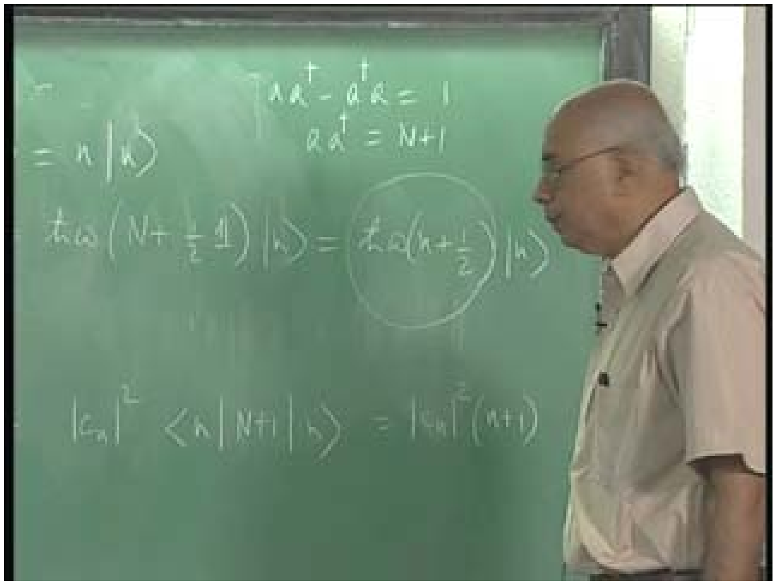

Can I simplify this (Refer Slide Time: 01:16:31)? I don't know a and what a dagger does on n. So i use the commutation relation which says a dagger - a dagger a = 1. I use the commutation relation here. So it says a dagger = (N +1) because a dagger a is the number operator and therefore this is n (N + 1) n but this is the Eigenstate of number operator with eigenvalue n. therefore this is equal to mod cn squared (n +1). And if I insist that should be equal to 1, then it immediately tells you that cn, apart from a phase factor is 1 over square root n +1. That guarantees that all my Eigenstates of the number operator are normalized. I start by saying I have a set of normalized Eigenstates and now I am asking how do you go from one Eigenstate to another. By applying a dagger, you move upwards but there is a constant factor multiplying it.

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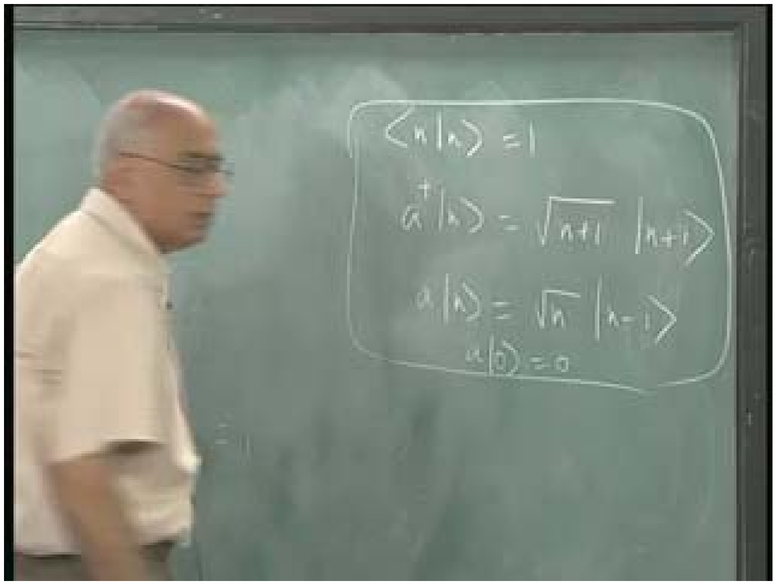

So it gives me the first piece of information. That's how it raises preserving normalization in this fashion.

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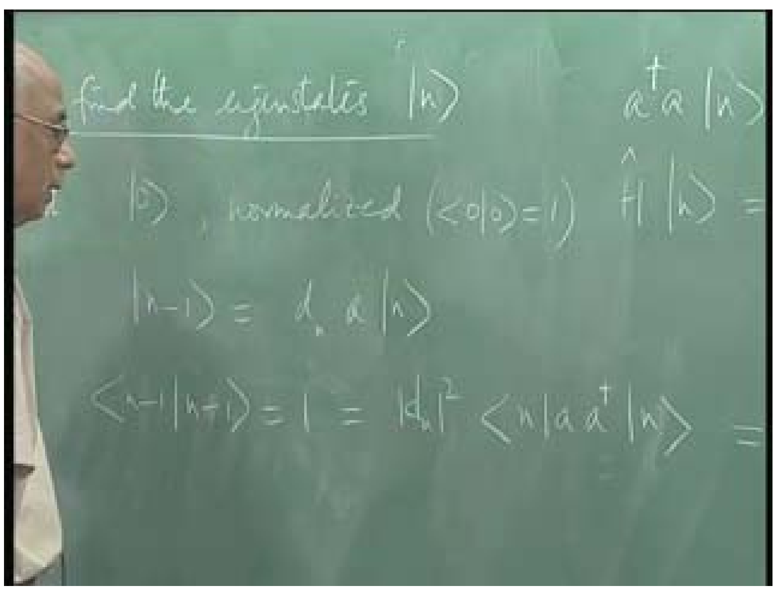

