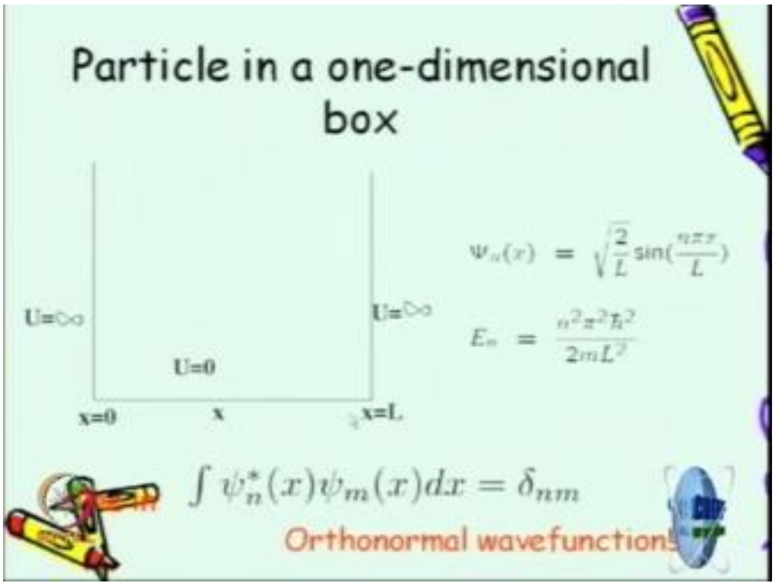
Quantum Mechanics
Prof. P. Ramadevi
Department of Physics
Indian Institute of Technology- Bombay

Lecture – 07
Bound States - I

Summarizing whatever we did take stock of what we did for the particle in a box slowly getting onto bound states, many of these things you know but I am just trying to recap and get you onto the clarity of what we know okay. So, bound states as I said if the energy of the particle is less than potential at + ∞ and – ∞, then we will have these 1 dimensional bound state.

(Refer Slide Time: 01:03)

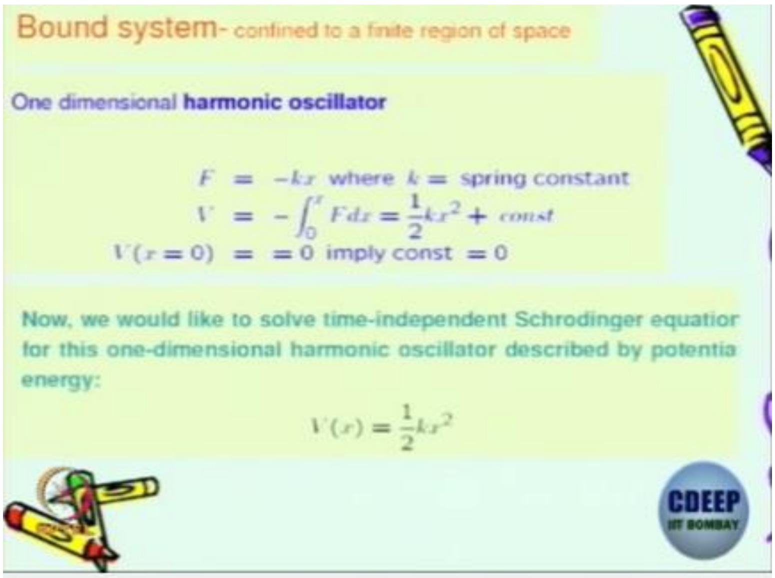


So, particle in a box definitely satisfies that condition right, everybody agrees, so it is a bound state solution, so all the solutions if we find the wave functions and the corresponding energy, they are all bound state solution, can you get scattering states in a particle in a box; yes or no; no, particle in a box, solutions are all bound state solution, okay and a couple of things which you would have mechanically done in the last semester or last year is taking the 2 wave functions, they are called orthonormal wave functions.

If they satisfy this property, I am confining myself to one dimensional potentials and they satisfy this property, this delta nm is the Kronecker delta, I assume everybody knows, if n = m, it is 1, if n ≠ m, it is going to be 0 and this is what we call it as the normalized function when n and m are equal, it is normalization condition and when n and m are not same, they have to be orthogonal.

