Chemistry Atomic Structure and Chemical Bonding

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Lecture – 22
Problems and Solutions for Harmonic Oscillator

Welcome to the lectures in chemistry on the topic of Atomic Structure and Chemical Bonding. My name is Mangala Sunder; I am a professor in the department of chemistry in the Indian Institute of Technology in Madras Chennai.

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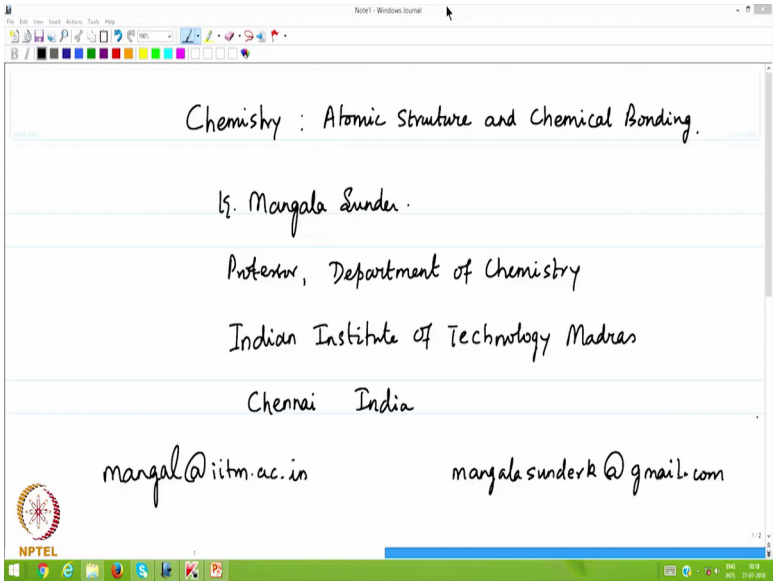

And my email ids are given in the screen here for you to contact. This is a video tutorial help for the lecture on simple harmonic oscillator which you have already seen.

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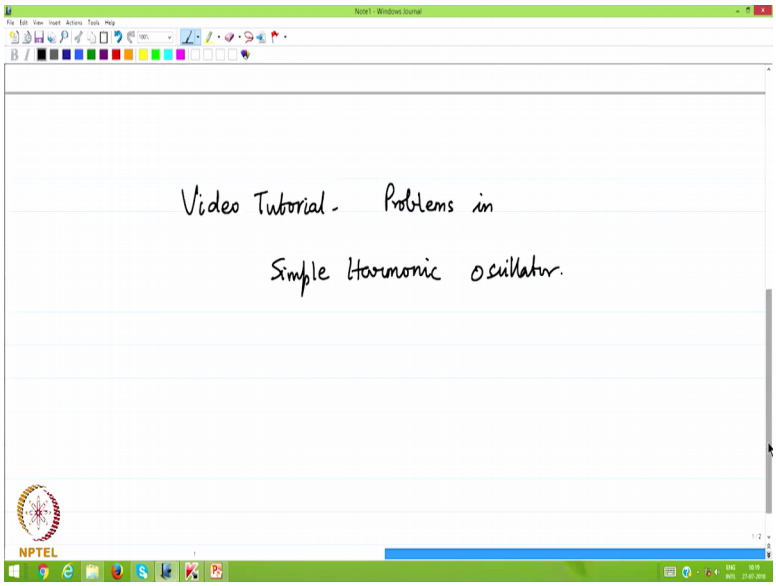

And there are a few simple problems and I would solve these problems and these problems also illustrate elementary methods in calculating and also understanding the basic principles ok.

So, following the practice we have been doing sequenced here, you will see the problems and then I will give you indicate the solutions to each one of them. So, this is on harmonic oscillator.

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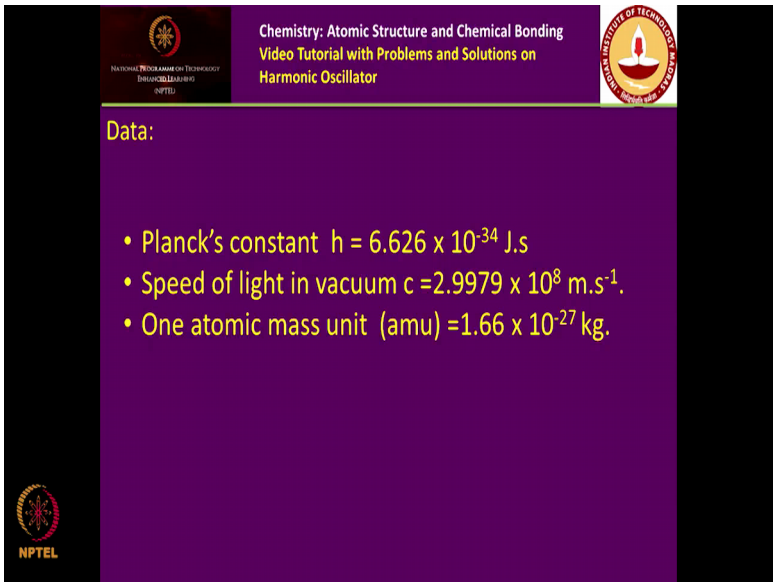

Remember the data that you have to keep in mind and you also have to use this the Planck's constant speed of light and the atomic mass unit are the three important fundamental constants we will need for this lecture.

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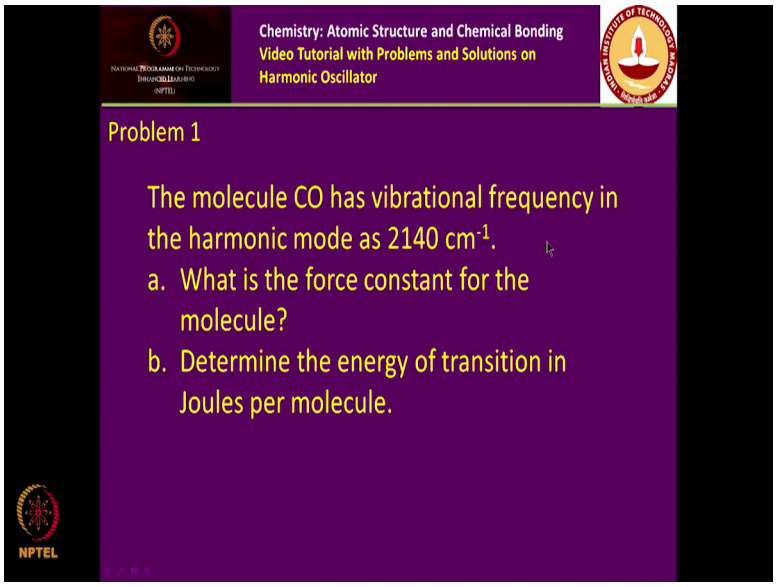

So, the first problem is using the harmonic oscillator model and approximating the molecular vibration as a simple harmonic motion. That is possible at low temperatures and also at moderate temperatures when the molecular vibrational states are such that most molecules are in the ground vibrational state. And we can model the vibrational energies and the vibrational wave functions using harmonic oscillator model ok.

Now, assuming that the model is valid, the question is the following the molecule carbon monoxide has a vibrational frequency in the harmonic mode as 2140 centimeter inverse. It is a safe frequency, but you know it is a wave number unit that we are giving. Question is what is the force constant for the molecule and the second question is on the determination of the energy of transition in joules per molecule ok?

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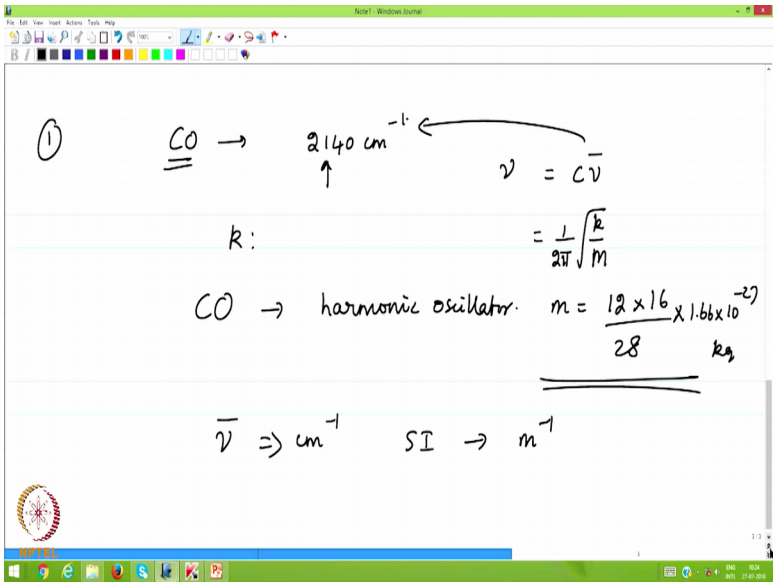

So, value given is problem 1. So, the CO molecule it is important because we need to know the mass of the molecule. The CO molecule the vibrational frequency is given as 2140 centimeter inverse. And we are asked to calculate the force constant for the molecule.

So, the force constant k is related to the frequency nu which is connected with the wave numbers through the relation the speed of light multiplied by the wave number and this is what you have here. The frequency nu is given by this formula 1 by 2 pi into square root of k by mu or m the mass. Here in carbon monoxide as a vibrating molecule the harmonic oscillator, we cannot use the total energy. But we have to use the reduced mass m is the carbon atomic mass unit 12, oxygen is 16 atomic mass unit and the total is 28.

And of course, you have the conversion 10 raise to minus 27 kilograms ok; this is the mass that we have to make use of. The other thing that you have to remember is that the nu bar is given in centimeter inverse. But SI units for joules and others will involve meter inverse. So, this problem is also about using the units carefully.