In exactly the same way, n - 1 is found by applying a on n here and there is some coefficient d $_n$ which I would liked to find out. Then if these states are normalized, (n - 1) is 1, this is mod d_n squared and this is just a dagger a. I don't even have to apply the commutation relation and this is equal to d_n squared.

So it gives you the other piece of information that this d_n is root n. this is why when it hits zero, it stops. So a on zero is zero. There is no state - 1, so it's completely consistent with that. So these are these are the pieces of information you need. Now let's see what the wave function looks like. You put in all the x's and p's and things like that see what happens.

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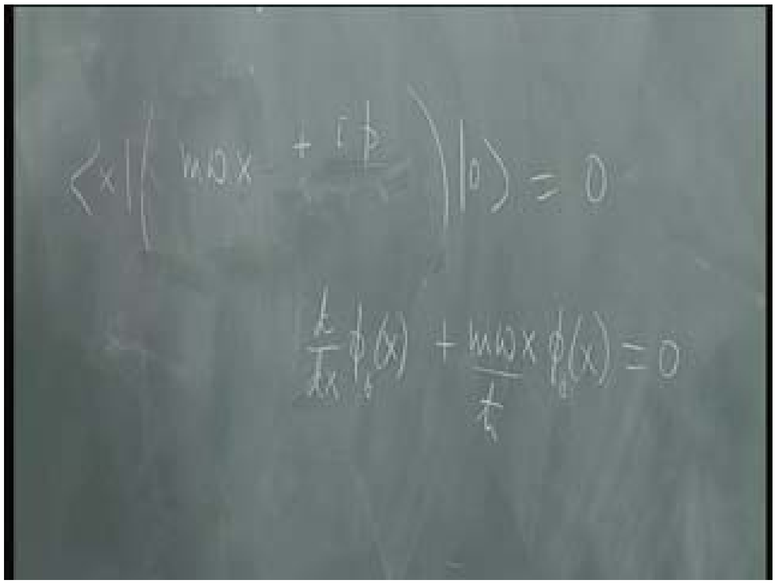

To avoid solving a second order differential equation, I simply choose this equation, a on zero is zero. But what's a in terms of x and p? this is x divided by root 2 h cross over m omega + ip over root 2 m omega h cross, that operator acting on zero is zero. Can we get rid of some of these constants? This is root m omega by 2 h cross. so we can get rid of x root m omega over 2 h cross and this 2 h cross so let's just write m omega x. i would like to find out what the ground state wave function is. What's phi zero of x?

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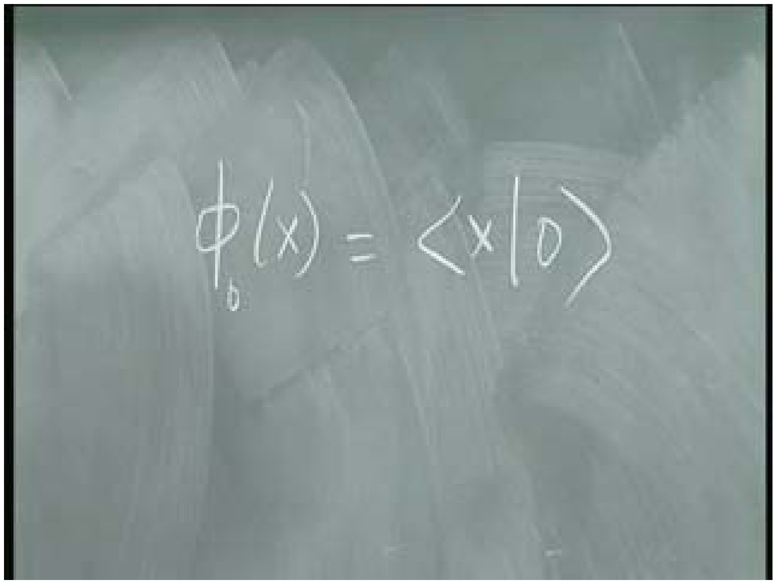

