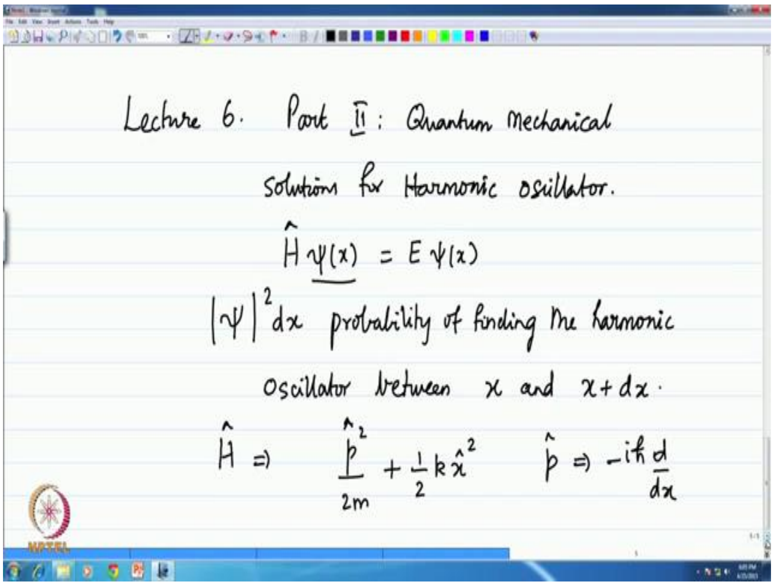
Introductory Quantum Mechanics and Spectroscopy
Prof. Mangala Sunder Krishnan
Department of Chemistry
Indian Institute of Technology, Madras

Lecture - 6
Part II

Quantum Mechanical solution for Harmonic Oscillator

In this segment, let us look at the solutions for the harmonic oscillator using the quantum mechanical methods.

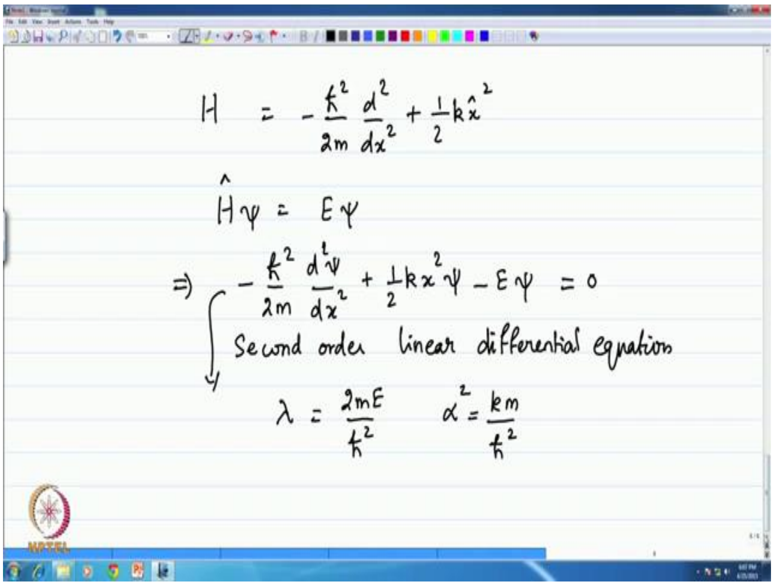
(Refer Slide Time: 00:24)



And the solution of the Schrodinger equation, time independent H psi x is equal to E psi x. The x is the position coordinate for the harmonic oscillator motion and the wave function is, a wave function is a function associated with the harmonic oscillator. And it has the same probability interpretation as you have with the particle in a one-dimensional box, namely psi square dx, represents the probability of finding the harmonic oscillator between x and x plus dx, x and x plus dx.