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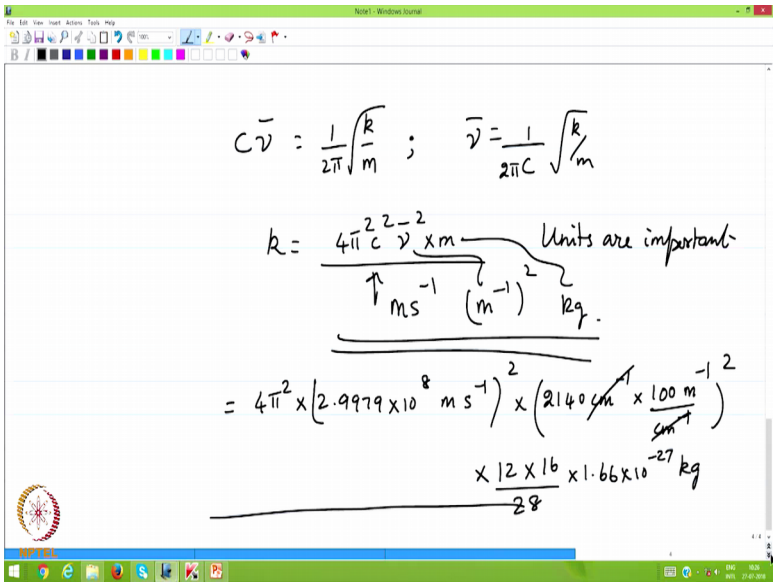

So, if I write C nu bar as 1 by 2 pi square root of k by m then nu bar is 1 by C 2 pi square root of k by m. And therefore, k is 4 pi squared C squared nu bar squared times m units are important ok. C is in meters per second nu bar is in meter inverse and m is in kilograms ok.

So, these are the only things that you need to do. Therefore, let me just put the numbers in and leave it to you to get the answer the numbers that we have are 4 pi square into 2.9979 into 10 raise to 8 meters per second whole square. And nu bar square is 2140 centimeter inverse into 100 per meter inverse centimeter inverse. So, this goes away and that is nu bar square into the mass that we calculated namely the 20 12 into 16 divided by 28 into 1.66 into 10 raise to minus 27 kilograms ok. So, this is pure big and numerical exercise.

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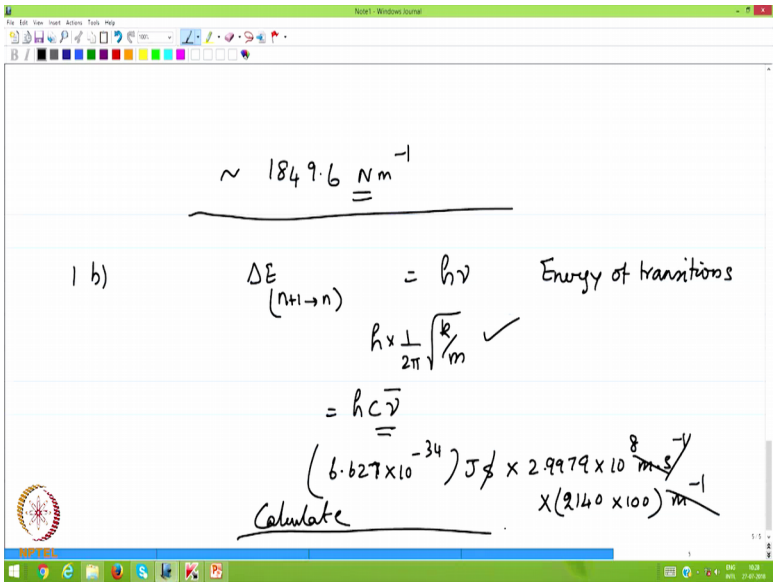

And I will leave it to you to calculate I think what I calculated the number to be is somewhere around 1849.6 Newton meter inverse Newtons per meter ok. This is the solution to the force constant in problem 1 ok. In the same problem it is also asking you to calculate the energy of transition in joules per molecule. If you recall the harmonic oscillator this is b, delta E is between any level n plus 1 to n. There are no transitions between levels which are separated by more than 1 level.

Therefore, this delta is h nu, this is the energy of transition, because you remember that the harmonic oscillator energy levels are equally spaced and they are half h nu 3 half h nu 5 half h nu and so on. Therefore, the gap between any successive pairs of levels is h nu and you already have calculated the force constant. Therefore, it is h times 1 by 2 pi into square root of k by m the you can use that or you can also use straightforward this number h into C nu bar, which is already given to you as 2140 centimeter inverse. Therefore, the answer is 6.627 into 10 raise to minus 34 joule seconds into 2.9979 into 10 raised to 8 meters per second 2140 into 100 per meter. And you can see that the answer will turn out to be the second goes away and the meter goes away. And therefore, what is left over is the joules and therefore, you can get this answer that calculated. So, this is a very straightforward problem ok.

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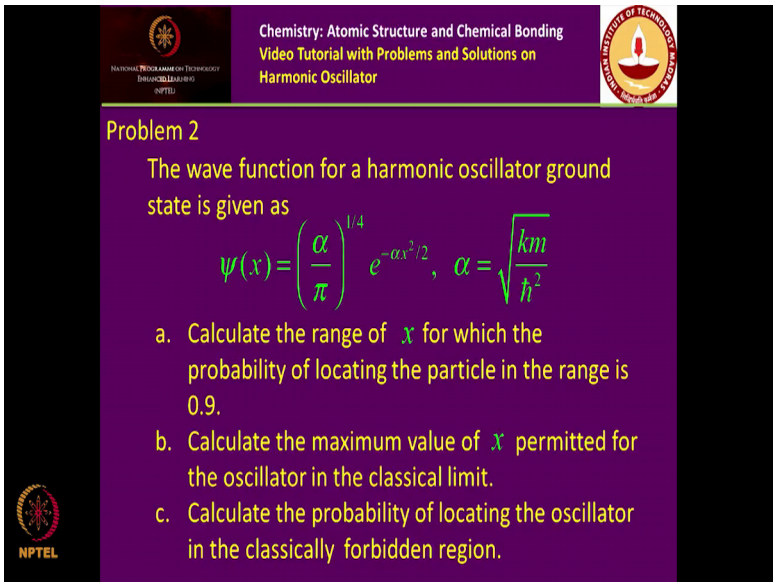

The second problem is a little more involved, the second problem uses the wave function for a harmonic oscillator ground state. Which is given here in the screen and you are asked to calculate the range of x for which the probability of locating the particle in the range is 0.9.

Recall that if 1 takes the square of the wave function and plots it as a function of x the area under the entire graph is the total probability of finding the particle in any of that region from minus infinity to plus infinity. And that area is 1 ok, because the wave function is normalized. Therefore, the square of the wave function d x psi squared d x between the limits will give you 1. Now you have to find that area for which the probability is 0.9 ok.

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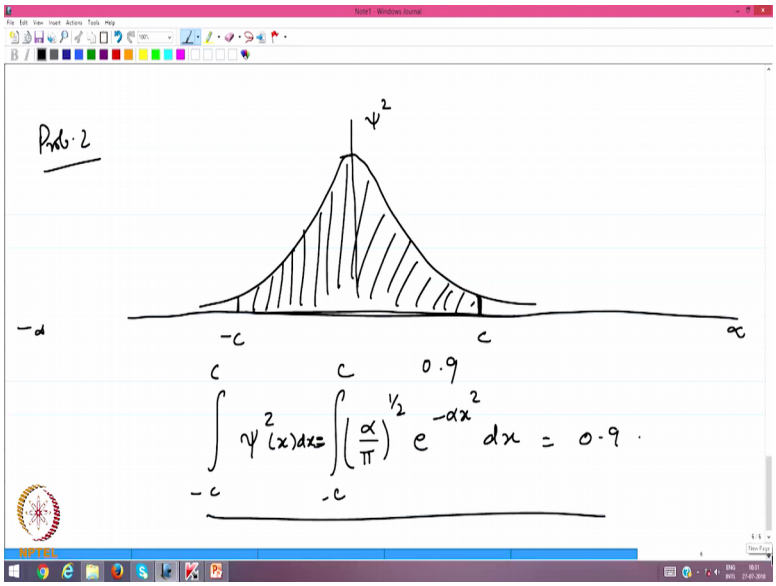

Problem 2, since the ground state wave function is given psi squared if you plot as a function of x is going to be like that and the entire area from minus infinity to plus infinity the area under the graph is 1.

But you have to find that value of x this is minus some c this is plus c that the area here this is 0.9 ok. Psi square is given to you already as psi square x is alpha by pi 1 by 2 e to the minus alpha x squared and psi square x d x is that. Therefore, you have to calculate the area from minus c to plus c minus c to plus c such that the answer is 0.9. one of the reasons for giving this number is that this cannot be calculated analytically.

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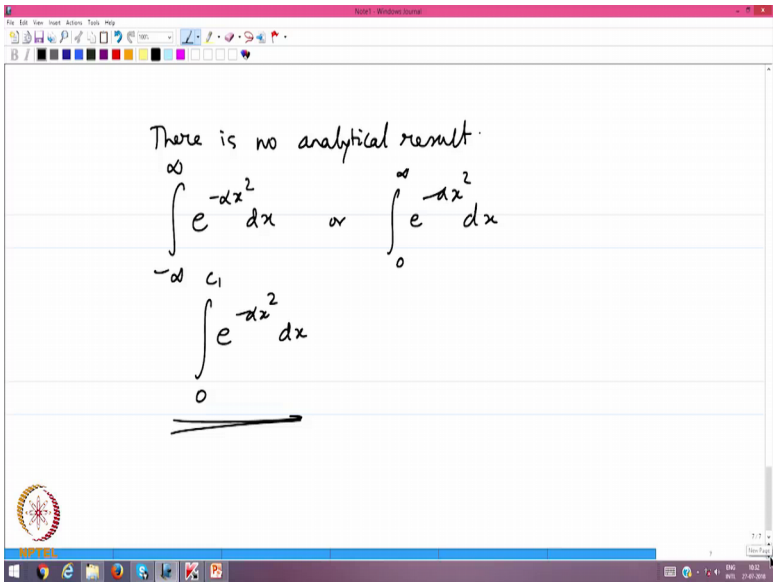

You need to know there is no analytical result; you need to use numerical tables. There is analytical result only for this integral minus infinity to plus infinity e to the minus alpha x square by d x or 0 to infinity e to the minus alpha x square d x.

If you have to calculate to this from say minus 0 to some constant c e to the minus alpha x square, this function is actually known as the error function ok. Therefore, the calculation for these numbers for these integrals has to be done numerically and there are numerical tables available ok. So, let us just quickly convert it in a form that they can get this area for the numerical value.