So, this whole thing is called as an orthonormal condition or these wave functions, these stationary state solutions of the particle in a box are supposed to be called as orthonormal wave functions, if they satisfy this problem is that okay, so that is the definition and we always tried to do this, we always try to find a set of stationary states which are normalized and also orthogonal to each other for convenience.

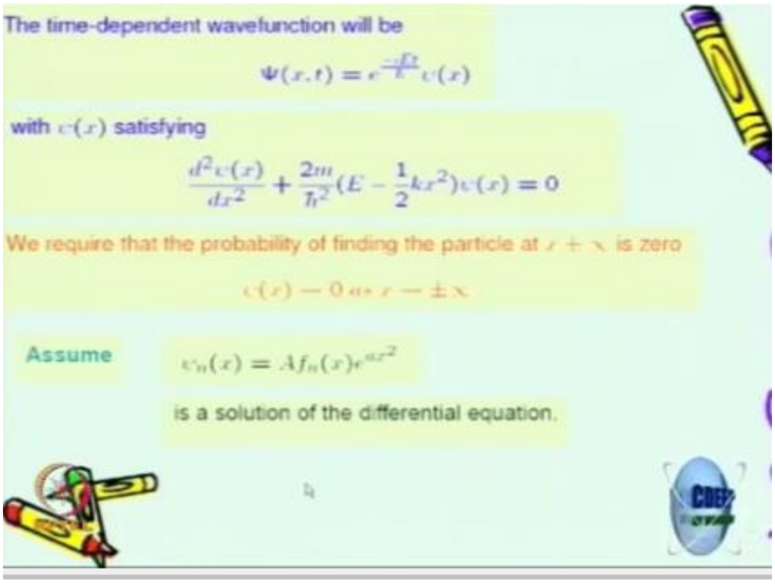
(Refer Slide Time: 03:05)



Because we write any arbitrary state as a linear superposition of these stationary states, okay, so this I did go through in the last lecture, I thought for continuity, let me put in here, so bound system is confined to a finite region and the familiar harmonic oscillator, where the force should be proportional to the displacement with the negative sign here, proportionality constant is a spring constant from which you can derive, what is the potential energy.

And putting in a boundary condition like x = 0, we want the potential to be 0, they will give you a potential energy to be $\frac{1}{2}kx^2$, okay, so we would like to solve the time independent Schrodinger equation for this one dimensional harmonic oscillator and this one also satisfies the boundary condition that V had + or – ∞, is infinity and your energy is always going to be < V at + ∞ and V at – ∞.

(Refer Slide Time: 04:01)

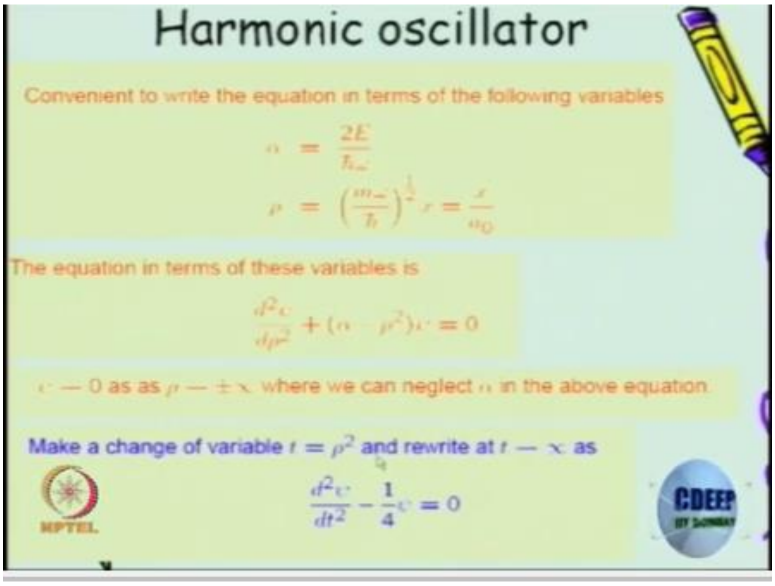


So, this one is also a bound state solution, okay, so since it is time independent potential energy, we can write the time dependent wave function with the appropriate energy of the stationary state multiplied, so how do we go about it? We try to substitute in the time independent Schrodinger equation and they also impose wave function to vanish as we go to the boundary which has + or – ∞, is that right.