By definition, this is x zero by definition. That's the representative in the position basis of the ground state vector zero. That's the definition of ground state wave function in the position basis. So let's take ket x on both sides. What is this (Refer Slide Time: 01:22:11) represented by? This is represented by - ih d by dx acting on x or zero. So this says - i +i cancels. So you get h cross d over dx phi zero of x. that's this on that (Refer Slide Time: 01:22:33) + m omega x. phi zero of x must be zero because this (Refer Slide Time: 01:22:43) operator acting on this ket vector just gives you the label x. This is the equation that must be satisfied by the ground state wave function. And it's a first order differential equation and they are trivial to solve.

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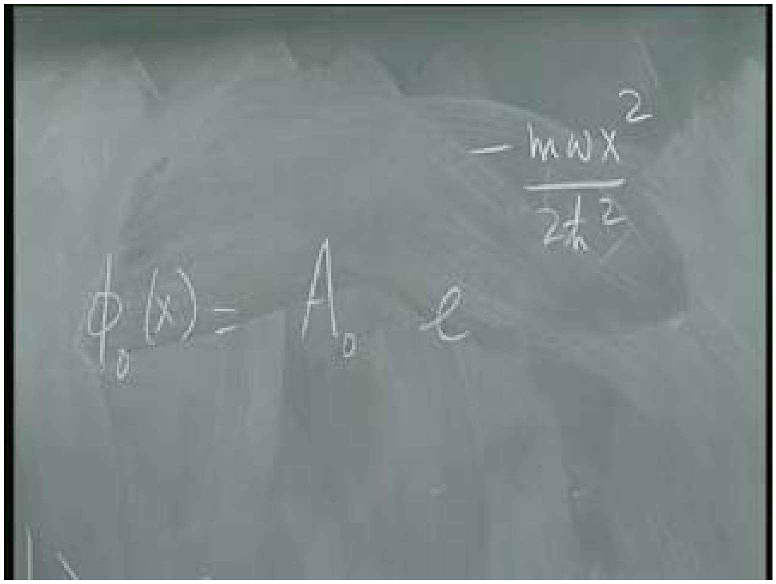

It says phi $_0$ of x = some normalization constant, A $_0$. This is m omega over h cross (Refer Slide Time: 01:23:17) and this goes away. So you have got d phi over dx + constant times x phi = zero. What sort of solution is this? e to the power minus the integral of this quantity (Refer Slide Time: 01:23:37) and that's x squared over 2. So it immediately says A $_0$ e to the power - m omega x squared over 2 h cross squared. That's the solution. What kind of a function is that? It's a Gaussian function since it has no nodes and it's a bell shaped curve. That's guaranteed to be the ground state wave function of this problem. It was completely painless since it did not involve second order equations. What's A $_0$ and how do we find it? All we have to do is to normalize it.

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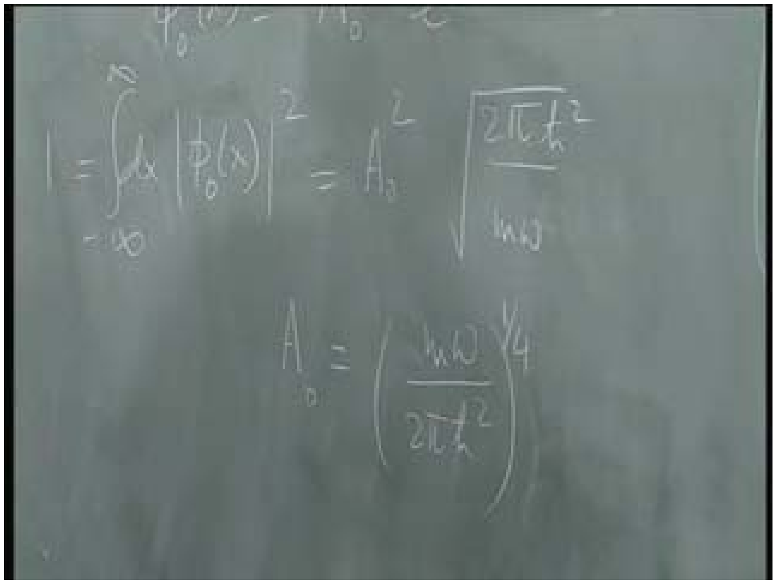

So phi zero of x norm squared dx, - infinity to infinity = A $_0$ squared I will choose the phase to be zero, so this is just A $_0$ squared. That's a Gaussian and you know the integral of a Gaussian e to the power - Ax squared is square root of pi over A. so this is square root of pi over A. A in this case is m omega and then a 2 h cross squared and I want to normalize this. So A $_0$ = m omega over 2 pi h cross squared to power one quarter.