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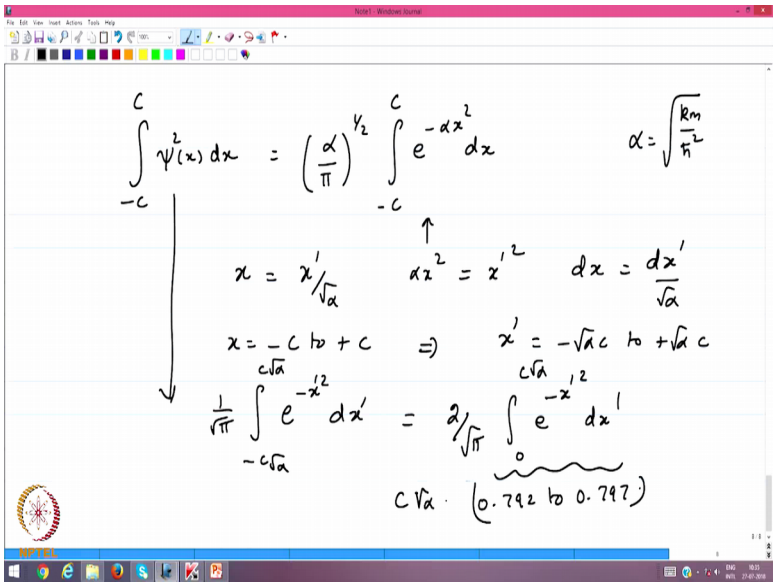

So, what we have is the following namely, the integral psi square x d x between minus and minus c to plus c is alpha by pi to the one half integral minus c to plus c e to the minus alpha x square d x. They are called as the wave function x d x and alpha is already known to you as square root of k by square root of k m by h bar square ok, these are the harmonic oscillator parameters.

So, what you have is this to calculate this integral do you a very simple transformation to say x prime such that it is x prime over root alpha. So, that alpha x squared becomes x prime square and d x is d x prime by root alpha. Therefore, the integral and also the limit x is equal to minus c to plus c implies x prime is equal to minus root alpha c to plus root alpha c.

And then you have you are set namely that the integral this integral transforms to the following minus c to plus c 1 by root pi e there is a root alpha here ,there is a root alpha here, e to the minus x square d x it is x prime square d x prime, but it does not matter. And so, the answer is its root 2 by root pi between 0 to c e to the minus d x prime this is the error function integral.

And if you locate from the tables numerical tables I mean you can look up to the tables from the internet or from any of the text books, which give you error function integrals. The value for this c root alpha for this is c root alpha; the value c root alpha is between 0.792-0.797 ok. Therefore, c is 1 by this number divided by the root alpha.

Alpha is dependent on the molecular system and or the actual problem because, the force constant and the mass are dependent on the model problem that you choose. Therefore, this is the formula that you have to use to calculate the probabilities on any finite value, any finite number and the probability being 1 is means it covers the entire area ok. Now, the second part of this question is calculate the maximum value of x permitted for the oscillator using classical limit.

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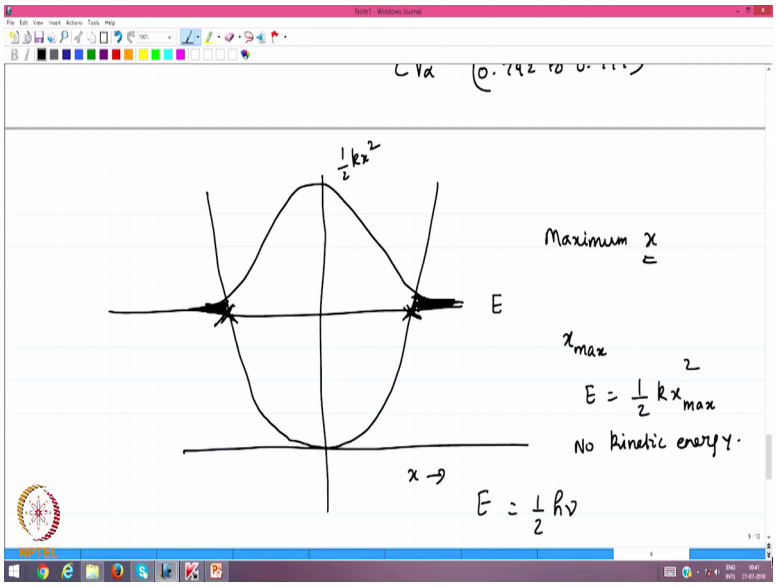

This is an interesting question; recall that the potential energy for the harmonic oscillator that we use is a parabolic configure something like the half k x square symmetric ok. Now, this is half k x square as a function of x plus or minus x. The maximum value for the potential, maximum x please remember if you take harmonic oscillator the energy to be some value E.

The extremes for the classical these two extremes which are called the turning points, mark the point or the points at which the oscillator velocity is 0 ok. The harmonic oscillator oscillates swings between the two ends like a you know recall the pendulum and at either ends the velocity is 0 and there the potential energy is the maximum and that is the energy of the oscillator.

Therefore, if the oscillator has a higher energy its things faster to a larger amplitude it is picking up somewhere at the top here instead of. So, if you pick up any energy E the classical value x max is when E is all potential energy half k x max whole square no

kinetic energy. This is classical therefore, the point is this point x max and at the ground state E is half h nu ok.

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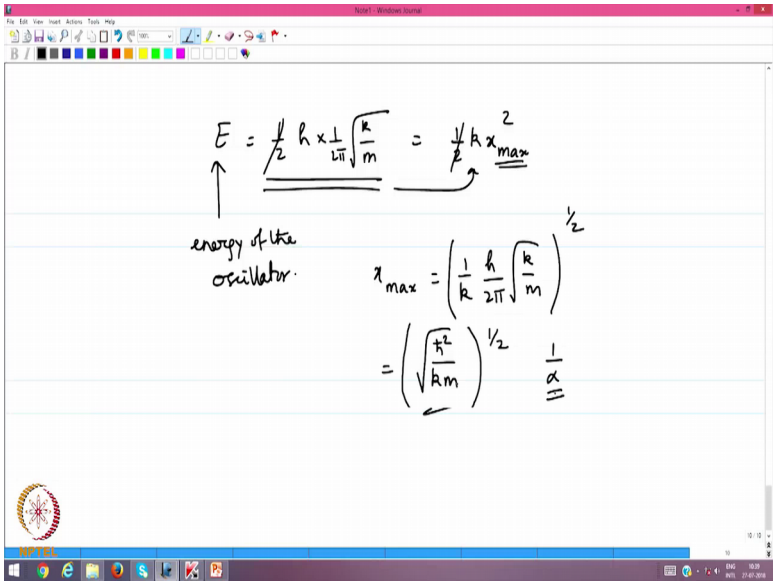

And the E half h into 1 by 2 pi square root of k by m that is half h nu and that is equal to half k x max square. This is what is meant by the entire energy of the oscillator quantum mechanical in the limit of this oscillator behaving classically if all its energy is potential energy this is the maximum value of x.

But we know that this is not true, this is only an analogy because a quantum mechanical oscillator has all the x values from minus infinity to plus infinity you are aware of tunneling and so on. Therefore, here we are simply looking after the limited this I mean application assuming that there is a classical system equivalent to that what is the x max x max value is then you know what the x max is this is given by the half goes away.

So, you have h by 2 pi square root of k by m into 1 by k ok. And the whole thing square root and if we simplify this, this is h bar square by k m what this is? This is nothing, but 1 alpha. Third problem calculate the probability of locating the oscillator in the classically forbidden region. Which is if you go back to the previous graph here, the probability of the oscillator being in the forbidden region is all these values supposing the wave function has for the ground state. It has the square of the wave function has the same ok.

Then what you see is all values of x beyond the x max, which is this region which is this region ok. They are symmetric therefore, you have if you calculate either this or this and then you say to twice that. This is the probability that the oscillator is in the forbidden region this is what is called to the tunneling probability and it is a straightforward answer to write because, once you know what the x max is.

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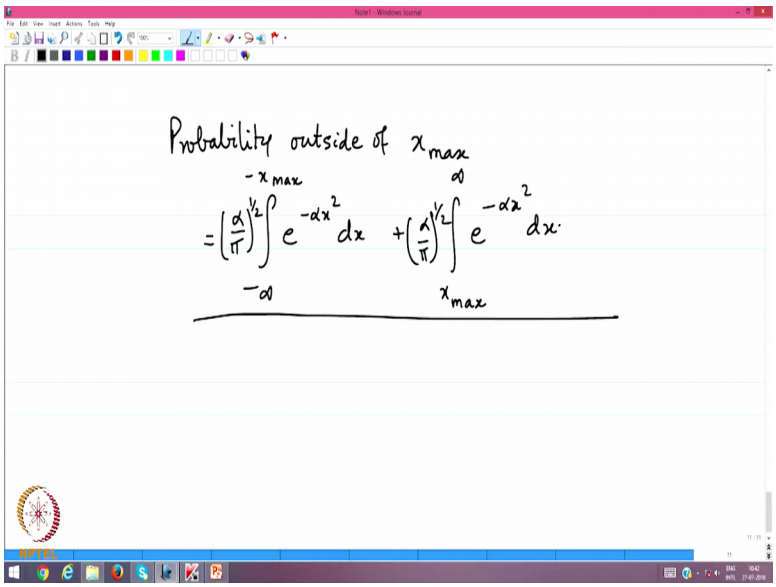

The probability outside of x max is the integral minus infinity to x max alpha by pi to 1 by 2 e to the minus alpha x square d x plus x max to plus infinity e to the minus alpha x square d x alpha by pi 1 by 2 ok. This is the probability that the system is outside the classically for is indeed classically forbidden region or outside the parabolic potential region, this is what is meant by the question.