So, we could formally assume a solution, which is you know which is having a some kind of an $f_n(x)e^{ax^2}$, it is just the formal solution, you can call it as a trial solution, you can try and find out whether it fits into the equation, so as of now let us assume that this trial wave solution, will allow us to fix what is the a value, what is the small a value? what is the capital A value?

What is the $f_n(x)$, where this n denotes the stationary states of energy E_n, okay, is that clear, okay. So, for n = 0, which is the lower state, we take $f_0(x)$ to be 1 and we want to verify whether this is an allowed solution, when we plug into this equation okay.

(Refer Slide Time: 05:35)



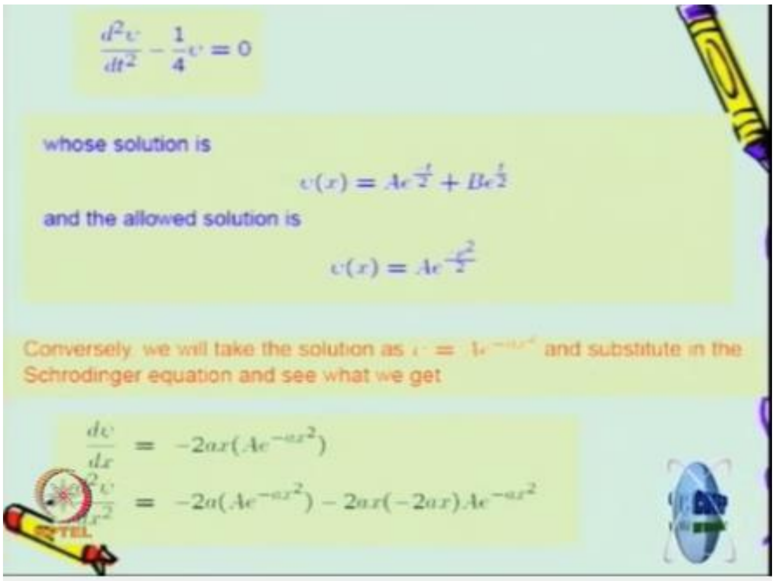
So, for convenience, just to make the equation look neater, we will redefine the energy to be proportional to α with these proportionality constant similarly, instead of x, we will put in a factor pre-multiplying it and call that to be P and also write x/a_0, where a_0 is this fact; a_0 is $\left(\frac{m\omega}{\hbar}\right)^{1/2}$. So, once you substitute into the time independent Schrodinger equation, please verify this in terms of the α variable and ρ variable, it looks in this simple form.

Please verify this from the previous slide here, it is e and also x, convert them into the ρ variable and instead of e, use the α variable and rewrite that equation, please do this okay, so the equation becomes simplified to be of this form, we are doing it for the lowest n =0, which we will call it as a ground state. So, now we will put in the boundary condition, what is the boundary condition?

Ψ vanishes as x tends to + or – ∞, which is also = ρ tending to + or – ∞, because the pre multiplying a_0 factor is just a constant factor, it is not x and you can also for convenience make another change of variable and make it look like your familiar equation, so our ρ tends to infinity, I can neglect α and rewrite in terms of another variable t, which I am calling it to be ρ^2.

Do not confuse this t with some time or anything, some other variable and rewrite it in terms of this variable t and take this is valid only for ρ tending to infinity and therefore, t should tend to infinity, okay, so this is not; this equation is the simplified equation when ρ is very large, you all agree because only when ρ is very large, I can ignore this α term, is that right. So, what is the solution to this equation, you have done this many times, right $e^{t/2}$, this is k squared is 1/4, right.

(Refer Slide Time: 08:08)

