Fundamentals of Spectroscopy
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Lecture-30
Harmonic Oscillator Eigenvalues and Eigenfuctions-II

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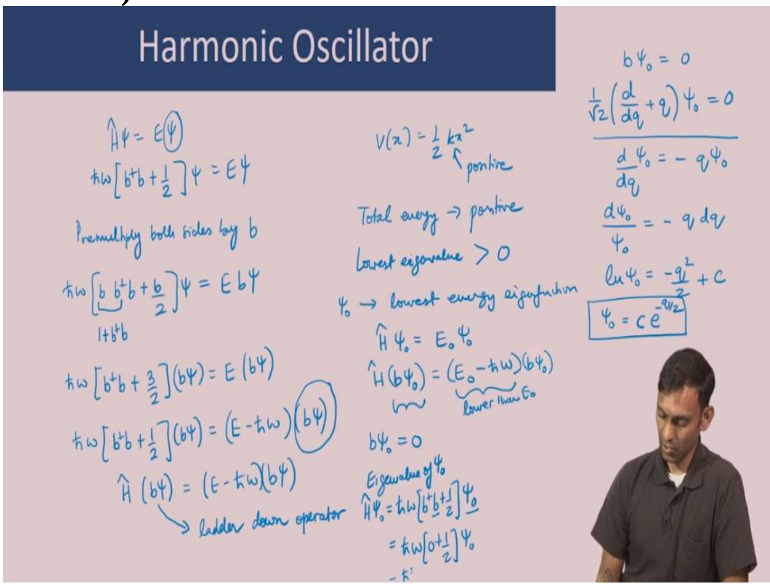

To get insight on the functional form of the eigenfunctions and the precise energies let us now again start with the Schrodinger equation, it is psi = E psi, but now pre multiply the equation on both sides by b instead of b dagger. So the Schrodinger equation is h bar omega b dagger b + half psi = E psi and we pre multiply both sides of the equation by the operator b. This gives h bar omega b b dagger b + b / 2 psi = E times b of psi, we want to make the left hand side of this equation look like the Hamiltonian.

We now use the commutation relation and write this bb dagger as 1 + b dagger b. So, this becomes h bar omega b dagger b + 3 / 2 and we write the b psi outside is equal to E times b psi. And if we make the operator on the left hand side look like the Hamiltonian operator, then we get h bar omega b dagger b + half b of psi = E - h bar omega b of psi. So, we see that if psi is an eigenfunction of the Hamiltonian, then b of psi is also an eigenfunction of the Hamiltonian.

Because here we have h of b of psi = E - h bar omega b of psi, but, the b of psi has an eigenvalue which is less than the eigenvalue of psi / h bar omega. This operator b acts on an eigenfunction of the Hamiltonian and gives a new eigenfunction with eigenvalue lower by h bar omega. And since this lowers the energy, it is called the ladder down operator we now make an argument that for a harmonic oscillator with potential energy v of x = half k x square.

Where k is positive the total energy is thus positive and this implies that the lowest eigenvalue of the Hamiltonian must be greater than 0. So, the eigenvalues are have a lower bound and all values are greater than that lower bound. Now suppose that psi 0 is the lowest energy eigenfunction. So, H of psi 0 is let us say E 0 times psi 0 and we have seen that b of psi 0 is also an eigenfunction of the Hamiltonian with an eigenvalue E 0 - h bar, omega. So, that implies that there is another eigenfunction which has energy lower than E 0.

So, there is a contradiction here on the one hand we are saying that psi 0 is the lowest energy eigenfunction and on the other hand, there seems to be another eigenfunction b of psi 0, which is having an energy lower than E 0 this contradiction can be resolved and this equation can be satisfied if b psi 0 = 0 b psi 0 = 0 implies that one over square root of 2, I am just writing the definition of the operator b here this is equal to 0.

So, psi 0 satisfies the following equation here. And this implies that d / dq of psi 0 = - q times psi 0, this is a differential equation for psi 0 and to solve it, we can take d psi 0 / psi 0 so we do a separation of variables is equal to - qdq integrating this equation gives ln of psi 0 = - q square / 2 plus a constant of integration, which implies that psi 0 is equal to some Constant e to the power of - q square / 2.

