Atomic Structure and Chemical Bonding
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Lecture – 20
Particle on a Ring: Expectation Values for Angular Momentum

Welcome back to the lecture. We will continue with the second part that is about it I think this is with this part I shall conclude the particle in a ring in a rather elementary introduction that I have given.

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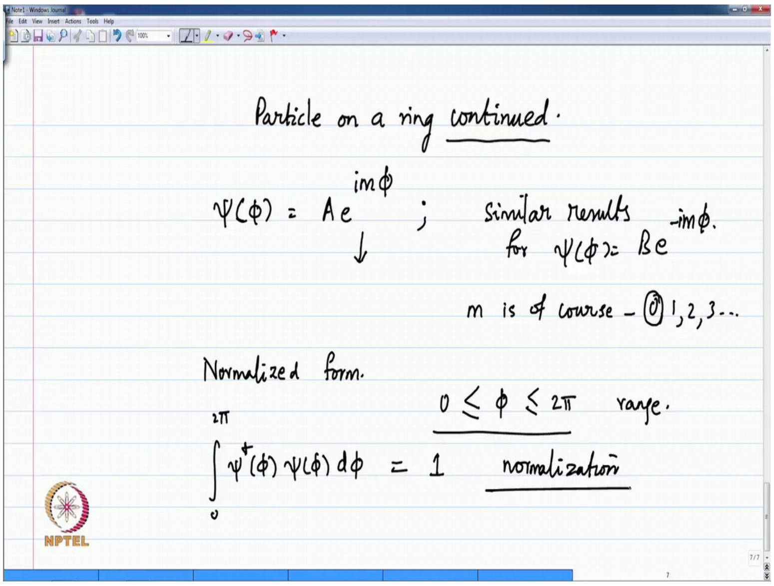

So, we shall look at a little bit more from what we left. Namely we have this the wave function being given by an exponential m phi or phi I mean I keep it a changing them, but you know what it means. And m is of course, we are taking positive values here 0, 1, 2, 3 etcetera. Now, the 0 is something that we have to consider a little bit later let us just worry about 1 2 3 and as integers.

If this is the wave function what about it is normalized form? A is a normalization constant because we always concerned ourselves with the making sure that the wave functions are normalizable. Therefore, the square of the wave functions can be associated with the probability description and the probability density.

In here the normalization is done in the fashion in which I mentioned namely the all the values of phi for which the wave function is unique for different values of phi the wave function is different. It has one value for one phi and of course, you know that with that particular range is between 0 and a 2 pi. Because after that the wave function simply repeats itself therefore, this is the range even though other values are considered this is the range for normalization different values therefore, what you have is psi star phi, psi phi d phi between 0 and 2 pi that should be made equal to 1 for normalization, yes.

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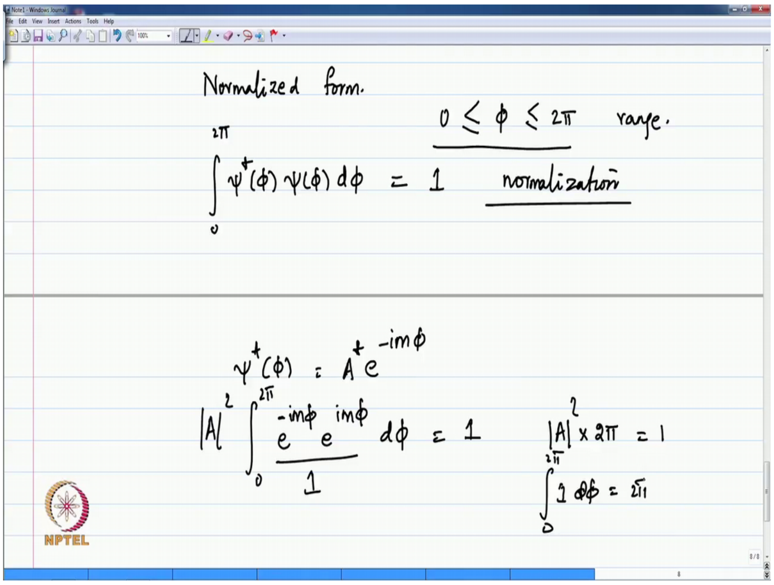

So, if you do that then essentially you know psi star phi is of course, A star e to the minus im phi because we do not know what A is, whether the A is real or imaginary. But we will write it as A star and therefore, what you have is the integral is the absolute value of A square, between 0 to 2 pi e to the minus im phi, e to the im phi d phi that is equal to 1. And this of course is 1 therefore, you have the absolute value of A square times 2 pi is equal to 1 because the integral of 1 d phi between 0 and 2 pi is of course, 2 pi.