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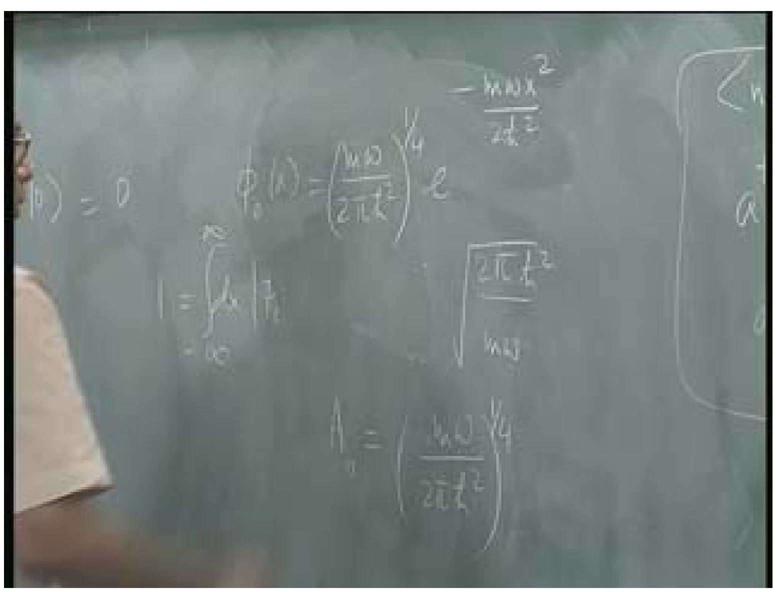
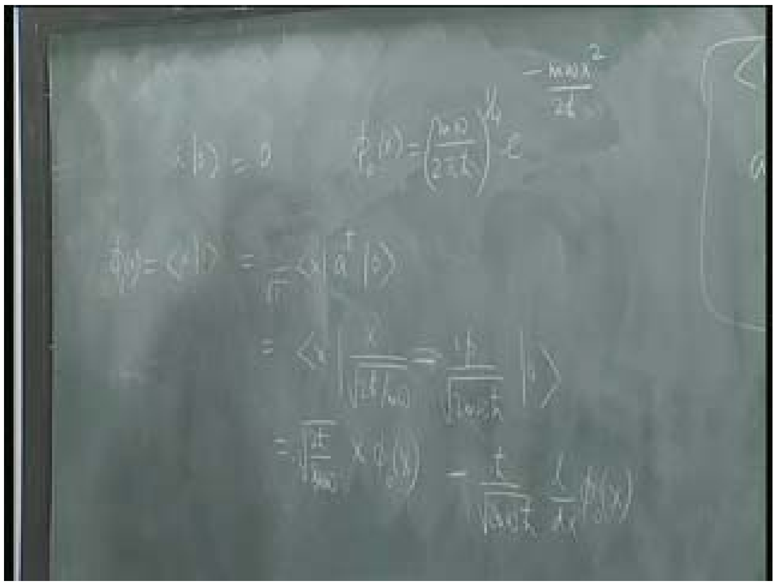


So I put that in here (Refer Slide Time: 01:25:29) and I get m omega over 2 pi h cross squared to the power one quarter times this. That's my ground state wave function. How do I find the first excited state without solving any differential equation? I use this relation here (Refer Slide Time: 01:26:37). So how should I use it?

(Refer Slide Time: 01:26:43 min)



I would like to find state one. This state is one over square root of 1 a dagger on state zero. The x representative of it is phi one of x and therefore I got to do this. This is 1 over root 1 x on this (Refer Slide Time: 01:27:24) quantity but this is x over square root 2 h cross over m omega - i p over root 2 m omega h cross on zero. but that's same as square root of 2 h cross over m omega x on phi $_0$ of x because this is going to act on this and just produce a number and the rest is phi $_0$ of x which you already found out there. And then i times - ih cross. So - h cross over root 2 m omega h cross d over dx on phi $_0$ of x. and we have phi $_0$ of x already. So all you got to do is to differentiate and that's guaranteed to give the normalized Eigenfunction.