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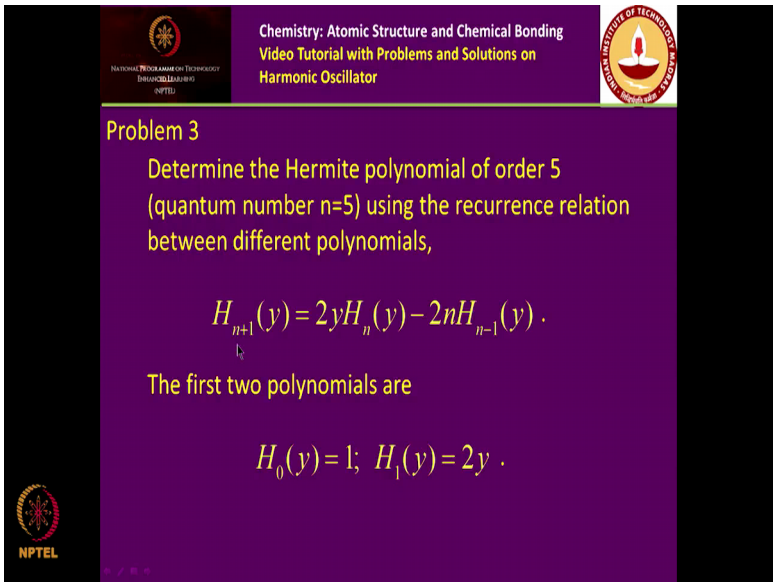

So, the next question is on calculating the harmonic oscillator Hermite polynomials, which are the polynomials as part of the wave functions to different orders, say order 5. And order 5 essentially means quantum number n equal to 5. There is a formal recurrence relation between the Hermite polynomials I think I mentioned this in the lecture.

And the recurrence relation is given by the index n the Hermite polynomial index n plus 1 and n minus 1 and the relations between them the Hermite polynomial with the index n plus 1 is connected to the Hermite polynomial that the index n and n minus 1 by this.

And to use this of course, you need to know n minus 1 and again for some value of y n namely n minus 1 equal to 0 and then n obviously, is 1. So, you have H naught is given H 1 is given therefore, what is H n plus 1 so, first we will copy this relation.

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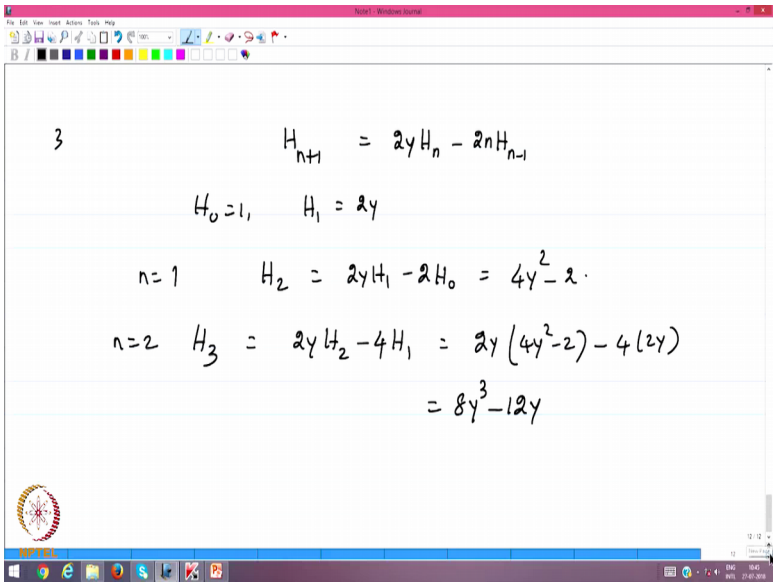

It is 2 y H n, 2 y H n minus 2 n H n minus 1 2 n H n minus 1 and that is equal to H n plus 1 ok. So, H 0 is 1 H 1 is 2 y. Therefore what is H 2 n equal to 1, H 2 is equal to 2 y H 1 minus 2 H 0 which is 4 y squared minus 2. What is H 3? H 3 is again n equal to 2.

Therefore, 2 y into H 2 minus n is 2 therefore, it is 4 2 n is 4 H n minus 1 is since given to this is H 1 and the answer is 2 y into H 2 is 4 y square minus 2 minus 4 into 2 y. So, the answer is 8 y cube minus 12 y. So, now, it is very easy to calculate the rest of it in a similar way and I will give you the answers.

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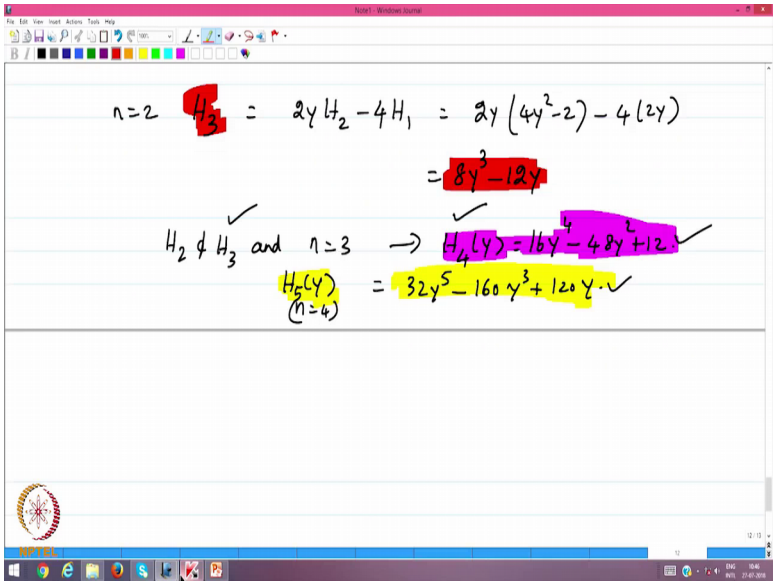

Use H 3 2 and H 3 and the n equal to 3 to get the answer H 4 of y is equal to16 y raise to 4 minus 48 y squared plus 12. And likewise H 5 of y using H 4 and H 3 and n equal to 4 to get the answer 32 y to the 5 minus 160 y cube plus 120 y. So, these are all the various Hermite polynomials of orders as per the quantum number n. So, this is H 5 and then you have this is H 4 and then you have H 3 and so on ok.

So, this recurring recurrence relation gives you how to calculate they have been polynomials of higher order from that of the lower order. So, this is just an exercise to understand that these relations the origin of these relations if you have to you must be in a position to solve our my differential equation which is not yet part of this lecture series.

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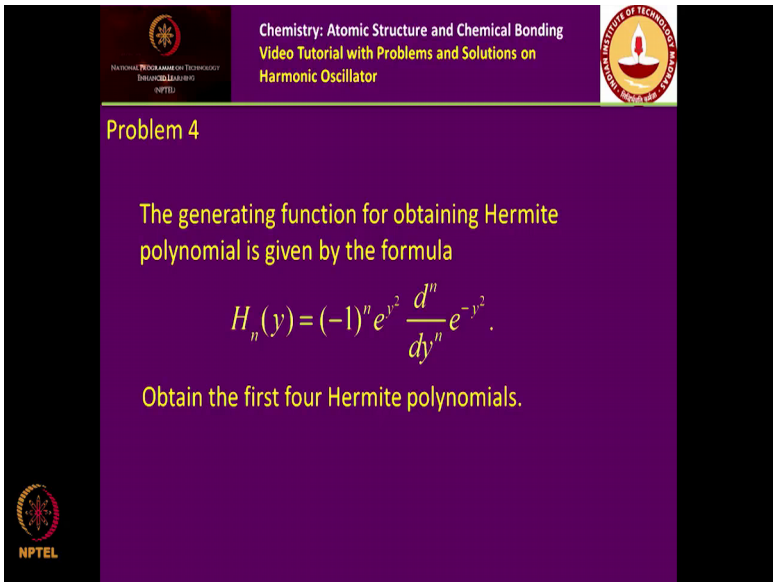

Problem number 4, there is another way of calculating the Hermite polynomial using what is known as a generating function. And the generating function now, involves the differentials and you can see the polynomial generating function for the Hermite polynomial is given by this formula from mathematics of the Hermite equation H n of y is minus 1 raise to n exponential y square and the derivative nth derivative of exponential minus y square.

And using this obtain, the first three or four Hermite polynomial it says four Hermite polynomials. But again its simply application of the differential the derivative to the exponential minus y square ok. So, let us see that quickly for one or two of them ok, it is minus 1 raise to n let us copy this formula.

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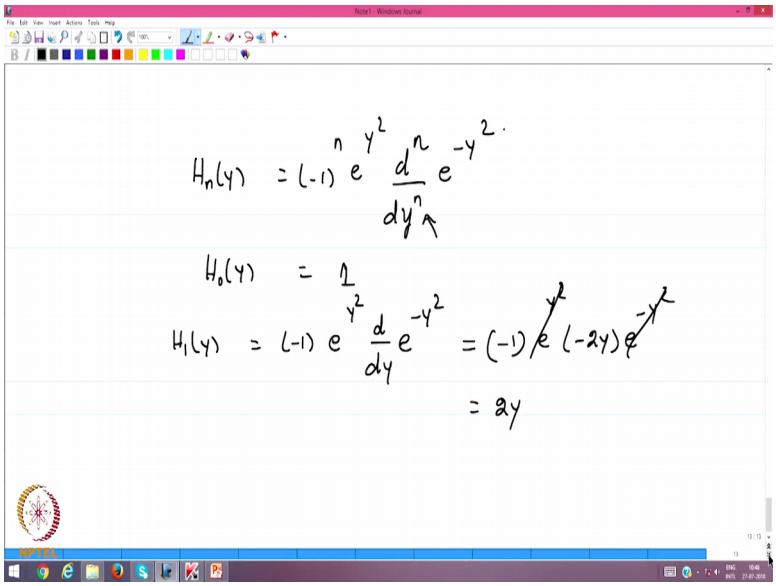

H m of y is minus 1 raised to the n e to the y squared the derivative nth derivative d d y to the nth of e to the minus y square. So, H naught it is easy because, the n is 0. Therefore, this whole thing is one the derivative and the exponential y square and minus y square cancel out therefore, you get the simple answer it s 1.

What about H 1 of y? H 1 of y is minus 1 e to the y square d by d y of e to the minus y square and that you know immediately the answer is it is minus 1 e to the y squared into minus 2 y e to the minus y square. They cancel off so you get the answer 2 y that you are already familiar with.