So, this gives us a functional form for the lowest eigenfunction of the harmonic oscillator Hamiltonian. Furthermore, the eigenvalue of psi 0 the lowest eigenfunction is h of psi 0 = h bar omega the Hamiltonian b dagger b + half times psi 0 and we have seen that be operating on psi 0 = 0. So, that is h bar omega 0 + half psi 0. So, the eigenvalue is simply h bar omega / 2 times psi 0 and the eigenvalue is simply h bar omega / 2.

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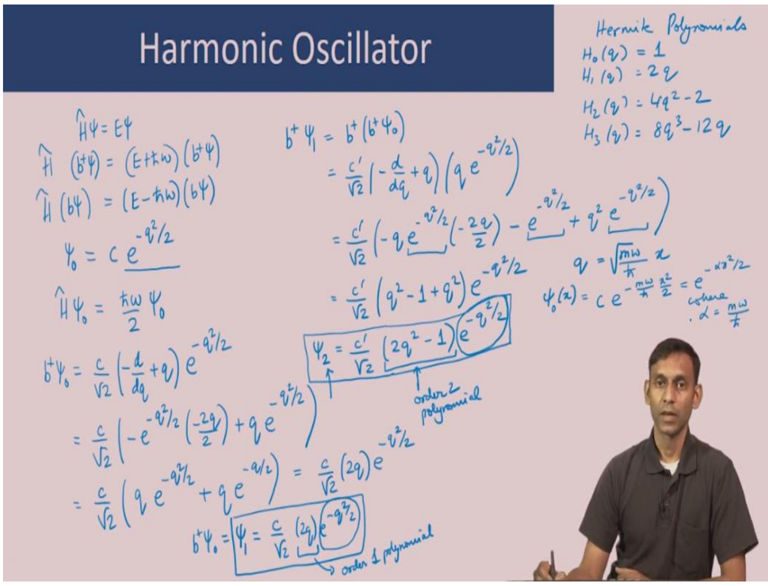

So far we have seen that if psi is an eigenfunction of the harmonic oscillator Hamiltonian, then b dagger psi is also an eigenfunction with eigenvalue e + h bar omega. And we have seen that b of psi is also an eigenfunction with a lower eigenvalue e - h bar omega. Moreover, we have seen that the lowest eigenfunction has the functional form c e to the power of - q square / 2 and this has an eigenvalue 8 psi 0 = h bar omega / 2 psi 0.

The question now is what is the functional form of the other eigenfunction besides the lowest eigenfunction of the harmonic oscillator and for this we can operate with the ladder up operator on the lowest eigenfunction of the harmonic oscillator and get all the other eigenfunctions. So, let us do that now. So, we operate with b dagger on the lowest eigenfunction psi 0.

And we write this explicitly, c is the constant associated with the psi 0 and the square root of 2 is part of the b dagger operator d / dq / q e to the power of - q square / 2. And when we take the derivative and write this, we get c over square root of 2 - e to the power of - q square / 2 - 2q / 2 + q times e to the power of - q square / 2 and on simplifying this becomes c over square root of 2q e to the power of - q square / 2 + q e to the power of - q square / 2.

Which is c over square root of 2 2q multiplied / e to the power of - q square by to the functional form for the first excited eigenfunction, b dagger psi 0, we can write this as psi 1 is does c over square root of 2 2q e to the power of - q square / 2. Let us find the next higher eigenfunction and for that we operate with the b dagger operator on psi 1 that is in other words b dagger on b dagger of psi 0. And that is some c prime / square root of 2 - d / dq + q, operating on q times e to the power of - q square / 2.

That is equal to c prime / square root of 2 - q e to the power of - q square / 2 - 2q / 2 - e square e to the power of - q square / 2 + q square e to the power of - q square / 2 we take e to the power of - q square / 2 common because this is there in all the terms and then this becomes c prime / square root of 2 q square - 1 + q square e to the power of - q square / 2, and that gives c prime / square root of 2 2q square - 1 e to the power of - q square / 2.

And this is the functional form of psi 2, or the second excited state of the harmonic oscillator. We notice that the eigenfunctions of the harmonic oscillator have certain pattern in their functional form. So if you look at psi 0, first, you see that this is simply the Gaussian function e to the power of - q square / 2 the psi 1 here is a Gaussian function e to the power - q square / 2 multiplied by a polynomial 2q.