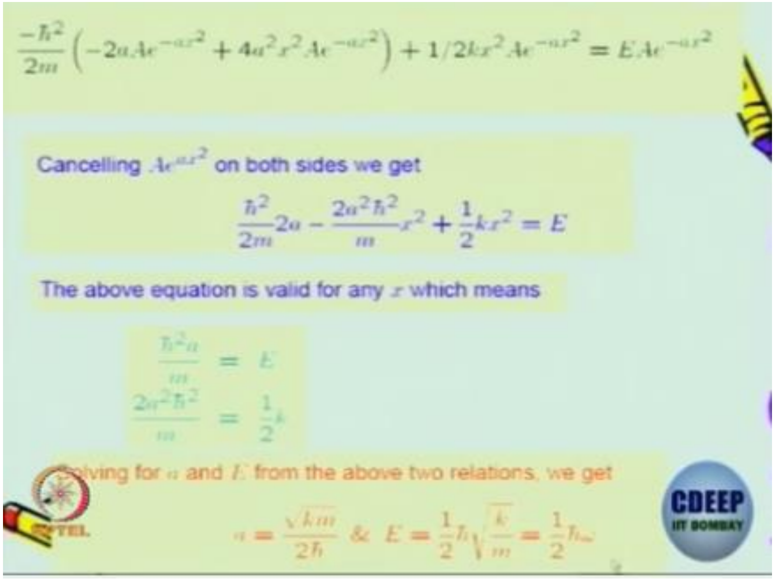


So, e^{kx}+ e^{-kx}, is that right, so the solution will be A $e^{-t/2}$+B $e^{t/2}$and out of this as t tends to infinity, which is allowed only the first term, so you have to put B = 0, right, so you get the allowed solution as $A\ e^{-\rho^2/2}$, so this is; this I have done with some kind of a trial solution putting into the equation and what is the trend when ρ is very large or x is very large?

I find the trend has to be this way and this is normalisable, from there you can find what is the normalization constant conversely, this you would have done in your first year course, you are given this wave function right, here we found the solution by looking at the time independent Schrodinger equation in the large role limit but instead you can assume this is a solution and substitute, right this you have done as far as I know.

What do you do; you substitute, take the derivative; again you take the double derivative because that is what is required in your time independent Schrodinger equation right.

(Refer Slide Time: 09:30)

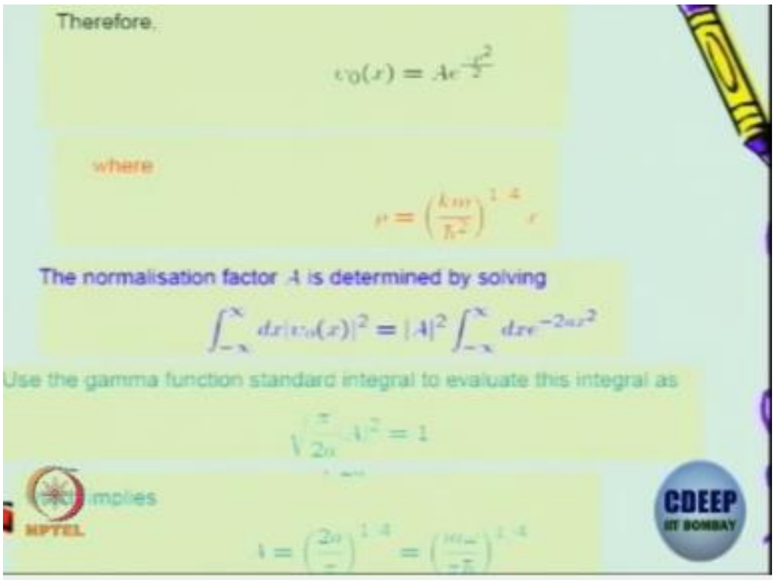


After you have done this, you have the time independent Schrodinger equation with this incorporated solution given to you to check whether it satisfies but this is what you get, then what do you do? Still not clear to me that this is a solution, how do I check that? You have to compare both sides for every power of x because this is valid for any x, so you should be able to compare left hand side and right hand side for every value of x.

E to the a x^2 anyway cancels throughout, you can remove it and compare powers of x on both sides okay, so from there what can we fixed; we can fix the small a, we can also fix the energy is that right, the term which is e, there are 2 x^2terms, the 2 x^2 terms can be set to 0, the sum of these 2 terms similarly, this is a constant independent of x, this should be equated to e, so do that.

Equate the constant term to e and equate the x squared term, this equal to this, so from there you can solve for what is A, small a and what is capital E and it turns out to be $\frac{1}{2}\hbar\omega$ and the a can be fixed to be this constant.