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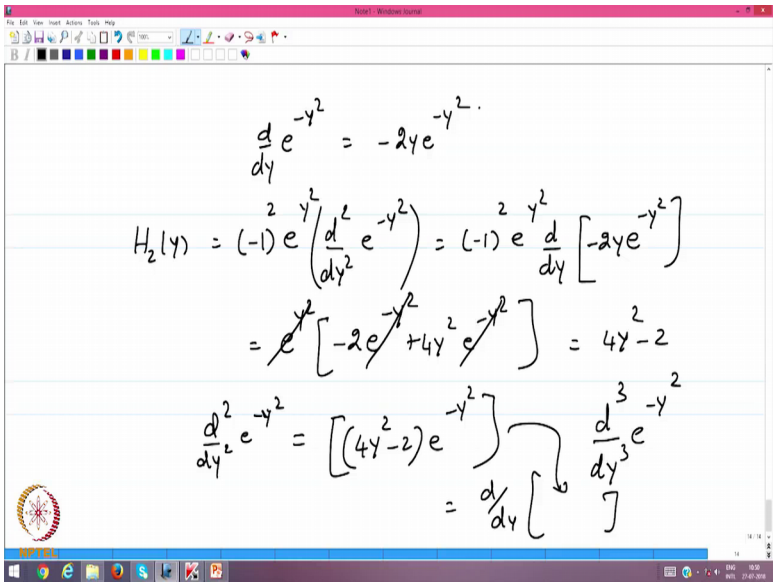

Now, remember the d by d y of e to the minus y square is minus 2 y e to the minus y square to calculate H 2 of y you will need this because, it is minus 1 square e to the plus y square. And its d square by d y square of e to the minus y square, which I would write as minus 1 square e to the y square d by d y of the previous result namely minus 2 y e to the minus y square ok.

Keep this in mind and then the answers will come out immediately because, this is minus 1 squared is plus 1 e to the y square and this is the derivative is minus 2 e to the minus y square and then there is another minus 2 y when you differentiate the exponential. So, this becomes 4 y square e to the minus y square. And obviously, this goes away with that and the answer you get is 4 y squared minus 2.

But what is important is, remember d by d y d square by d y square of e to the minus y square is 4 y square minus 2 e to the minus y square. And use this to calculate to the third order Hermite polynomial d q by d y q e to the minus y square as d by d y of everything that you have here. So, it is important to keep this order in mind and therefore, the rest of it is easy that you can calculate H 3 of y and plus 4 Hermite polynomials mean only that.

So, this is again an algebraic exercise to calculate Hermite polynomials using a generating function.

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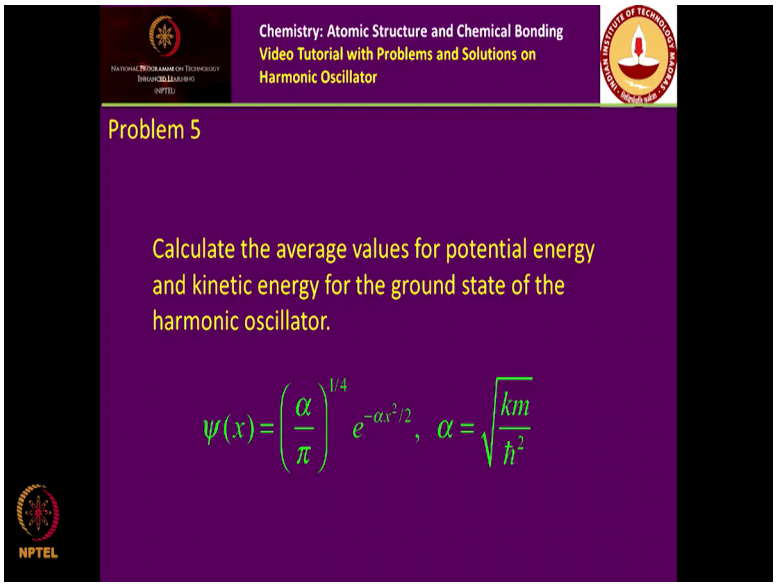

Next problem, this is an extremely important problem fundamental, calculate the average values for the potential energy and kinetic energy for the ground state of the harmonic oscillator. You need to know the exponential formulas for doing this. And it is also important that we can only calculate the average values, and not the exact eigenvalues of the potential energy and kinetic energy for the harmonic oscillator in quantum mechanics because, the operator for the potential energy and the operator for the kinetic energy do not commute.

And therefore, it is not possible for you to have the eigen functions for both these operators which do not commute. And this is exactly the same thing as saying that the position and the momentum operators do not commute. Therefore, position and momentum cannot have simultaneously exact eigenvalues same process.

It is not necessary that we should always have exact eigenvalues we will have only those operators which commute among themselves. And therefore, the state of the system will always be specified by only those sets of operators, which commute among themselves and those are the properties. Here potential energy and kinetic energy are not properties. In fact, position is not a property; momentum is not a property with respect to the total energy.

If you specify the harmonic oscillator to be precisely in an eigen state, you can only calculate the average value for the position which turns out to be right in the middle there

the harmonic oscillator do not say it is a maximum ok. Now for position momenta they are all only average values that you can calculate. So, let us do that here for the oscillator this problem 5.

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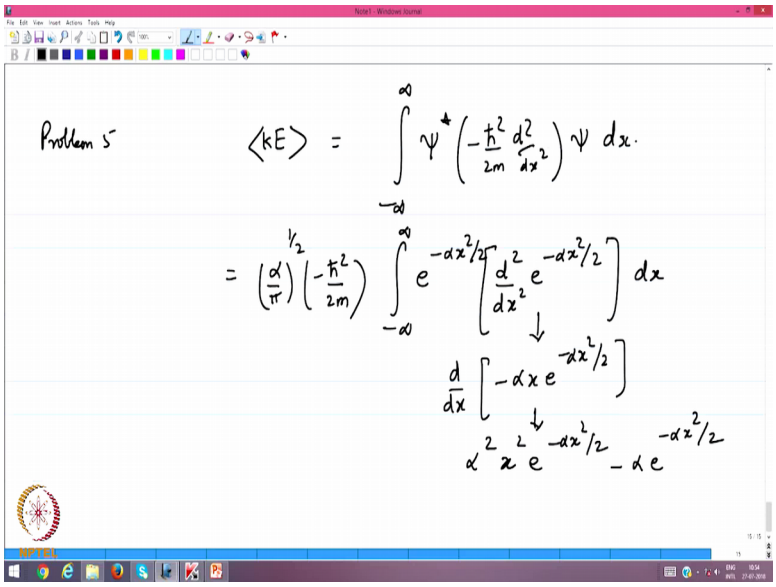

Average value for the kinetic energy yes, psi star, a kinetic energy operated is minus H bar square by 2 m d square by d x square psi d x. Here of course, this is minus infinity to plus infinity so the answer is the expression is alpha by pi to 1 by 2.

And you have the minus H bar square by 2 m and the integral minus infinity to plus infinity e to the minus alpha x square by 2 the derivative of d square by d x square e to the minus alpha x square by 2 times d x ok. Now, it is easy to calculate these derivatives the first derivative is of course, minus 2 alpha x divided by 2.

So, you get only the minus alpha x e to the minus alpha x square by 2. And the second derivative is minus so it will give you alpha square x square e to the minus alpha x square by 2 and the other 1 is minus alpha e to the minus alpha x square by 2 ok.

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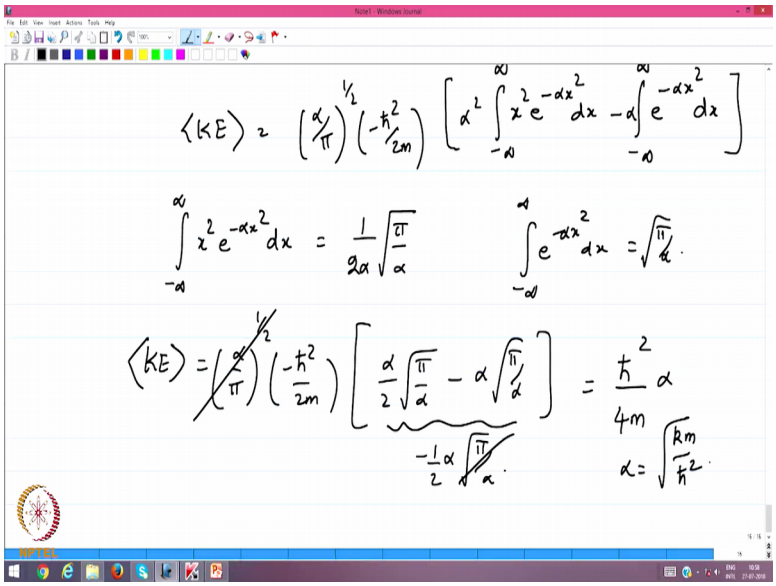

So, this is the derivative and therefore, the kinetic energy average value of the kinetic energy is alpha by pi 1 by 2 into minus h bar square by 2 m. And then you have two integrals to calculate namely, alpha square integral minus infinity to plus infinity x square e to the minus alpha x square d x. And then you have another 1 minus integral minus infinity to plus infinity alpha e to the minus alpha x square d x ok.

So, the integral x square e to the minus alpha x square d x this is standard integral the formula is 1 by 2 alpha into root over alpha ok. And the integral e to the minus alpha x square by 2 d the alpha x square d x in minus infinity this is root pi over alpha ok.

Therefore, the kinetic energy is calculated as follows namely, it is alpha by pi 1 by 2 minus h cross square by 2 m into alpha square divided by this. Therefore, alpha by 2 root pi over alpha and the other is minus alpha root pi to over alpha ok. So, this is minus 1 by 2 alpha root pi over alpha and that cancels off that the minus sign what you have is h bar square by 4 m into alpha. And alpha is square root of k m by h bar square.

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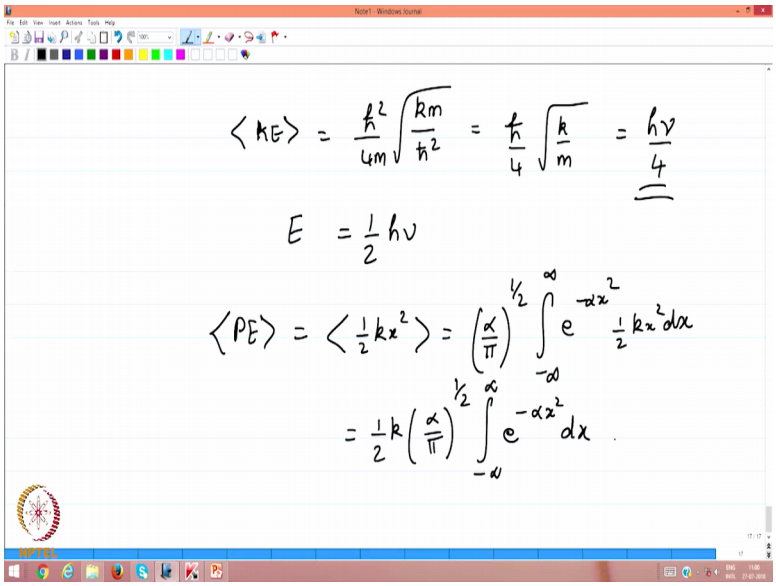

Therefore to simplify the average value of kinetic energy is h bar square by 4 m into square root 4 m into k m by h bar square it gives you h bar 1 h bar goes away and then km if you do this becomes by 4 square root of k.