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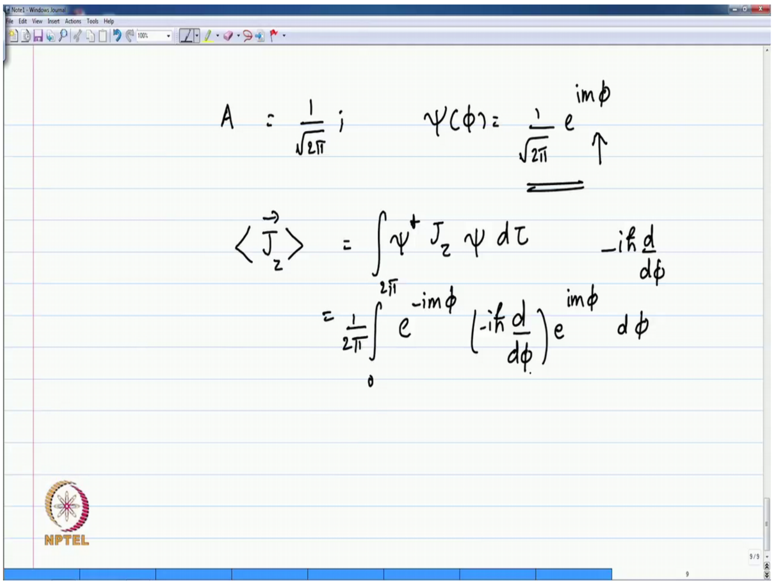

So, you have A, we will take it as real as 1 by root 2 pi. This is the normalization constant therefore, the wave function psi of phi is 1 by 2 pi e to the im phi. It is independent the normalization constant is independent of m unlike in the case of the harmonic oscillator where you found out that the normalization constant is also a function of the quantum number m because of the Hermite polynomials involved.

This is the wave function of course, in rotational motion the two things that we are concerned which is the rotational kinetic energy and the angular momentum of the particle. Now, if the wave function is given by this alone as we have chosen, then it is possible for us to calculate the angular momentum J. Since it points in a direction perpendicular to the actual plane of this circular motion and we shall call that as the z component, if he assumed x and y as the coordinates of the motion of the particle or the ring that we consider, the angular momentum is in the direction perpendicular to that. And that you know is nothing, but psi star the operator J z psi d tau which in this case the operator is minus ih bar d by d phi this is the angular momentum operator that you use to actually derive this result.

Therefore, if you calculate that you see it is exponential between 0 to 2 pi 1 by 2 pi because you have psi star psi. Therefore, this is the square of 1 by root 2 pi and then you have exponential minus im phi you have minus ih bar d by d phi exponential im phi d phi this is psi star psi I do not need the denominator because the wave function is already normalized.

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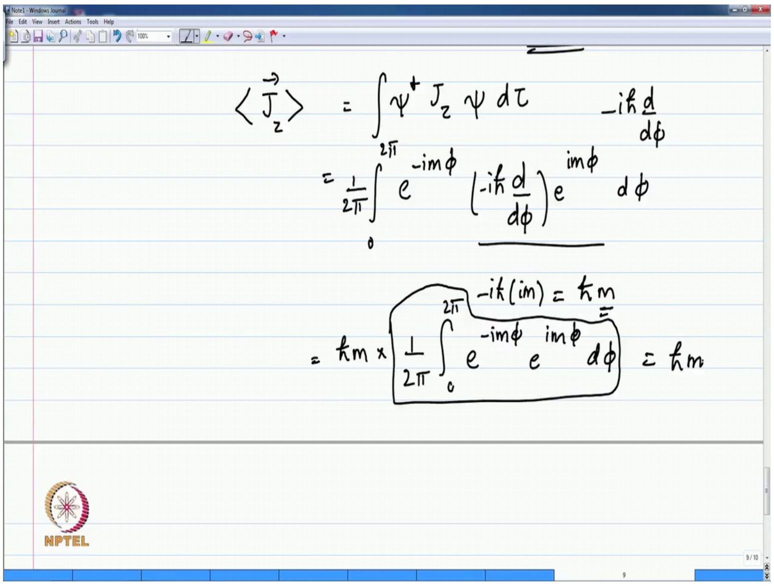

And it is easy to calculate this. This is minus ih bar d by d phi s i e m therefore, you have minus ih bar multiplying i e m which gives you h bar m and m is a quantum number, h bar is a constant. So, you can actually take that out therefore, you have h bar m times 1 by 2 pi between 0 to 2 pi e to the minus im phi times e to the im phi d phi and that is of course, you know that is nothing, but the normalization of this wave function itself. So, you get h bar m. So, the angular momentum is therefore, a quantized quantity.