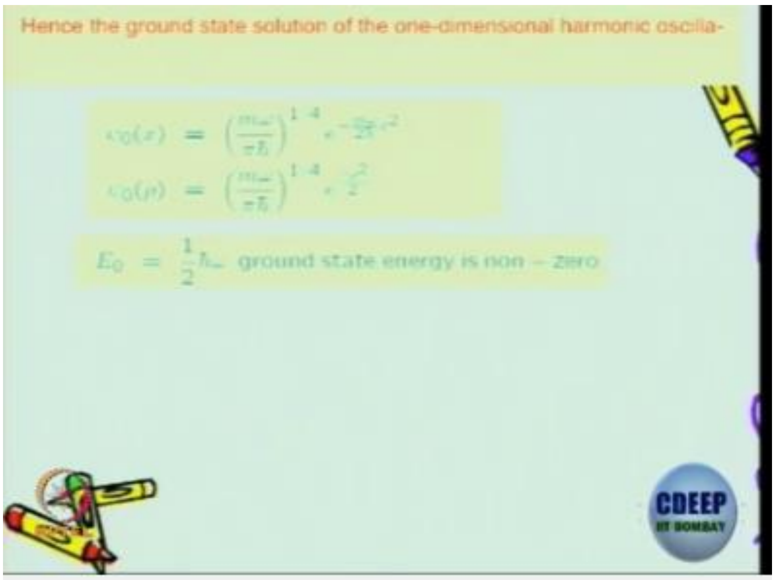
(Refer Slide Time: 11:12)



So, once you have this, you can write your most general solution, rewriting your x in terms of ρ as the solution, so I have given you 2 ways of finding the solution and we have verified that this is a valid solution okay, so ρ is up to those factors proportional to x and normalization condition will fix for you, what is the normalization factor, what is this integral going to give you? $\sqrt{\frac{\pi}{2\alpha}}$, right everybody knows the gamma function, can I assume, okay.

So that gamma function if you use, then you can fix the normalization condition, what $|a|^2$, is that okay, okay, so that is the normalization condition.

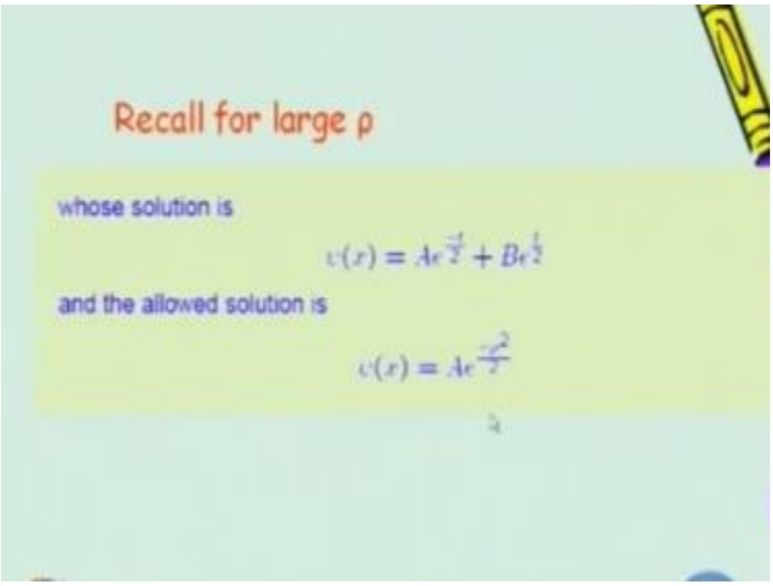
(Refer Slide Time: 12:11)



And this gives us a complete solution for the ground state $\Psi_0(x)$, you can rewrite it in terms of ρ for convenience but you can replace it back and rewrite it in terms of the physical x coordinate and there is a normalization factor, so E_0 is a ground state energy and unlike your classical physics, where if I ask you what is the ground state energy for a harmonic oscillator, you would have said it is 0, right, classical energy is 0.