And this is of course, you know h bar is h by 2 pi and 1 by 2 pi of this is k, but this 1 is nu. Therefore, this is h nu by 4 this is the average value. And remember the energy for the harmonic oscillator, which is an eigen function for the sum of the kinetic energy operator and the potential energy operator the energy is half h nu for the ground state.

And so, what you see here, is the kinetic energy is exactly half of this the average value not the kinetic energy at any given instant of time that you cannot calculate the average turns out to be h nu. It is easy now to see the potential energy in a similar way the potential energy average is obviously; the average of half k x square and that is again the integral is alpha by pi to 1 by 2 e to the minus alpha x square.

Now, we do not need to put these things in between so, we can write this as 1 by 2 k x square d x between the limits minus infinity and plus infinity. So, what you have is 1 by 2 k alpha by pi 1 by 2 the integral e to the minus alpha x square d x.

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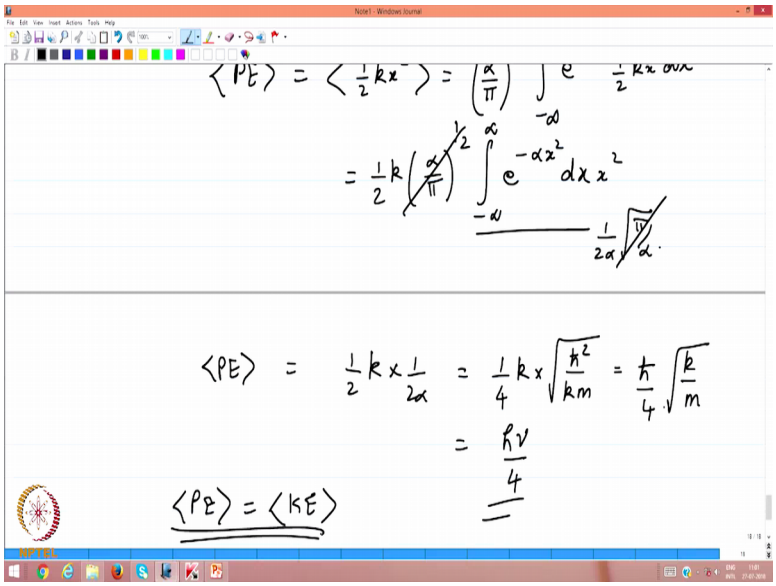

And this value you know already that this is a and also there is d x square here. So, this integral is 1 by 2 alpha square root of pi over alpha. So, the answer is for the potential energy. If you substitute that its 1 by 2 k it is alpha and this in, this way you have 1 by 2 alpha which is 1 by 4 k into square root 1 by alpha. 1 by alpha is obviously, h bar square by k m and that is given as h bar by 4 square root of k by m.

And so, that is also h nu by 4 because h by 2 pi times 4 and 1 by 2 pi times that is 4. So, the average value of the potential energy for the ground state is equal to the average value for mean kinetic energy also partly known state.

This is an extremely important and interesting result that you have to and they both are equal to half the energy of the harmonic oscillator the total energy of the harmonic oscillator.

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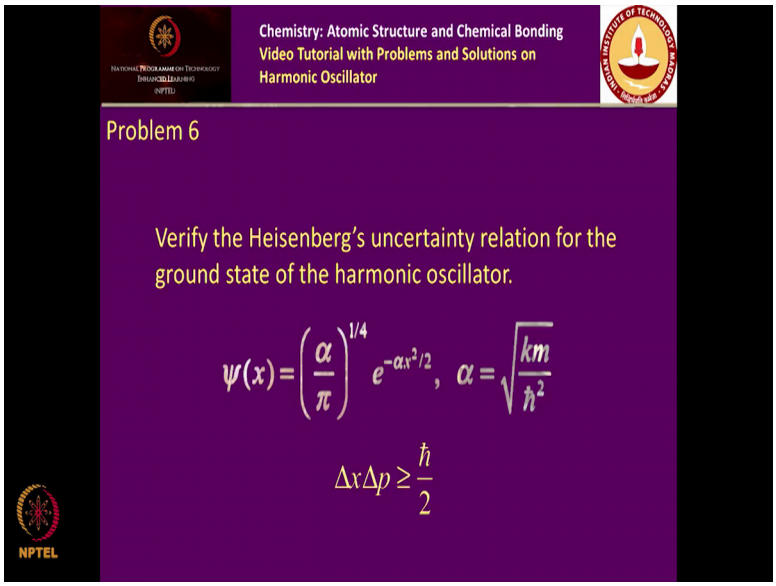

Next problem, verify the Heisenberg's uncertainty relation for the ground state of the harmonic oscillator. I have actually done all the elements of integration that you need for calculating this quantity. And therefore, I will indicate to you and you would find out that in this case the delta x delta p is exactly equal to h bar by 2.

And the ground state of the harmonic oscillator is also known as the minimum uncertainty state for the harmonic oscillator. You will just quickly see that result and the calculations can be done by you as I have already done that in this tutorial that is right.

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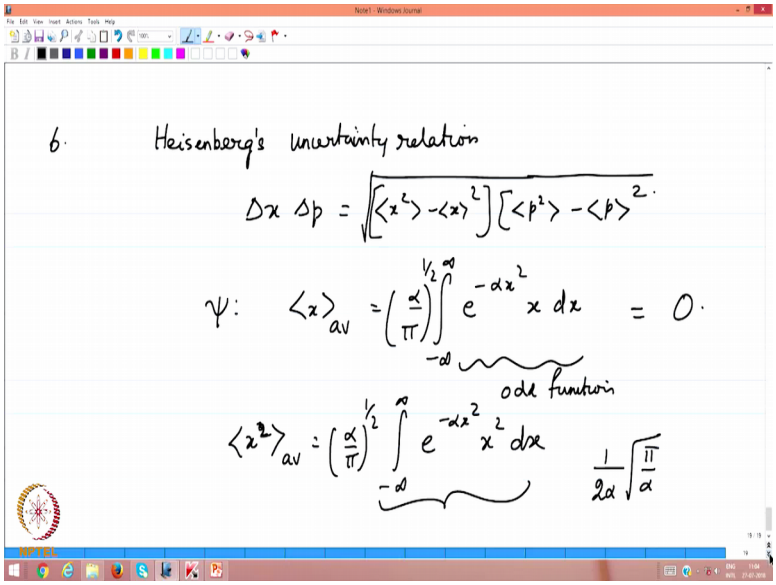

Now, Heisenberg's is this problem I believe 6 yes, problem 6 Heisenberg's uncertainty relation delta x delta p is square root of x square minus x average square multiplying p square average minus p average square.

Now, for the harmonic oscillator psi the x average is alpha by pi 1 by 2 e to the minus alpha x square x d x between minus infinity to plus infinity you know that this is an odd function. And it is between symmetric intervals and for this answer is 0 and x square average if you have to do that that is again alpha by pi 1 by 2 from minus infinity to plus infinity you have e to the minus alpha x square x square d x. This integral I have already told you is 1 by 2 alpha into root pi over alpha.

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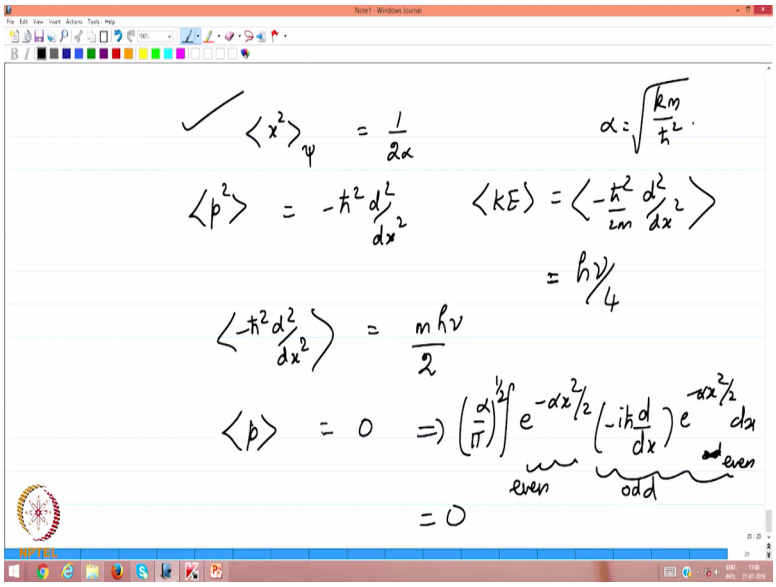

Therefore the x square average for this ground state is 2 pi alpha and this alpha by root psi will go away this is 1 by 2 alpha ok. And you know alpha is square root of k m by H bar square. So, this is known p square average please remember, p square is minus h. bar square d square by d x square And we just calculated that the average value of the kinetic energy which is the average value of the operator minus h bar square by 2 m d square by d x square is h nu by 4 ok.

Therefore you can immediately see that the p square average is minus h bar square d square by d x square should be 2 m times this therefore, you have 2 m h nu by 4 which is m h nu by 2 this is the p squared average. What is a p average? It is also easy to see that this is 0 because, the p average is you put the operator between the 2 e to the minus alpha

x square the wave function. And you have minus i h bar d by d x acting on the e to the minus alpha x square by 2 d x.

You know this will change the even function to an odd function and the product of this or this is even this is odd this is even. And therefore, the product will be odd and the answer is 0. Therefore, you have p square average is 0 a sorry p average is 0 you have p square average is given by the 2 and you have x square average is given x average is 0.