And again, if you look at to it is again the Gaussian function e to the power of - q square / 2 multiplied by another by another polynomial and the order of the polynomial is equal to the quantum number of the function. So, the psi 2 has a polynomial of order 2 and the psi 1 has a polynomial of order 1 and the psi 0 has a 0 order polynomial or just a constant multiplying the Gaussian function.

The polynomials which are part of the functional form of the harmonic oscillator eigenfunctions are called her meet polynomials and some of the lower ones have the following functional forms. So, H 0 of q is just 1 H 1 of q = 2q H 2 of q = 4q square - 2, H 3 of q = 8q cube - 12q. And these forms of the Hemite polynomials can be very easily looked up in any textbook on spectroscopy or quantum mechanics.

The last thing to remember is that the variable q, which is the dimension this coordinate was introduced by us to simplify the derivation and q is actually related to x in the following manner h bar x. So, all of these functional forms are actually functions of x psi of x. And for example, the lowest eigenfunction psi 0 of x would become c e to the power of - m omega / h bar x square / 2, when we write it in terms of x by replacing q with x, this can be further simplified as c e to the power of - alpha x square / 2, where alpha = m omega / h bar in terms of k the alpha is equal to square root of km / h bar.

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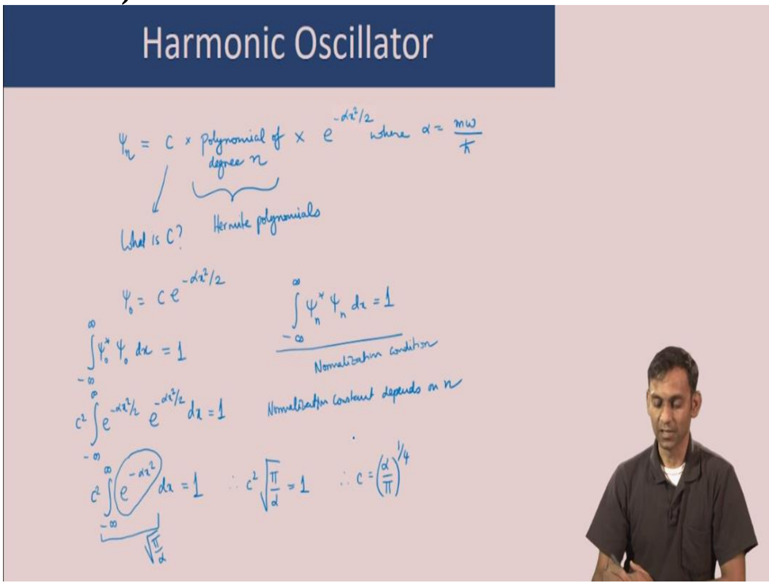

The eigenfunctions of the harmonic oscillator Hamiltonian have the following functional form. So, if you take the eigenfunction, this is some constant multiplied by a polynomial of degree n multiplied by the Gaussian function e to the power of - alpha x square / 2, where alpha = m omega / h bar, we have seen that this polynomial of degree in are the Hermite polynomials and we have looked at the functional forms of some of these.

Now, the question is what is this constant C? Now, the C just comes from the normalisation of the eigenfunction. So, for example, let us do this for the lowest eigenfunction. So, the lowest eigenfunction is psi 0 = c e to the power of – alpha x square / 2 and to get C we impose the normalization condition that is psi 0 star psi 0 dx limits from - infinity to infinity = 1. This implies that c square - infinity to infinity e to the power of - alpha x square / 2 multiplied / e to the power of - alpha x square / 2 dx = 1.

And that means c square - infinity to infinity e to the power of - alpha x square dx = 1. The function here is just the Gaussian function and the integral of this from - infinity to infinity is a standard integral with value square root of pi over alpha. So, therefore, c square times square root of pi divided by alpha = 1 and this implies that c = alpha divided by pi to the power of 1 / 4.

The normalisation condition for all other eigenfunctions can be similarly found and they in general depend on the quantum number of the eigenfunction, but the condition to normalise them is always the same, which is minus infinity to infinity psi n star psi n dx = 1, this is the normalisation condition. The normalisation constant depends on N and can be found by applying this condition.