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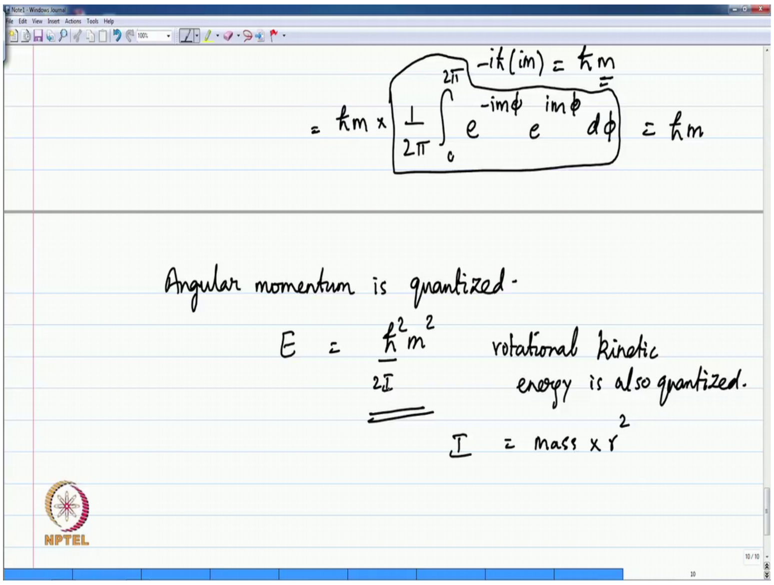

Angular momentum is quantized; you already have derived the energy E as h bar square m square by 2I. Thus energy is rotational kinetic energy is possible quantized, is also quantized. I have been careful enough not to include the rotational the potential energy, see there is a potential energy as I said in the last lecture rotational motion is in is an accelerated motion it is a non inertial motion.

And the particle or the system keeps moving around a point only because there is a central force directed towards the center of the rotation therefore, the potential energy cannot be ignored, we have ignored it because we assumed that the radius of the system is a fixed value. And for that given radius we found out that the energy is given by h bar square m square by 2I. Where is the information on the radius? Is actually in the value of I because that is nothing but the mass m times the r square where r is the radius, therefore it is already given in here.

If the radius is also a variable then the potential energy is actually a function of the radius and then whatever we have done cannot be done you have to solve the full Schrodinger equation in which that is the kinetic energy given by whatever we did namely minus h bar square by 2 I d square by d phi square that is one. Then you have to actually include the potential energy and then it is a two dimensional motion because it involves radius and the angle. That is something else, we will do that if you have to study in rotational motion as an internal degree of freedom in spectroscopy.

Here, we have not considered that we have only worried about the rotational kinetic energy as the total energy neglecting the potential energy and then you find out that the angular momentum is given by h bar m and that is a quantized quantity.

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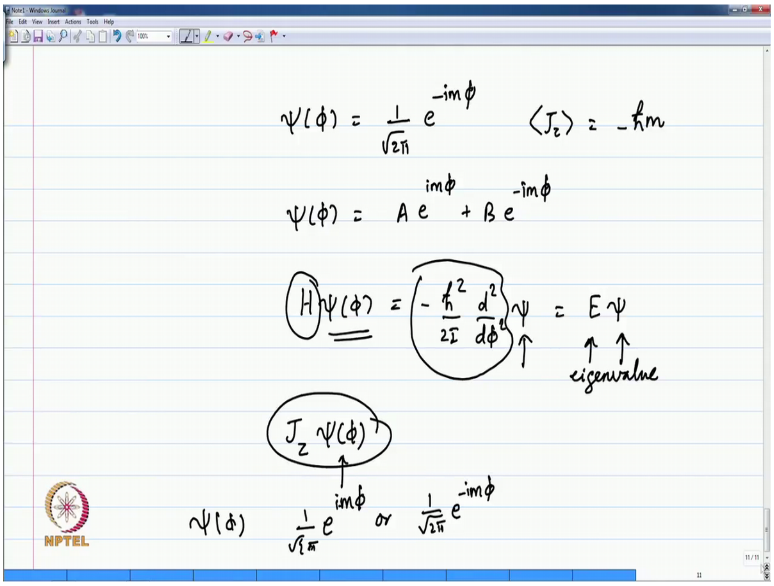