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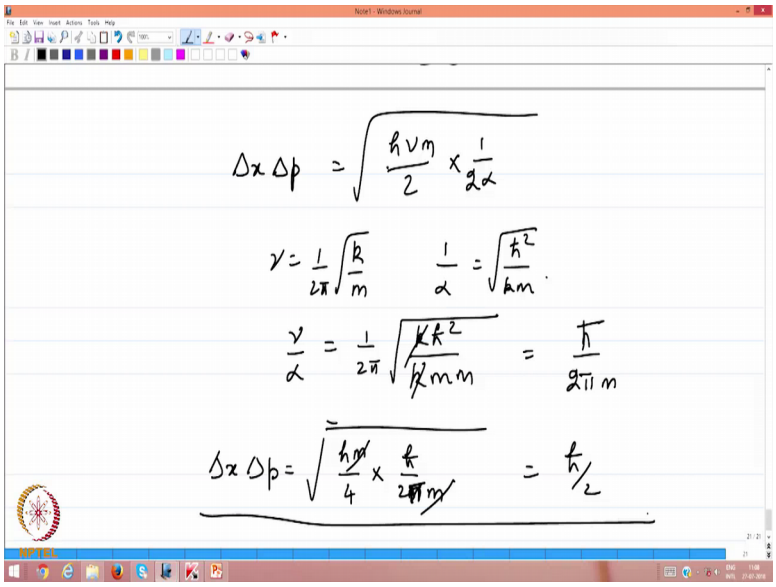

Therefore it is very easy to calculate the delta x delta p as square root of h nu by 2 m m by 2 into the other answer x square average is 1 by 2 alpha 1 by 2 alpha ok.

Now, all you know is that substitute all these things, nu is 1 by 2 pi square root of k by m and 1 by alpha is square root of h bar square by k m. Therefore, nu by alpha is going to give you 1 by 2 pi square root of k h bar square by k m m k goes away. And so you have 1 by 2 pi m h bar and there is already an m here.

Therefore, you can calculate this is only mu by alpha therefore; delta x delta p is square root of h m by 4. And the nu by alpha is obviously, h bar by 2 pi m and h by this is 2 pi h by 2 pi is h bar m goes away. And therefore, you have h bar square by 4 and the answer is h bar by 2.

You see that the delta x delta p is exactly h bar by 2 this is called the minimum uncertainty state. And it is an extremely important harmonic oscillator ground state obeys

the Heisenberg's uncertainty principle to it is limit. It is not a higher uncertainty, is not a lower uncertainty it is the minimum given by Heisenberg's formula that is important.

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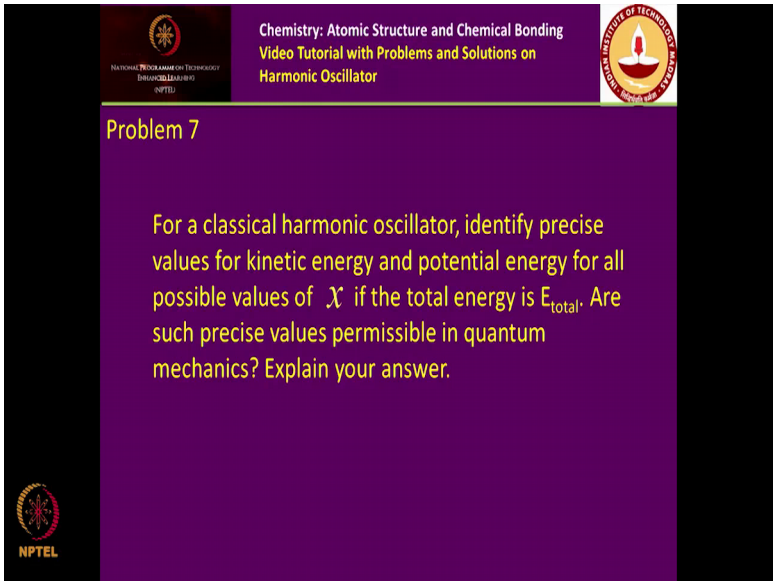

Now, the next problem is the problem of some concept for a classical harmonic oscillator, identify the size values for kinetic energy and potential energy for all possible values of x. If the total energy is E total, that is a fairly straightforward thing from the parabola that we can calculate, but then the question is are such precise values permissible in quantum mechanics explain your answer. And the answer is of course, no such precise values are not permissible in quantum mechanics so, let us see what these classical values are in the first place.

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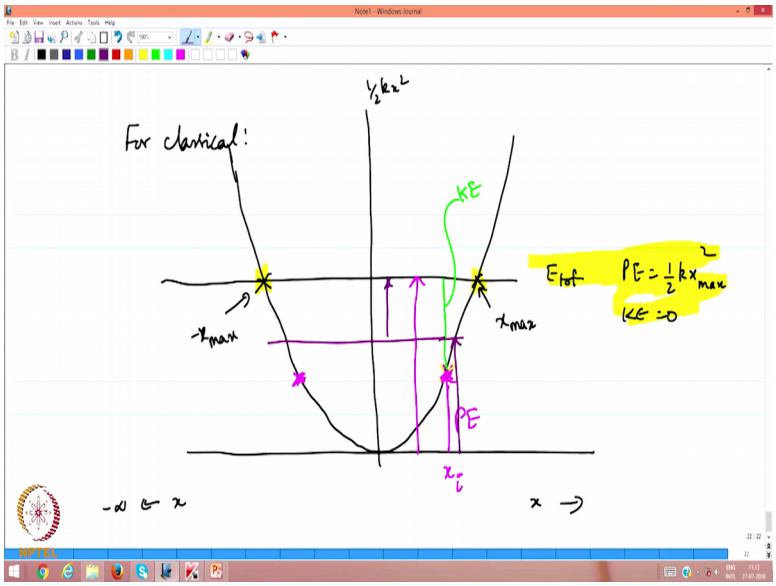

For a classical oscillator the potential energy as a parabola is something that you have to the potential energy as a parabola is something that you have to remember ok. This is the v of x is half k x square and this is x positive x to the negative minus infinity and the parabolic curve is something like that ok; it is the symmetrical oh myself.

So, if we have an E total which is given by some value E total. Then you remember this value of x max which is the turning point for the classical oscillator, where the kinetic energy is 0 gives you the maximum value for the potential energy. So, at this point the potential energy is half k x max square ok, this is x max this is minus x max kinetic energy is 0 ok. So, this is item one and that corresponds to this point.

Now, let us take any point in between let us take this point let us take this point, so, let me use a different color ok. Let us take this point and the corresponding point here ok. The potential energy is given by half k x value square, which is the x value here ok, some x intermediate i. So, the total energy still of course, this because that is the E total.

Therefore, if this is the potential energy quite, obviously, this is the kinetic energy potential energy, but remember for a classical oscillator every point of the harmonic oscillator the parabolic curve is well defined because, we know the graph the point as well as its velocity at that point the steepness we know. Therefore, classically we know the position and the momentum of the particle very very clearly at each and every instant of time therefore; we can say that the oscillator goes around like this.

And at each such point, we know that the kinetic energy is the difference between the total energy and the maximum potential energy bounded by the graph this point ok. So, if you have to do any other point again, if you have to take this then you know that this is the kinetic energy and the corresponding value this is the potential energy. So, it is very precisely defined for each and every x max, why it cannot be done in the case of quantum mechanics for this.

First of all this parabolic curve for a quantum mechanic system is not a very meaningful thing. Because the harmonic oscillator can have any value of x classically forbidden value it does not mean that the kinetic energy is negative. The kinetic energy or the potential energy as individual attributes or individual measurement quantities are not available you only can measure the total energy.

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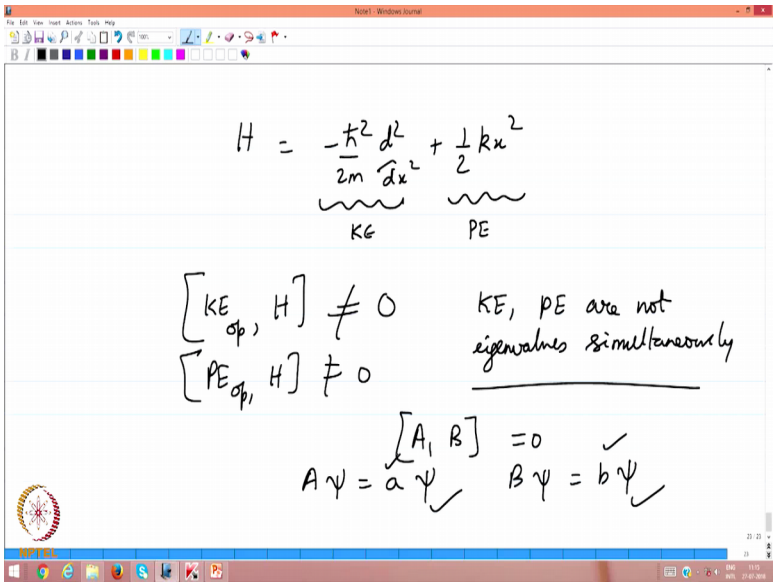

Therefore the quantum mechanical result says very clearly that the Hamiltonian, when it is written with minus h bar square by 2 m is square by d x square plus half k x square. Remember operator for the kinetic energy is this is the operator for the potential energy the kinetic energy operator does not commute with the overall Hamiltonian. Because it may commute with itself, but this operator does not commute with the x square term.

And likewise, the potential energy operator does not commute with the H go to 0 is not 0. Because k x square will commute with the k square part of the Hamiltonian, but k x square will not commute this. Therefore, K E P E are not again values simultaneously.

So, what is important for you is to remember that, when two operators A and B, when they commute Aon psi x can have an eigenvalue a psi B on psi x can have an eigen value psi, same eigen function different eigenvalues are possible.

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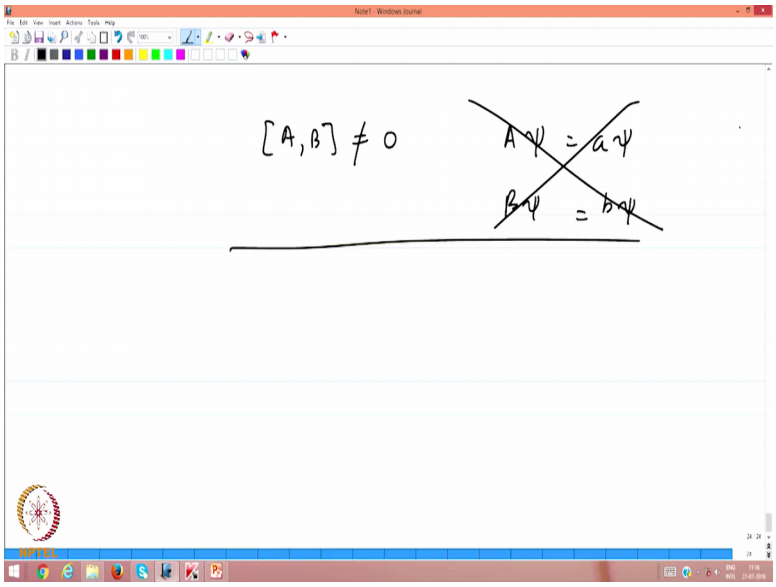

However, if the operators do not commute then it is not possible for you to define the same size such that A of psi is given by the eigen value equation and B of psi is given by another eigenvalue equation.