The H is, of course, the Hamiltonian operator and the Hamiltonian operator in quantum mechanics is obtained from the classical Hamiltonian, which is p square by 2 m by changing the momentum to the operator and also half k x square, where x is the position operator. In quantum mechanics, of course, in this case p is to be replaced by the standard representation in coordinate with the derivative minus H bar d by dx. It is one-dimension, so we do not need the partial derivative.

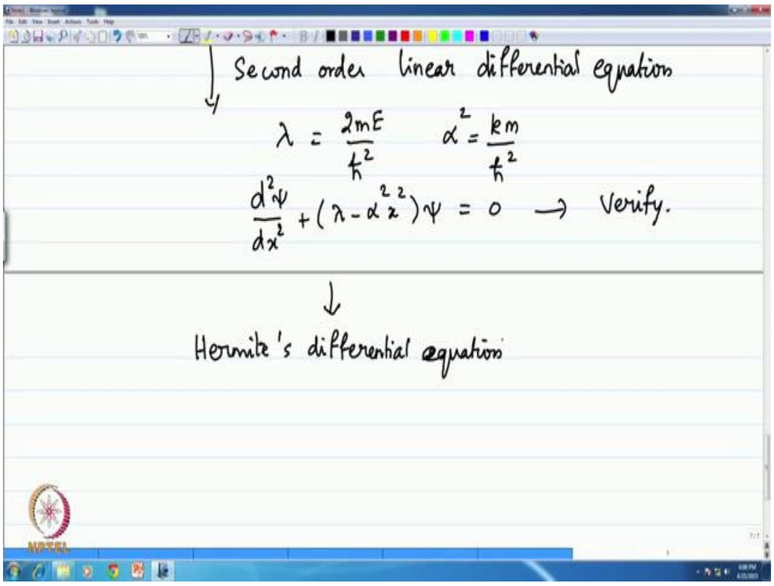
(Refer Slide Time: 02:27)



It is h bar d by dx, which leads to immediately this formula, namely h is minus h bar square by 2 m d square by dx square, as you had it in the particle in the one-dimensional box with half k x square, which is the potential energy associated with the harmonic oscillator. Therefore, the solution that you have to obtain is the solution, that H psi is equal to E psi, sorry, no cap on the psi, is equal to E psi, is the solution of the differential equation, namely minus h bar square by 2 m d square psi by d x square plus half k x square psi minus E psi is equal to 0. So, second order linear differential equation.

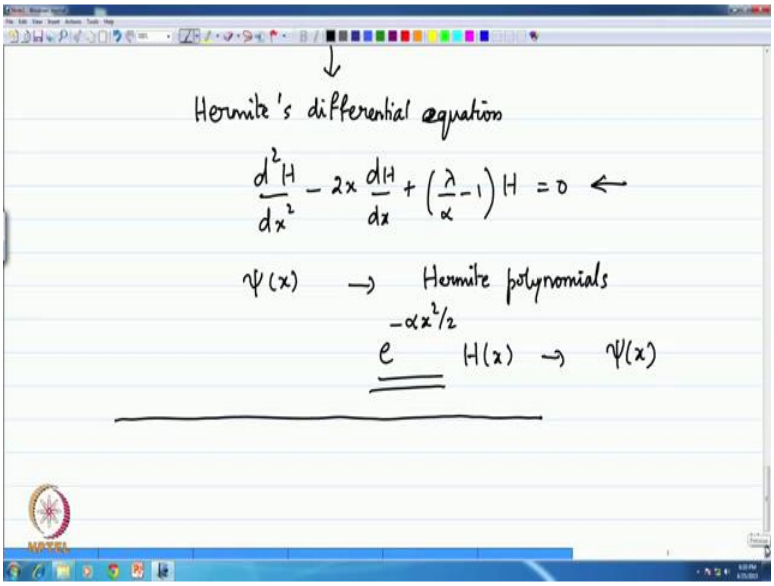
This lecture will not tell you how to solve a differential equation, but it will tell you, that if you rewrite this by introducing a simple parameter, say for example, lambda is equal to 2mE by h bar square and another constant alpha or alpha square as km by h bar square.