What about if you use the wave function e to the minus i m phi, e to the minus im phi? Should be obvious that if you calculate the angular momentum it is obviously, minus h bar m so, negative value.

The angular momentum therefore, has a directional sense either towards the perpendicular to the plane up or perpendicular to the plane down. But what is interesting is, what is if we use the general wave function namely A e to the im phi plus B e to the minus im phi because we do not know whether the particular motion is clockwise or anti clockwise we do not know what it is. Then we also do not know what the value the J z is not a fixed quantity.

Please remember when you wrote the kinetic energy H of psi phi was minus h bar square by 2 pi d square by d phi square psi and you wrote this as E psi. Therefore, you see that the Hamiltonian acting on the wave function, the Hamiltonian operator, acting on the wave function gave you the wave function and the energy and you remember that this was the eigenvalue equation.

Therefore, the energy was an eigenvalue for this problem and the psi is an eigen function likewise, if you write the J z operator and write psi phi. If psi phi is either exponential e im phi 1 by root 2 pi or 1 by root 2 pi minus sorry 1 by root 2 pi exponential minus im phi, if the wave function is either this or that. Then you also see that the angular momentum J z acting on psi phi gives you that angular momentum value which is as you remember minus h bar d ih bar d by d phi 1 by root 2 pi exponential plus or minus im phi.

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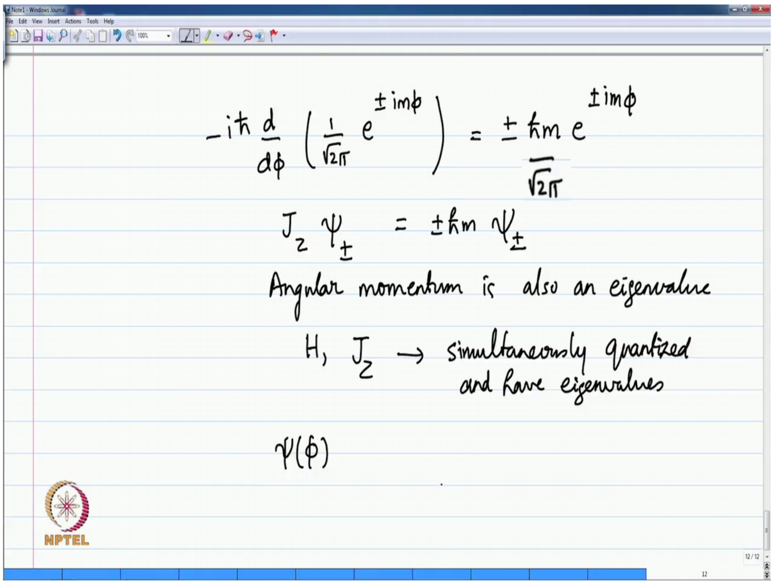

If I put that in then you will get the answer minus r or sorry what do you get plus or minus yes, plus or minus h bar m e to the plus or minus im phi. So, the pluses for the plus and the minus is for the minus therefore, you see that the angular momentum operator J z acting on psi gives you plus or sorry yeah plus or minus h bar m psi and I will write it as plus minus, plus minus here to say the plus component is e to the im phi the minus component is e to the minus power im phi.

Angular momentum is also an eigen value, is also an eigen value that is H and the angular momentum are simultaneously quantized and are observables and are eigenvalues of psi and have eigen values, simultaneously I have to think about this. If the wave function is not given by one or the other component of the exponential im phi, if the wave function is given by a linear combination of the 2, these are the two possibilities in the m of course, takes different values. And therefore, the psi is what you have infinite number of wave functions and infinite number of energies for the particle fixed to a particular radius because that radius fixes the value of I the moment of inertia.