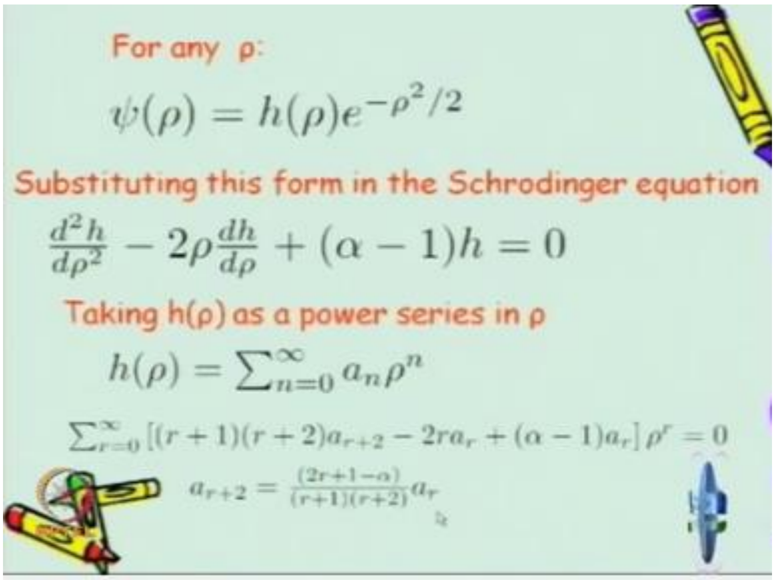
But quantum mechanics solving time independent Schrodinger equation, the lowest energy turns out to be non-zero, which is 1/2 $\hbar\omega$.

(Refer Slide Time: 13:01)



So, just to get you back to the time independent Schrodinger equation, they saw that for large ρ, you can try to simplify the equation and write the most general solution as this and taking t tending to infinity will force us to look at only ψ(x), which is $Ae^{-\rho^2/2}$, this we have seen as few transparencies behind, okay.

(Refer Slide Time: 13:31)



So, what is my aim? My aim is to try and find, so that is a trend for large ρ but for finite ρ for any ρ, I should be able to write my solution to the time independent Schrodinger equation, which we have not done, so far we have looked at the solution for large ρ and there was a trial solution also of the same form and we verified, we found the energy and the energy was $\frac{1}{2}\hbar\omega$.

Ideally, you should do the solution to the Schrodinger equation for any ρ, which we did not do, so lets us assume that the wave function which we have okay, is some function of ρ multiplying $e^{-\rho^2/2}$, later on we input what is ρ in terms of x that is just a matter of redefinition for convenience, we will work with the variable ρ, okay, you plug this into the time independent Schrodinger equation which is what we will do.

Substitute this in the time independent Schrodinger equation, α is proportional to energy looking at this, can we say what is the solution; it is not obvious, take go and look at the mathematical special functions, you can determine what the solution is but we would like to do this from first principles, how to find the solution. To do that what do we do; you had an exponential factor here, you would like to put this to be some kind of a polynomial function.

In principle, it could be an infinite series, call it as a Laurent series if you want, this is the most general h(ρ), I can think of taking in a polynomial form, so once I have this h(ρ) in this polynomial form, I plug this back into the simplified time independent Schrodinger equation where this factor got cancelled out throughout, right. Then, what do you get; you get kind of a series which are dependent on the coefficients, a_n's are the coefficients.

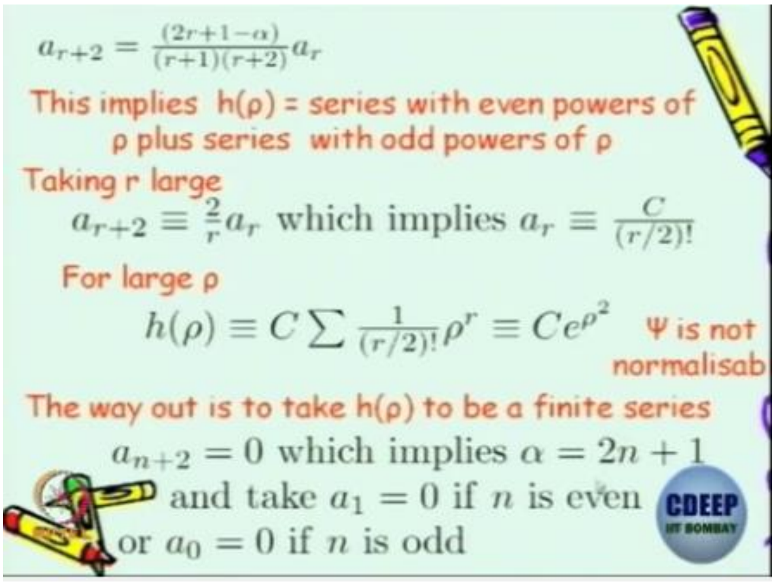
You get a series like this for every power of ρ, you can group the terms accordingly, please do the step, go from this step to this step by substituting $h(\rho)$, is substitute $h(\rho)$ and then for a particular ρ^r, group all the terms which I have written it in square bracket and then the r is running from 0 to infinity, why have I done this, what is the reason for doing this?