(Refer Slide Time: 04:19)



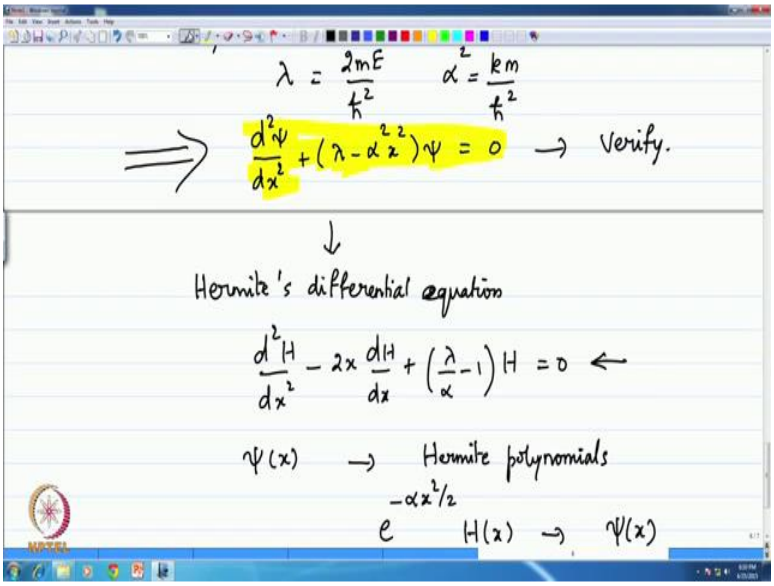
If you introduce two new constants, then it is possible for you to write the differential equation as d square psi by d x square plus lambda minus alpha square x square psi is equal to 0. I think, verify, this will be one of the items for you to check. It is possible to transform this into what is known as the Hermite's differential equation for which solutions have been known for more than hundred years when this itself was proposed.

(Refer Slide Time: 05:12)



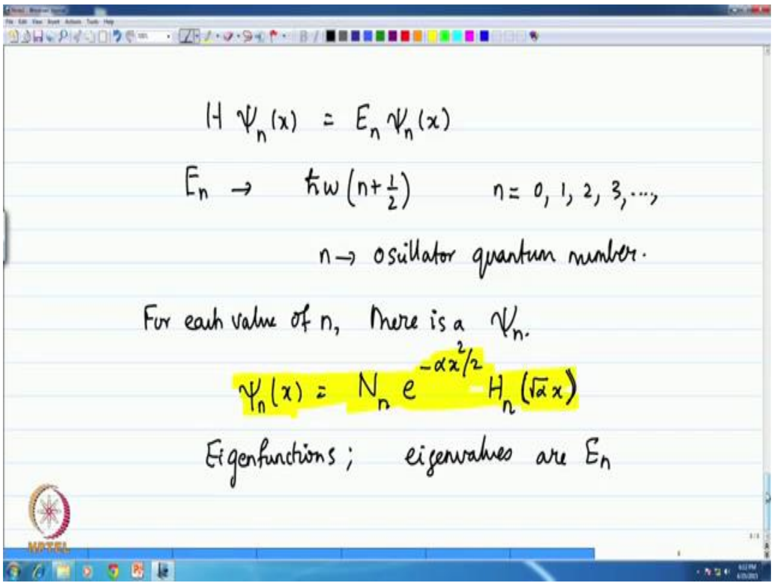
In fact, the Hermite differential equation, let we write that down, the Hermite differential equation is d square H, the Hermite function d x square minus 2 x dH by dx plus lambda by alpha minus 1 H is equal to 0. Now, I just pulled this out of nowhere, but it does not matter. What is important is the wave function psi are going to be associated with what are known as the Hermite functions or Hermite polynomials and will also have a component called the Gaussian, which is e to the minus alpha x square by 2.