Therefore the energy is given by that unit h bar square by 2 I that is the fundamental unit for that problem, but if the wave function is the linear combination of the plus or minus im phi then the angular momentum operator does not rather an eigen value. Because if you write psi phi is A e to the im phi plus B e to the minus im phi if you write that and you can normalize this.

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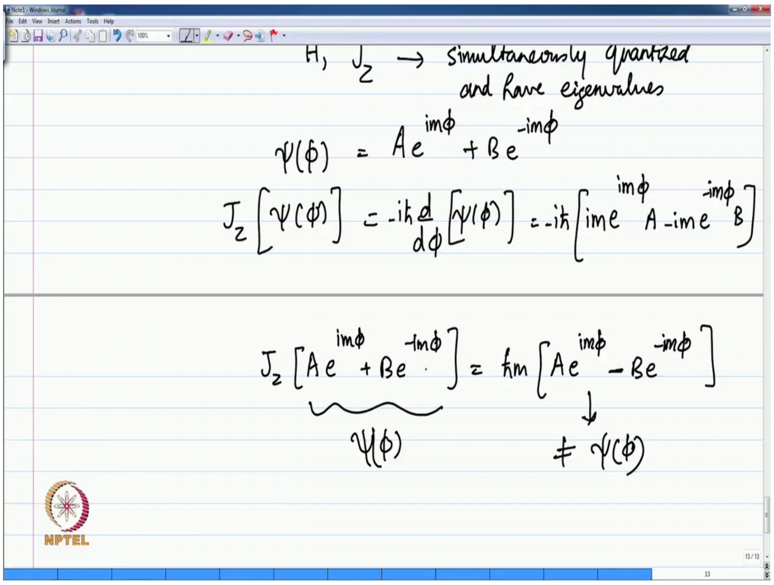

If you try to calculate the expectation value sorry, if you calculate J z acting on this psi phi please remember J z is minus ih bar d by d phi on this wave function psi phi. And please note that this is going to give you the d by d phi acting on im will give you plus im and therefore, you will get minus ih bar im e to the im phi with A of course, and then you will have for the B you have minus im e to the minus im phi B. Therefore, you see that you are going to get J z acting on A e to the im phi plus B e to the minus im phi gives you now h bar m times A e to the im phi, but with a minus sign B e to the minus im phi.

This is psi phi, this is not equal to psi phi this is something else therefore, you have an operator acting on a function giving you something else, not the function back. So, it is not an eigenvalue equation. What does that mean? Angular momentum does not have a precisely defined value if the wave function is a linear combination A to the im phi plus

B to the im phi does that mean angular momentum cannot be defined, it cannot be defined as to have a unique value. And the average value can always be calculated, an average value in quantum mechanics is essentially the wave function star the operator associated with the wave for the a measured value and acting on the wave function integral you remember that.

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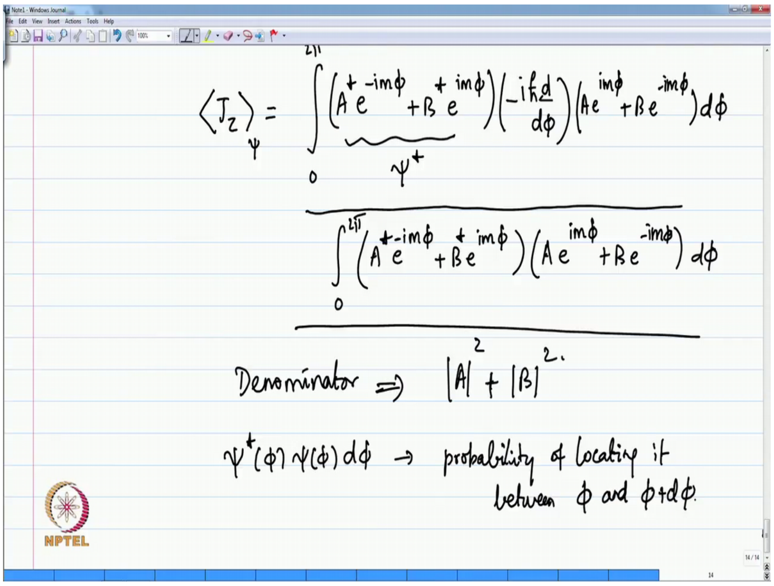

Therefore, the angular momentum does not have a unique value. But an average value of the angular momentum can always be calculated for such linear states, linear combination states by the same thing 0 to 2 pi you will have A star e to the minus im phi. Because this is psi star plus B star e to the im phi this is the psi star acting on now with the operator minus ih bar d by d phi, acting on the psi which is A e to the im phi B e to the im phi d phi. But please remember this wave function we have not yet normalized therefore, we have to make sure that we write the psi star psi in the denominator namely 0 to 2 pi A star e to the im phi plus the B e star A star minus im phi plus B star e to the im phi, multiply by A, e to the im phi plus B e to the minus im phi d phi.