This should be the solution for arbitrary ρ, so that is bracket; square bracket coefficient should be 0 for every power of ρ, just like earlier we did comparing x independent and x^2 dependent term for a simplest $A\, e^{ax^2}$ now, we are going to do it for substituting in this which is a most general solution, valid for any ρ, so what are the things which you will have?

So, you can try to rewrite, if you see from this, this is always the square bracket involves coefficients which are in steps of only 2, okay so, this relation setting it to 0 will relate a_{r+2} in terms of a_r, okay, everybody is with me, is that right, you do not get a_{r+2} in terms of a_{r+1}, what does that tell us? I can split my $h(\rho)$ into 2 pieces, one involving odd powers, one involving even powers and the coefficients of even powers are related by this.

Similarly, the odd powers are related by this, when r is even, the coefficients are related by this with r being even and when r is odd, the coefficients are related by this, where r is odd.

(Refer Slide Time: 18:49)



Okay, so, this is the data we get by taking h(ρ) as a polynomial series plugging into the Schrodinger equation, we find that the coefficients are not independent, the coefficient of the respective powers; even powers or odd powers, they are related to the lower coefficients, with this factor which depends on α, α is proportional to energy, right that is the definition we had, okay.

So, what was the α proportional to? α is proportional to the energy okay, okay, so this I have already said that you can from this condition, you can write h(ρ) with series with even powers of ρ with the coefficients of the higher powers related to the lower coefficients and similarly, another series with odd powers of ρ, so do not confuse this r with any radial coordinate or position, this r is the subscript r in the coefficients which are there in the power series which we wrote for h(ρ), okay, a subscript r.

Let us take r; this subscript r to be very large, if I take r to be very large, then this r is very large, you can ignore these constants and you will end up saying that when the coefficients of large subscript r, they will be related to the lower coefficients by 2 over r. My aim is to find the solution that is why I am trying to do from first principle rather than looking at the Schrodinger equation and going and looking at the mathematician's literature to find the solution.

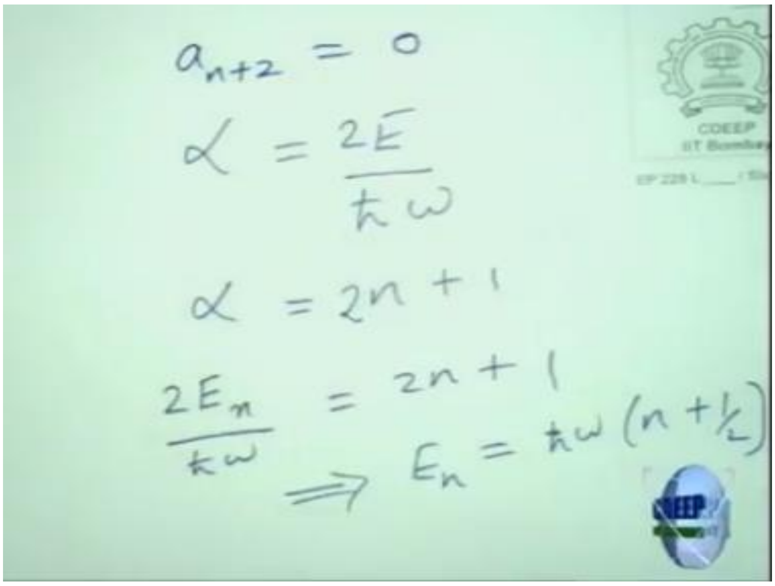
I am not doing that I am giving you a way in which we can try to actually find the solution by taking a general power series h(ρ) times $e^{-\rho^2/2}$ and $e^{-\rho^2/2}$ happened for large ρ in the Schrodinger equation we saw it, is that okay, so then what next? You have to; this solution should also be a valid solution for large ρ when you take ρ to be large, the an coefficients, the dominant contribution will come from an square n is very large, right, is that right.