(Refer Slide Time: 06:44)



This Gaussian and the Hermite polynomial x will determine the solutions of the harmonic oscillator. The mathematics is involved, we do not need to worry about it. What I would do is to right down directly the solution of this equation, which you have here, this equation and then we will only examine the nature of the solutions and the consequences of the solutions rather than solving the differential equation itself. This can be referred to at a later time.

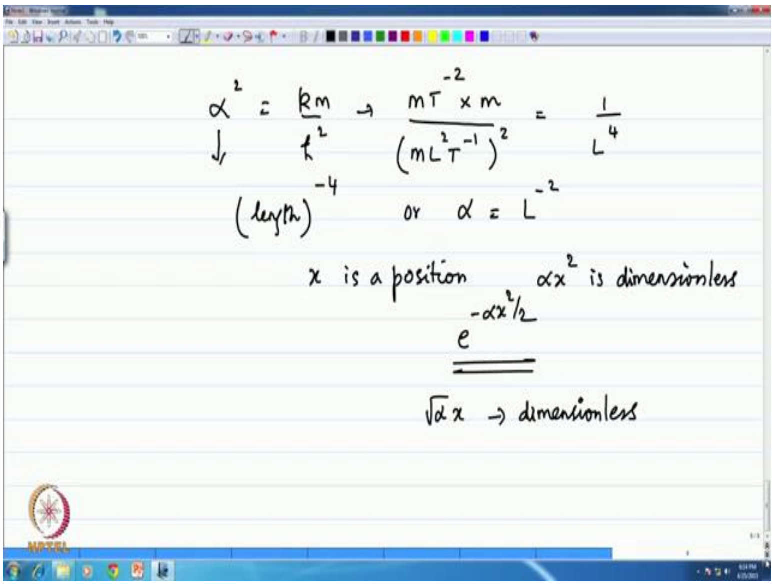
(Refer Slide Time: 07:29)



So, what are the solutions for the harmonic oscillator? First of all, there are an infinity of solutions. H psi n of x is equal to E n psi n of x and the formula for E n turns out to be, when you have solved the Schrodinger equation, E n is h bar omega times n plus half and n is the quantum number, which can take values 0, 1, 2 to infinity, n is the oscillator quantum number. And for each value of n there is a psi n, there is a wave function psi n.

The general formula for psi n, when you do the mathematics is given by a normalization constant, which also depends on this quantum neuber n and an exponential of minus alpha x square by 2 times the hermite polynomials H n root alpha x. This is, these are the solutions or in whatever we have described so far. These are also known as the Eigen functions of the harmonic oscillator, Hamiltonian. The Eigen values are E n, E n.

(Refer Slide Time: 09:44)