This is a very elementary integral anybody can calculate that, I think with all the mathematics that you have done so far you should be able to calculate this. It is easy to see that this will give you the denominator will give you, A square absolute A square minus absolute B square, sorry plus B square B start a to the yeah plus B square. But the numerator will give you something else.

The average value can be defined, but and eigenvalue does not exist. What does that mean? That means, that if the wave function if the particle particles motion is not very clearly known as a clock anti clockwise or as clockwise then we do not know whether the angular momentum vector is pointing upward or point pointing downward this is an average value that is means you can only do this many times and every measurement gives you some result. And then you take the average and that is the sense in which the angular momentum plays a very definite role when you come to particle in the box, particle on a ring.

I think this exists also in the particle in a box, if the wave function for a particle in a box is not a precise eigen state of the energy, but it can be linear combinations of the eigen states of multiple eigen states of energy as you have here, you have a similar problem. Therefore, please remember this is also the first instance in which I am giving you a slightly more difficult problem that the eigenvalues and the expectation values need not have to be the same, when the state of the system is not precisely defined to be an eigenstate. Is this state an eigenstate of the energy operator this linear combination? Of course, it is please remember the energy operator has d square by d phi square second derivative operator.

The minus m which comes in when you operate the derivative on this function once it is at some it becomes plus m square. Therefore you get the energy of course, that is how you solve the Schrodinger equation and I gave this as a general solution therefore, this is a general solution what you have written here namely the A e to the im phi plus B e to the minus im phi that you have here on the screen. This is also an eigenfunction of the energy operator, but it is not an eigenfunction of the momentum operator for particle in the box, a particle on a ring I mean portion on the ring comes out with something you need.

The probability here is a problem because you know psi star psi is constant is 1 therefore, it is 1 by root 2 pi and the probability of finding the particle on a circle in any region is precisely proportional to that region and it is a constant. It does not vary like what you have for a particle in a box. If you say psi star psi define is the probability of locating the particle between phi and phi plus d phi and phi plus d phi between.

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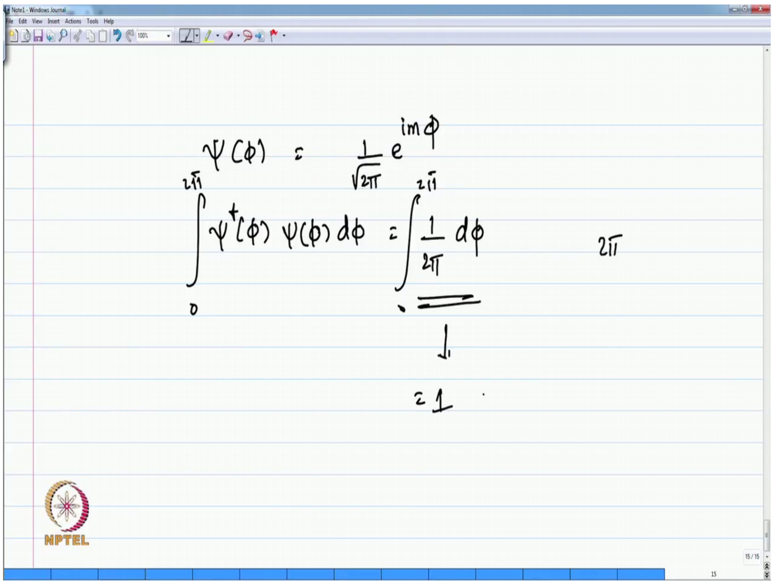

Then you know that if the wave function is psi of phi is A sorry it is 1 by root 2 pi e to the im phi then psi star phi psi phi d phi is 1 by 2 pi d phi because the exponentials concerned each other. Therefore, you see that the probability is proportional to the part of the ring, the length of the arc in a ring that we look at.