So please notice I am not normalizing each of these separately. I already constructed that one over square root of one it took care of it automatically. So this (Refer Slide Time: 01:29:13) Eigenstate is normalized. So it has got an added advantage that even the normalization of all these Eigenstates is done in one shot. What kind of function would it be? Well, x phi $_0$ of x has to be an odd function. We already saw it's got to be an odd function. This is a Gaussian and that multiplied by x and this is the derivative of a Gaussian. So it's again got an x outside. So it's of the form x e to the power - x squared. What would its solution look like?

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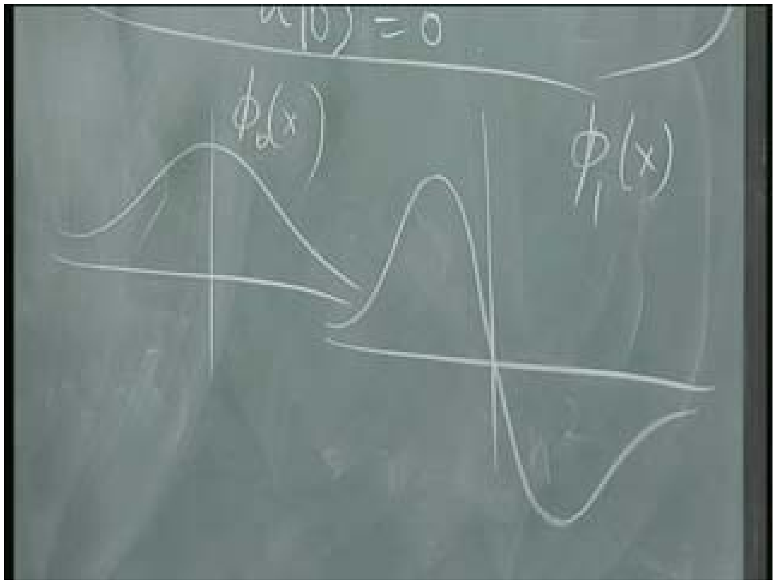

So phi $_0$ of x looks like that (Refer Slide Time: 01:29:59) and phi $_1$ of x looks like that and similarly for phi 2 and so on. I will leave you to find out what phi n of x is. It's a little painful to do this by differentiating and so on but the nth one is going to be an nth order polynomial.

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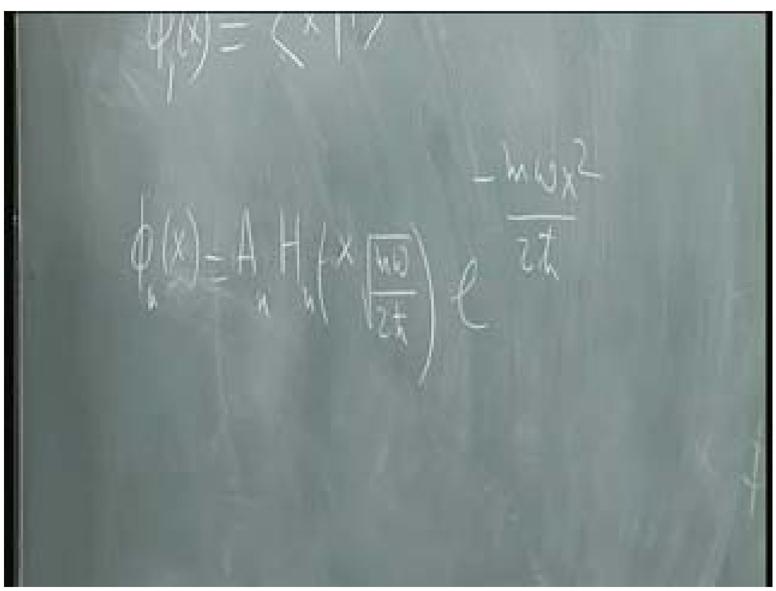

And phi n of x is, apart from some normalization constant, it's the Hermite polynomial x in these dimensionless units times this Gaussian. But this is the n th Hermit polynomial H_0 of x is 1, H_1 of x is 2 x and so on. Next time I will mention a few properties of these polynomials. This is one of a family of orthogonal polynomials and those are the solutions to the harmonic oscillator problem. We will also see why this is so significant. They turn out to have very interesting connections. What would their Fourier transforms be?

This problem is sort of symmetric in x and p. so you would expect the position space and momentum space Eigenfunctions to be exactly the same. So the Fourier transforms of these combinations are again Hermite polynomials times Gaussian's in p. they look exactly the same in units of square root of 2 m omega h cross. This also has implications for Fourier transforms itself because it says that the harmonic oscillators Eigenfunctions, in a sense are the Eigenfunctions of the Fourier transform operator in function space. So it's got close links with many other things and we will point out some of them. Let me stop here.