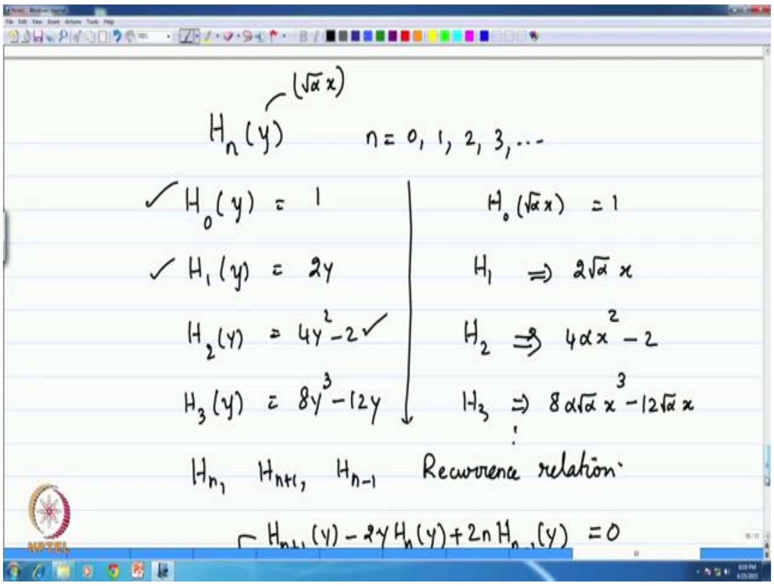


Go back and look at the constants alpha and lambda. Alpha square is km by h bar square, alpha square is km by h bar square; k is the force constant, which is mass T to the minus 2 multiplied by mass, m, and h bar is mass length square T to the minus 1, but it is a square. So, what you have is, 1 by L to the power 4.

Therefore, alpha square has the unit length raise to minus 4 or alpha has the dimension, I mean, alpha square has the dimension of length to the minus 4 and alpha has the dimensional of L to the minus 2. That should make sense because x is a position and therefore, it is also the length from the equilibrium, a distance from the equilibrium. Therefore, you see, that alpha x square is dimensionless, otherwise e to the minus alpha x square by 2 does not make sense.

So, the constants have been chosen to get some of these physical parameters clear and the Hermite polynomial, which is the function of position, is multiplied by square root of alpha. And you can see that square root of alpha is length inverse, length inverse, therefore, square root of alpha x is also dimensionless, so that you can add various powers.

(Refer Slide Time: 11:45)

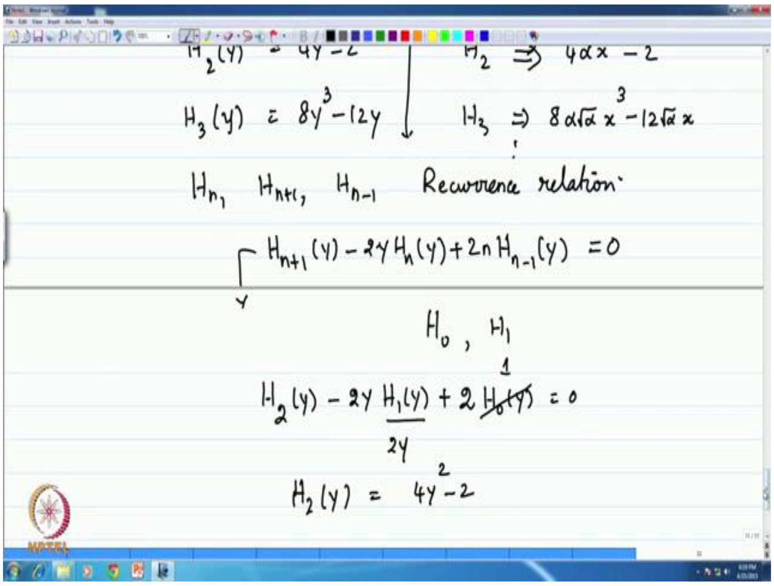


The Hermite polynomials or solution of what is known as the Hermite equation, which I wrote down earlier and the Hermite polynomials are defined for various values of, so let me write H and y. If I put the argument as y instead of root alpha x, y is root alpha x. In this case, if I write H and y and n equal to 0, 1, 2, 3, etcetera, then the result is already known, namely, H 0 of y is 1, H 1 of y is 2 y, H 2 of y is 4 y square minus 2, H 3 of y is equal to 8 y cube minus 12 y and so on.

So, if you write this in terms of root alpha, x is not root alpha, x is 1, H 1 is 2 root alpha x, H 2 is 4 alpha x square minus 2 and H 3 is 8 root alpha, no alpha root ((Refer Time 13:09)), that is, it is alpha to the 3 by 2 x cube minus 12 root alpha x and so on, ok.