What is the total length of the arc on the ring? What is the time? What is the circumference? 2 pi. Therefore, you see that the probability of locating the particle in any region is uniformly the same and is purely proportional to the length of the arc, unlike the particle in a one dimensional box where it is quite different. So, there is a subtlety here. As long as the particle is moving on a circle its probability of locating it instant certain medium is simply proportional to the length of the region. And of course, the total probability is 1 therefore, anywhere on the circle if you want to calculate you have to do for all values of phi it becomes obviously, 2 pi and therefore, psi star psi will be phi between the entire region is of course, that 0 to 2 pi and that is equal to 1.

So, the probability does not come up it, but please remember this is for e to the im phi, it is the same thing for e to the power minus im phi, and I will ask you to calculate the problem the inner problem in one of the quizzes what is the probability if it is a linear combination of the wave function. The mathematics is very simple you should be able to do that.

So, particle on a ring has 2 or 3 important summarized results, one would be summary. Let me write the final summary here.

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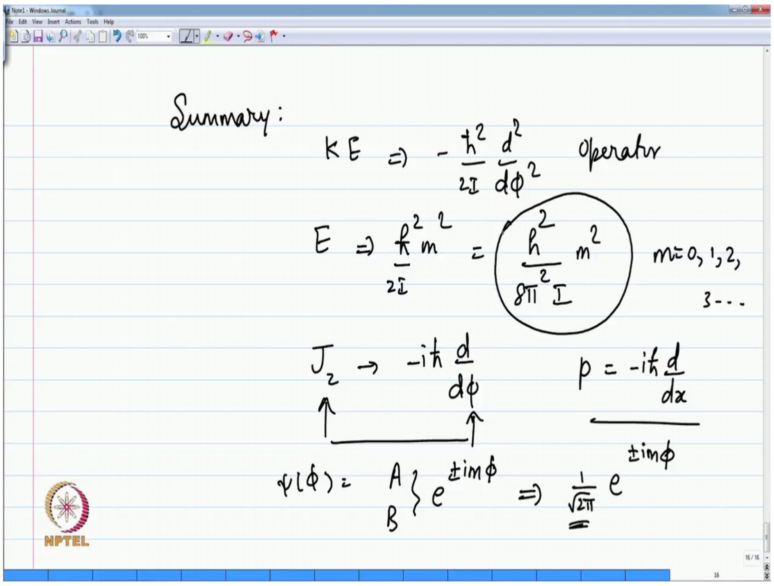

Kinetic energy, we wrote this as minus h bar square by 2 I d square by d phi square operator, kinetic energy operator. Energy is h bar square m square by 2 I which if you have to write it is h square by 8 pi square I m square m is 0, 1, 2, 3 etcetera.

M is equal to 0 is a perfectly acceptable quantum number here, because all it means is that the particle does not have the rotational kinetic energy it stays somewhere on the circle. It does not violate in the uncertainty principle because if you say that m is 0 we say that its angular momentum is exactly 0, if the angular momentum is 0 please remember angular momentum is given by this operator minus ih bar d by d phi. And therefore, the angular momentum and the angular coordinate have the same relation like the linear momentum and the linear coordinate that you have for a particle in a one dimensional box. They satisfy a commutation relation. Therefore, the location of the particle cannot be specified precisely if we know in a precise value for me the linear momentum.

The same thing here, if we know precisely the value of angular momentum we do not know exactly where the particle is it is anywhere on the ring therefore, it is as uncertain as the dimension that you are worried about. Therefore uncertainty principle does not violate is not violated. So, m is equal to 0 is allowed which means rotational energy is equal to 0 particle stationary, but you do not know on what part of the circle what is arc of the circle that it is in. So, the uncertainty rules are not violated in any way, unlike the particle on a in a box where since you do not have the possibility of the particle in a box having a very precise position and a very precise momentum or part for a particle in the ring we do not have that problem.

So, this is the other important variation from the particle in the box. And finally, the wave functions are given by A or B if you want to write e to the plus or minus im phi and m is of course, plus m is with the notation constant essentially it is 1 by root 2 pi e to the plus or minus im phi which is the normalization constant. So, these results are important, but this particular result will be very useful in what is known as the microwave or rotational spectroscopy. I do not know that I will talk about that in this course, but the particle in the ring is an extremely important model for understanding the elementary rigid body rotations of diatomic and polyatomic molecules.

Therefore, I hope I have introduced you to something slightly different from the usual the quantum results that you see, particle in ring is slightly more subtle than any other model. And that has to be kept in mind.

Until then thank you very much.