This is not permissible and therefore, the definition of potential energy and harmonic oscillator kinetic energy at each and every instant of the position is not simultaneously definable for a quantum oscillator.

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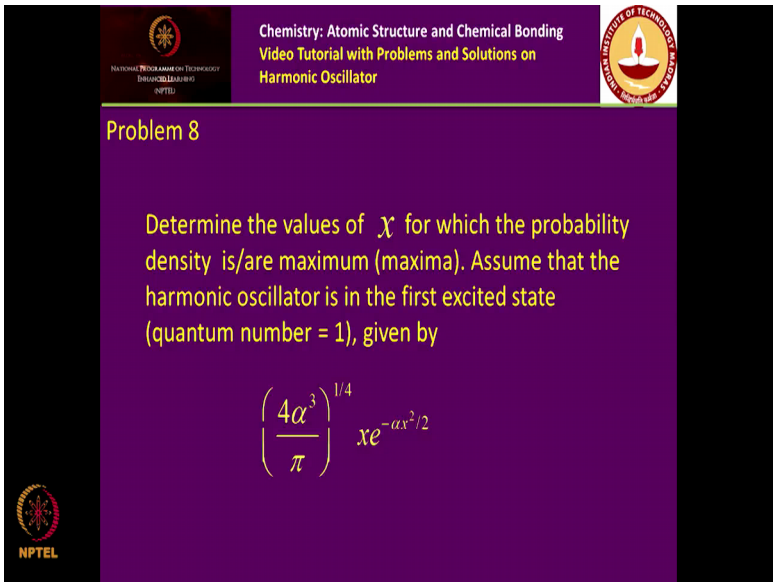

Determine the values of x for which the probability density is or maximum, I mean if there is more than one maximum, then you have to calculate all of them. And one example of a function given is the harmonic oscillator in the first excited state given by this formula that 4 alpha q by pi 1 by 4 x e to the minus alpha x square by 2 ok. Actually the numerical constant is not relevant for the problem, but anyway we will keep that. What we are asked to do is to so, for calculating the maximum or minimum in the probability.

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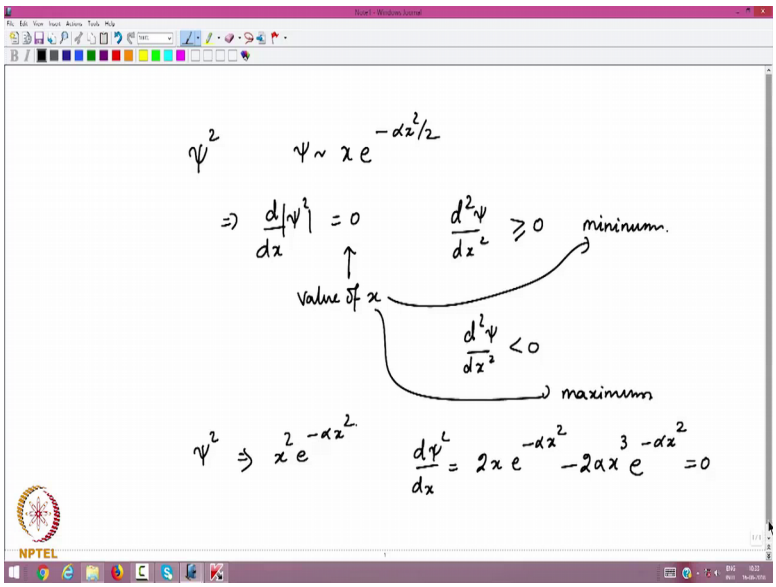

We need psi square and psi is given as x e to the minus alpha x square by 2. Therefore, we have to take the derivative of the psi square with respect to x that should be set to 0. And the second derivative d square psi by d x square for the value of x at which this derivative is 0, if the second derivative is greater than or equal to 0 this is a minimum. This value of x this value of x is a minimum. If d square by psi by d x square is less than 0, the value of x for which the psi square is your maximum.

So, what we will do is, let us calculate x psi square which is x square roughly, we do not need to worry about the constants. It is x square e to the minus alpha x square. Therefore, d psi square by d x is equal to 2 x e to the minus alpha x square minus 2 alpha x so 2 alpha x cube e to the minus alpha x square that should be 0.

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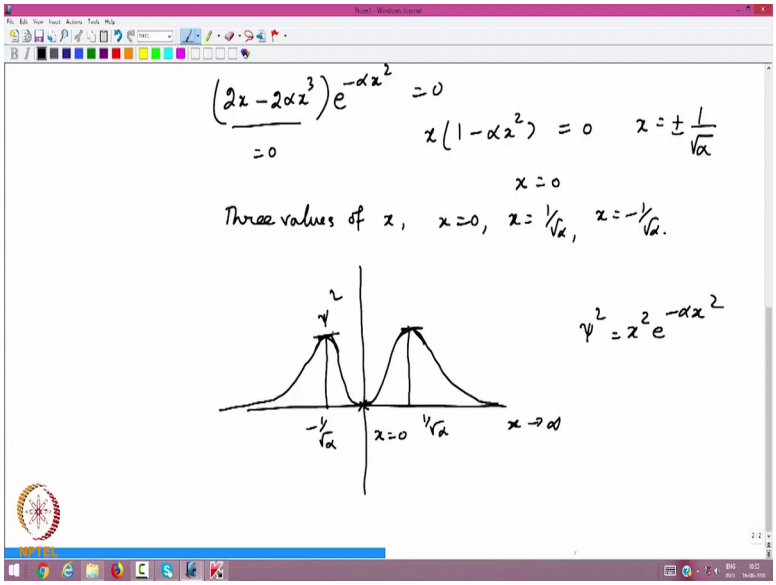

And you know that the exponential level goes to 0. Therefore, it is 2 x minus 2 alpha x cubed e to the minus alpha x square. If this is 0, this should be 0, or x into 1 minus alpha x square is 0 x is equal to plus or minus 1 by root alpha. So, if you recall the probability you also have one more result namely, x is equal to 0. So, there are three values of x for which the derivative is 0, three values of x x is equal to 0, x is equal to plus 1 by root alpha x is equal to minus 1 by root alpha.

So, now we have to find out which is maximum and which is minimum. Of course, one quick way to do that is to plot the function x square e to the minus x square this is x to infinity and this is psi square. And you know the psi square actually goes to 0 at x is

equal to 0. And you see that the function is x square into the function is x square e to the minus alpha x square and at x is equal to 0 this is 1, but this is 0.

But for all other values of x at least in the beginning x square increases and this decreases therefore, the function has a shape like that ok. And since it is in the properties this is an even function. It has a shape like that they are the same. If you want to look at they are symmetric anyway well as near me as you can. Now you would see right away that x is equal to 0 seems to be a minimum, this is the value and also this is 1 by root alpha and this is minus 1 by root alpha where, the function is a maximum and the derivative here is 0, the derivative here is 0.

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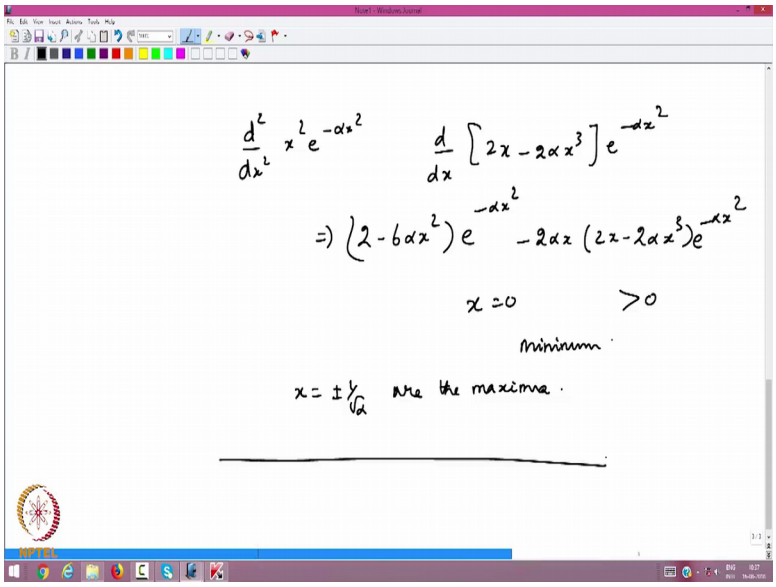

The other way is to look at calculate d square by d x square on x square e to the minus alpha x square. And since you know that it is already d by d x 2 x minus 2 alpha x cube e to the minus alpha x square. So, this will be 2 minus 6 alpha x square times e to the minus alpha x square that is one term. And the second term is minus 2 alpha x 2 x minus 2 x cube times e to the power minus alpha x square.

Therefore, if you put x is equal to 0, you can see immediately that this goes to 0 this is 2, this whole term is 0. Therefore, this is greater than the derivative is greater than 0, second derivative. Therefore, this is a minimum this is what you saw in the graph ok. Now, if you put x is equal to 1 by root alpha you can see that this is x square is 1 by

alpha and this is alpha cancels out this is 2 minus 6. And then you have x is equal to 1 by root alpha and if you do that the whole thing will turn out to be negative ok.

Whether you put plus alpha or minus alpha 1 by root alpha plus or minus 1 by alpha both will give you the second derivative to be less than 0. So, x is equal to plus or minus 1 by root alpha or the maxima for this function. I think that is what this problem is all about. The idea behind these problems that is being discussed in detail is that some of the mathematics, which you might find in your first attempt to do this.

If you find them difficult that is some help here, but ideally I would like you to do the mathematics yourself and then come back and check on the way it is being done. And if there are any mistakes, which have been made in the lecture please let me know and I shall correct the corresponding video lecture and we will replace it with the corrected one. We will continue with the lectures.

And until then thank you very much.