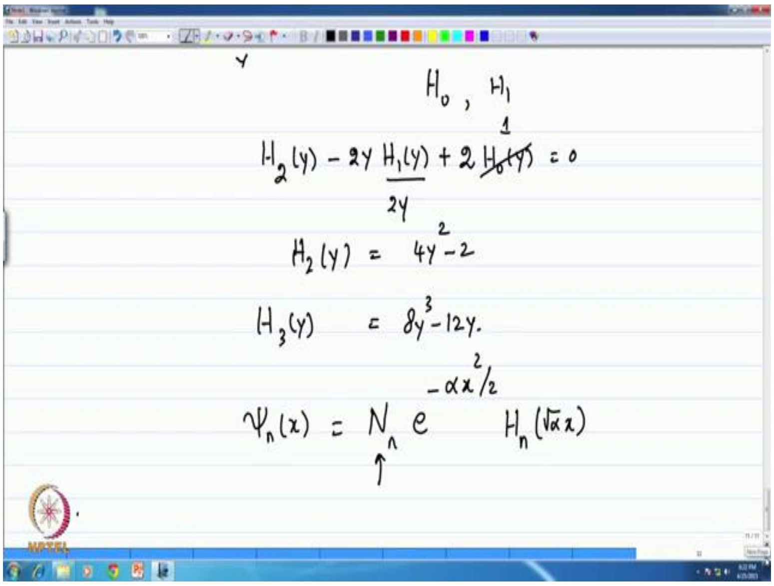
There are the relations that the polynomial satisfy between H n, H n plus 1 and H n minus 1. There is a relation called recurrence relation. Stop for a minute, ((Refer Time: 13:43)). The recurrence relation between these is also known. Mathematic, in mathematics it is H n plus 1 of y minus 2 y H n of y plus 2 n H n minus 1 of y is equal to 0.

(Refer Slide Time: 14:16)



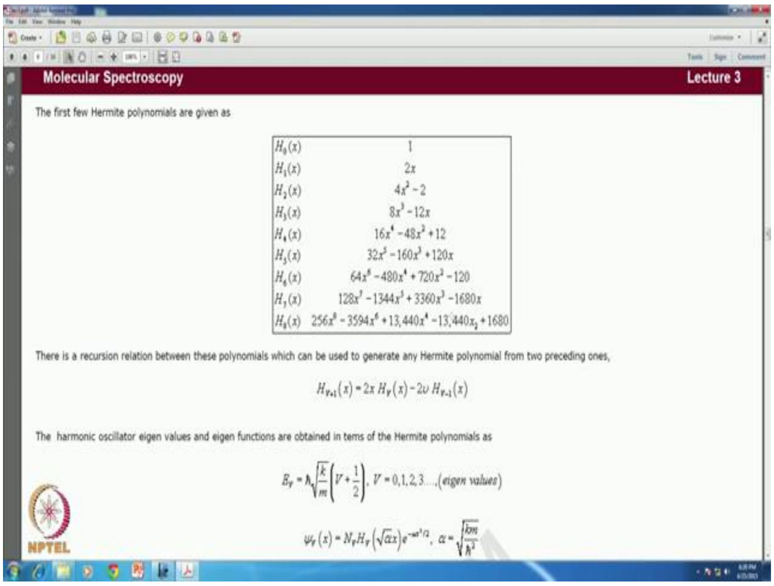
What this tells you is, to obtain harmonic oscillators for higher values, I mean larger values of n from, the harmonic oscillator, the hermite polynomials for smaller values. For example, H 0 and H 1, if you know, then you can calculate H 2 of y minus 2 y, H 1 of y plus 2, since n is 1 this is 2. H 0 of y that is equal to 0 and this is 1 and H 1 of y is known as 2 y. Therefore, you see, H 2 of y is 4 y square minus 2, which is what I had written down earlier, see that.

(Refer Slide Time: 15:28)



So, if you knew H 0 and H 1 from mathematics and also from the recurrence relation, if you know the recurrence relation, then in principle, we can calculate any Hermite polynomial H n from the previous two Hermite polynomials. And so, one exercise would be to show, that H 3 of y is equal to 8 y cube minus 12 y and so on. So, one can reproduce these tables and let me just show you from one of the lectures, that I have had earlier.