So, for large ρ, you can approximate h(ρ), it is not exactly equal, by taking this a_r, this you can do only for large ρ because the dominant contribution will come from those coefficients, so you can approximate h(ρ) for large ρ to look like Ce^{ρ^2} , is this allowed; is this allowed, is when ρ tends to infinity, blows up, so it is not allowed right, you all agree.

So, what is the way out of this, how? So, this is not allowed, if I am getting stuck if I take an infinite series polynomial solution for h(ρ), let us work with finite series polynomial solution that is the only way I can avoid my wave function not to blow okay, so this is not normalizable, the way out is to take h(ρ) to be a finite series but how finite you should take?

Whatever finite you want to take that means, at some point you have to put this coefficient for some specific part to be 0 that is the meaning of saying, it is a finite series, once you put that to be 0, then by this relation; recursion relation, all the higher powers will be 0, so let us put an + 2 to be 0, once I put an + 2 to be 0, then the only way this will be 0 is that α will be = 2n + 1.

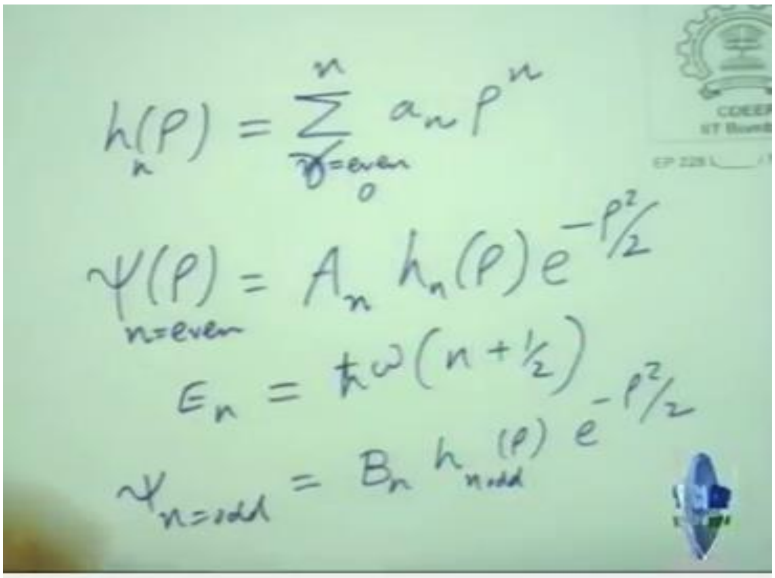
(Refer Slide Time: 24:09)



Once I get α = 2n + 1, can somebody tell me what will be the energy, so what is α? ${2E}/{\omega\hbar}$, right and α is n + 1, α is 2n + 1, so then E; let me put the E to be a subscript n now, $\frac{2E_n}{\hbar\omega}$ is 2n + 1, so which implies $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ so, the solution is to take if one normalizable solutions, infinite series for h (ρ) will not work, finite series will work.

And I can truncate wherever I want, okay by putting an appropriate n here, I started with an + 2 = 0, so what is the solution?

(Refer Slide Time: 25:27)



The solution is h(ρ) will be summation over n even from 0 to some specific value, so let me write it as r_0 to n, so you take it only in steps of even numbers an ρ^n, so that your ψ(ρ) is some normalization constant, let me call it as ψ_n, $h_n(\rho)$ $e^{-\rho^2/2}$ and the corresponding E_n is

$\hbar\omega\left(n+\frac{1}{2}\right)$. I have still not written these a_n's but I have given you a recursion relation here from which you can determine what is an in terms of a n - 2 and so on okay.

So, this is one possible solution, another possible solution is n could be odd, okay and you can write another solution where, so this is n is even, we can also have a similar solution for n = odd but the h_n series will involve only odd bounds, okay, so these are the possible solutions whose power series; finite power series can be determined also from the time independent Schrodinger equation and you can go and compare with the special functions literature, okay.

This is one route a person who does not know what is the solution to the complicated differential equation can actually do it this way, so the solution for the nth state, where n is even implies that the corresponding energy is this and you can set the odd powers, the lowest odd power to be 0, once you put the lowest odd power to be 0, by this recursion relation, odd powers do not show up at all, right.

And or you can do for the n odd where you can put the lowest even power to be 0, which is the ac, okay so those are the 2 solutions which I have written n is odd and n is even, okay.