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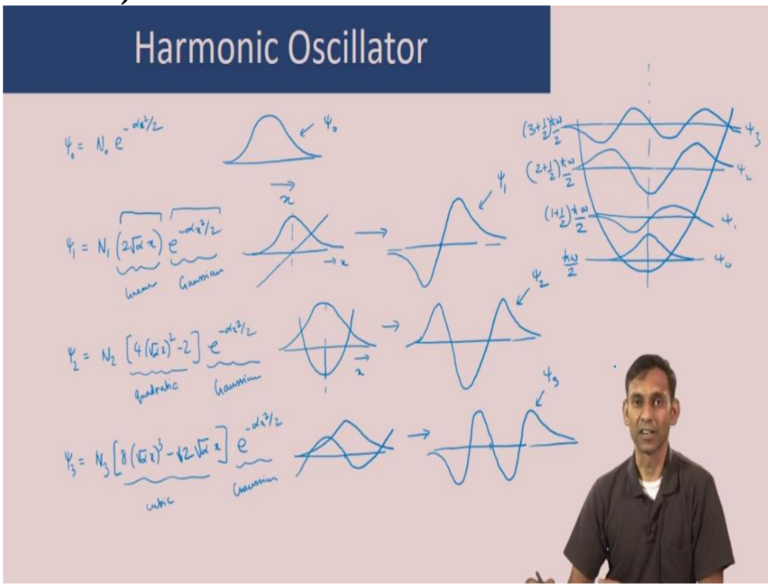

We will now look at the shapes of some of the lowest eigenfunctions of the harmonic oscillator. So, let us start with the lowest eigenfunction psi 0, which is a normalisation and N 0 e to the power of - alpha x square / 2, N 0 is a constant, which we can obtain by using the normalisation condition that we discussed. The functional form of this function is just the Gaussian function. So, if this is the x axis, then the function has the typical Gaussian shape like this. So, this is how psi 0 looks.

Let us look at the first excited vibration wave function. That is psi 1 is equal to the normalisation constant multiplied / 2 root alpha x e to the power of - alpha x square / 2. We note here that this is a function which is a product of 2 functions. This is a linear function. And this is a Gaussian function. So if we were to plot these, here is the x axis, the linear function is a straight line this 2 root of alpha x is just a straight line like this. And the Gaussian function, which is the second part, is a function like this.

And if you take the product of these 2 functions, then we get a function which looks like this which has 0 value at x = 0 and it has a negative value first and a positive value, and it looks like this. So this is the shape of the psi 1 eigenfunction. Let us look at the next eigenfunction psi 2, which is N 2 times 4 for a square root of alpha x square - 2 e to the power of - alpha x square / 2. So we notice that here we have a quadratic function multiplied by a Gaussian function.

And the first function is a parabola. But the value of the parabola when x = 0 is - 2. So if you were to plot that parabola, it looks something like this, where the value here is this match is - 2 and the Gaussian function is again like this, this is the x axis. So, the product of this function will be like this where it has value initially positive then negative then positive again and then goes like this.

So, this is the shape of the psi 2 eigenfunction psi 3 has the functional form in 3 multiplied by now a cubic polynomial so, square root of alpha x cube – 12 alpha x multiplied by the Gaussian function. So, here is cubic multiplied by Gaussian, the cubic function looks something like this. And the Gaussian function looks like this. So the product of the 2 gives a function which has 0 values at as the x = 0.

And it has a negative value initially it becomes positive goes through the 0. And it has a function for shape. And it has a shape which looks like this. So this is psi 3. If we write these functions and their energies, along with the potential energy function, then the entire picture looks something like this. Here is the potential energy the lowest function looks like that this is the energies are all equally spaced.

So, I can draw the energies like this is psi 0 psi 1 psi 2 psi 3 and if I draw the shapes, they look like this and like that and like the energies of these different states are h bar omega / 2 1 + half h bar omega / 2 and for the psi 2 it is 2 + half h bar omega / 2 and here it is 3 + half h bar omega / 2 This gives a complete picture of the eigenvalues and eigenfunctions of the harmonic oscillator.