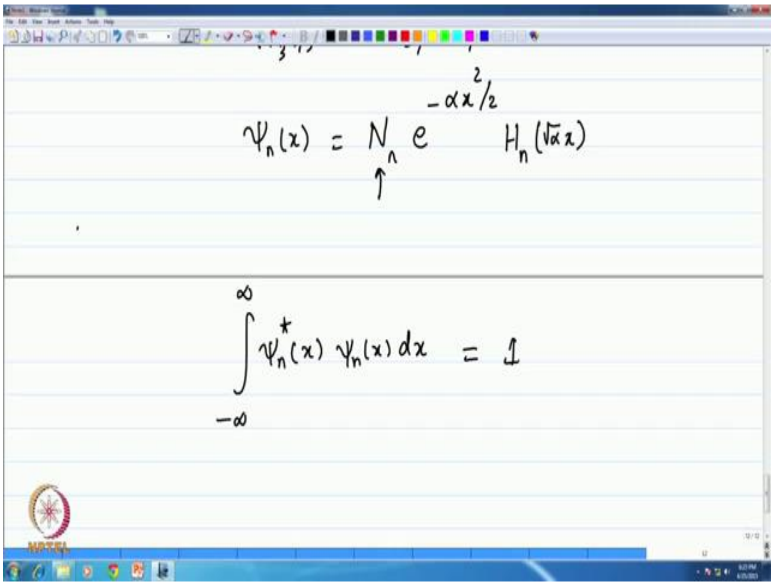
(Refer Slide Time: 15:54)



One can see the table here for various values of the Hermite polynomials. In this table, of course, y and x have been interchanged. You can see, that H naught of x and one can go on and calculate H naught, H 1, H 2 and what you see here is up to H 8. One thing, that should be noted is, that the even numbered polynomials 0, 4, 4, 6, 8 are all even function of x. H 0 of x is 1, H 2 of x is 4 x square minus 2, which does not change if x is negative or positive and is minus x or plus x. H 4 of x is again, is x raise to 4 x square. Therefore, it is an even function of x. H 6 of x is even.

Therefore, the Hermite polynomial also give us a series of functions, which are odd or even depending on whether the quantum number associated with the harmonic oscillator problem is odd or even. This is something that we have to remember when we do some of the computations regarding probabilities and average values using harmonic oscillator Eigen functions.

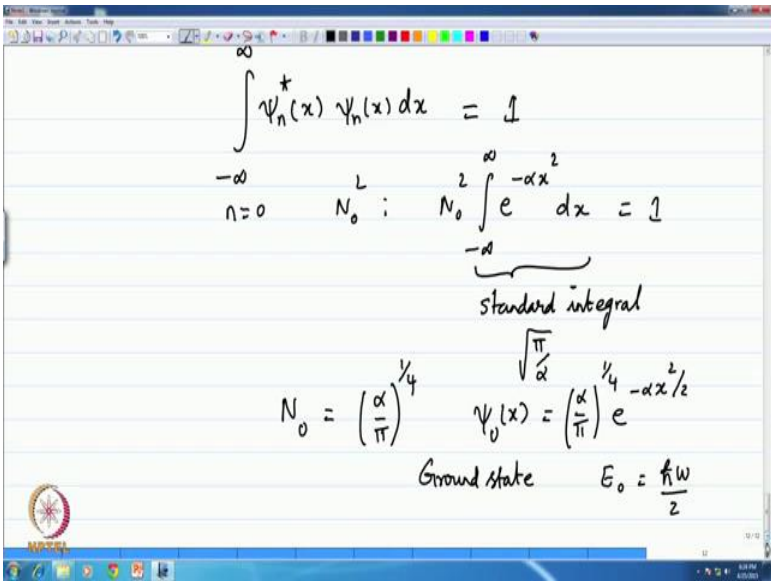
(Refer Slide Time: 17:48)



So, let me summarize this with the only other thing, that I have not yet mentioned, namely, if we write psi N of x as a normalization constant N and an exponential e to the minus alpha x square by 2 multiplied by the Hermite polynomial H n of root alpha x. The one more unknown quantity that we have is the normalization constant, and of course N is such that the integrals psi and star, which in this case is same as psi n of x psi n x dx between the limits minus infinity to plus infinity, because the harmonic oscillator position coordinate can go the negative direction as well as in the positive direction.

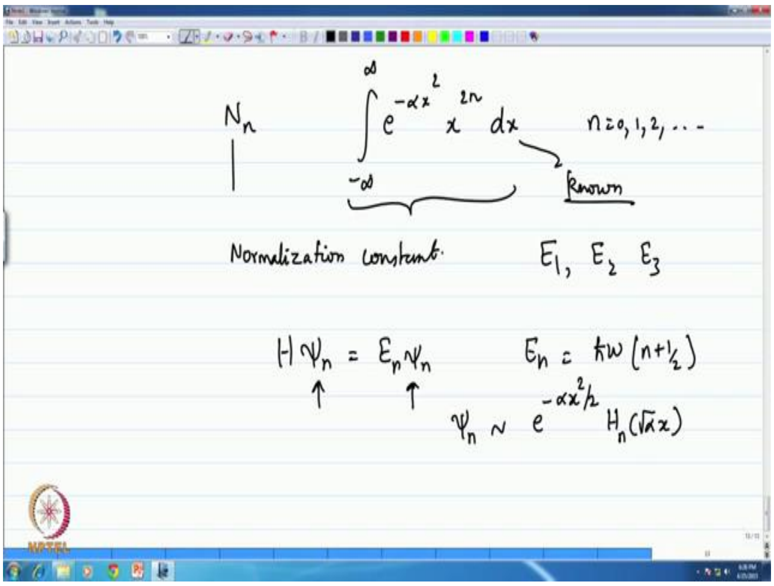
And if you take the theoretical limit, that the x can go all the way to minus infinity and to plus infinity when the normalization constant requires this condition, namely, can be obtained from this condition, namely psi star n of x psi n of x dx is 1, which for n equal to 0.

(Refer Slide Time: 18:35)



For example, if you want to know what the N 0 square is that is obtained as follows, namely, N 0 square integral e to the minus alpha x square dx between minus infinity to plus infinity is 1, because the Hermite polynomial for n equal to 0 is 1. And this is a standard integral, its value is known. This integral is root pi over alpha, therefore the harmonic oscillator normalization constant N 0 is alpha over pi to 1 by 4. Thus psi 0, what is called ground state wave function, are the lowest energy solution. E 0 is h bar omega by 2, because n plus a half will give you only half. n is 0, 0 is h bar omega by 2 and psi 0 of x is alpha by pi to 1 by 4 e to the minus alpha x square by 2.

(Refer Slide Time: 19:59)



In a similar fashion one can calculate any n by having the normalization constant evaluated using these types of integral, e to the minus alpha x square x raise to 2 n minus infinity to plus infinity dx. If you know the value of this integral for all values n equal to 0, 1, 2, 3 etcetera, then it is possible for you to calculate any normalization constant N n.

In some of the problems and quizzes that follow this lecture, I would suggest that you calculate these constants for the first excited state are the first, the second energy state like E 1, E 2, E 3, etcetera. You can easily calculate this are using simple integral formulas and this integral is not from integral tables. You can also calculate this using elementary integration.

So, the solution is therefore, H psi n is equal to E n psi n are given as h bar omega n plus half for the E and the psi n as exponential minus alpha x square by 2 H n of root alpha x. In the next part, we will see what these things mean in terms of a pictorial representation, and also what the probabilities and an important concept known as the zero point energy.

Thank you.