Quantum Mechanics
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Lecture - 37
Tutorial - 06 (Part I)

We are continuing with tutorial 6 and we are supposed to solve the 4th problem. So consider a particle in a Coulomb potential in three dimension, so the potential is a Coulomb potential and you have to evaluate the commutative bracket of the angular momentum operator Li and the Hamiltonian. So here the Hamiltonian will be the; will have the kinetic term plus the Coulomb potential term. So let us get started with this.

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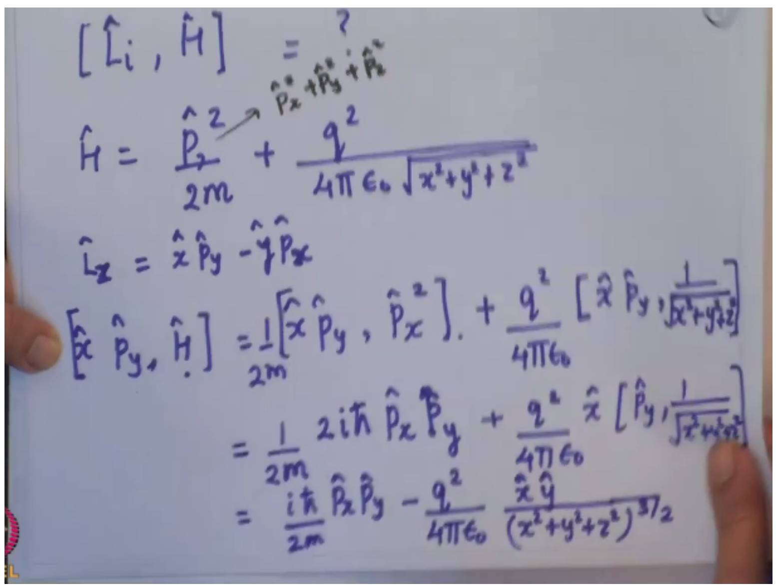

We have to obtain the angular momentum with the Hamiltonian. So expression for the Hamiltonian; this is the question. We have evaluated such question but the Hamiltonian what was different the potential term was different. So the Hamiltonian here is P square upon 2m this is the kinetic part. Now the potential is Coulomb potential so you have a q square upon 4pi epsilon0 square root of x square + y square + z square, okay.

And this p square when I write explicitly is Px square + Py square + Pz square, okay. So we will start by writing Lx as; Lx is or Lz is Lx Py – Ypx. Here we can evaluate first Lx or Ly or Lz. So first term first that is let us evaluate X P Y on the Hamiltonian. This term would give us X P Y.

This is X Px Py Pz okay. And we know from our previous experience that only Pz term contributes, so I will write Px square and 2/m I have it here.

And for the second term we have commutative of + q square upon upon 4pi epsilon0 commutator of; here you have X cap and Py so commutative of this would be 1/square root of y square + z square so this will be 1/x square + y square + z square. So here we have the first term we have seen that consists of Px square + Py square + Pz square upon 2m. The second term is the potential term Coulomb potential term which is q square upon 4pi epsilon0 square root of x square + y square + z square.

And we are finding out the commutator of X cap and Py cap with the Hamiltonian operator. So in the Hamiltonian operator we have two terms so correspondingly we will have two separate terms of the commutator. Then this we remember we can recollect that this was = 1/2m; remember this and X cap and Px square commutes. So we will have commutation of X and Px square that is 2i h cross Px cap and you have a Py.

So the first term is very simple to evaluate you have a computer of X and P; position and momentum which we very well know now. Second term is q square upon 4pi x0 so x cap we will take out because it will not contribute to the commutator bracket only term that will commute contribute to the commutative bracket is Py, so you have Py x square + y square + z square. Now there is a small trick involved here, you will have to find the commutator of this expression and that comes out to be I h cross Px cap Py cap upon 2m.

Commutator of this expression will be very simple you have to apply the momentum operator Py on this and the other time you will have the momentum operator this operating on the momentum Operator So this will come out to be -q square upon 4pi epsilon0 times x*y operator position operator x and position operator y upon x square + y square + z square the whole raise to 3/2, so this is the expression for commutator of X P Y with Hamiltonian. Similarly, you can evaluate Y P X on the Hamiltonian. We will get a similar expression.

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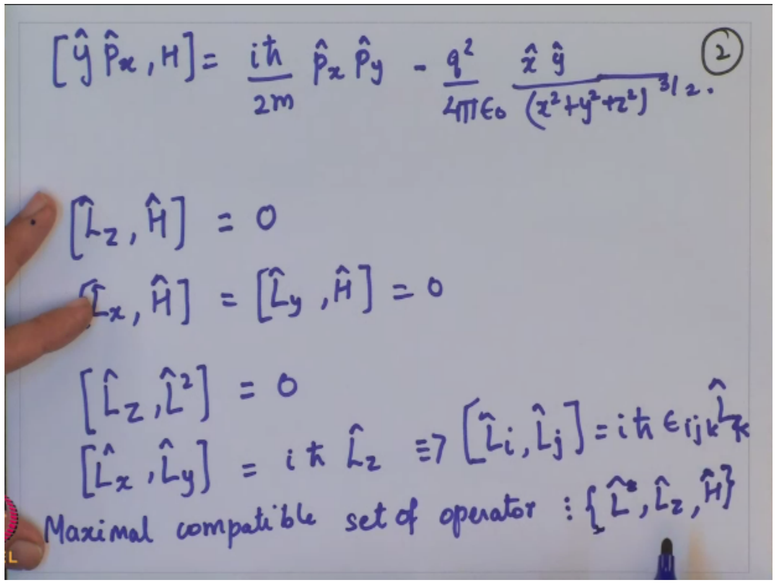

Y Px on the Hamiltonian I will get a similar expression -q square upon 4pi epsilon0 X cap Y cap upon x square + y square + z square the whole raise to 3/2. Okay. So this expression we obtain for the Lz so Lz precisely that is the angular momentum along the z direction will be precisely 0. Similarly, you can obtain for Lx Ly and commutator of Ly, commutator of Lz with h to be 0. So we have to also do in the second part what will be the list of maximum or maximal compatible set.

So what you can think of is one more thing you can help you know or you have seen commutator of Lz with L square is 0. So the; and you also know this relation i h cross Lz. In general, this is Li Lj I h cross epsilon Ijk Lk this expression you know. When you make a cyclic rotation you will have three commutation relations which will result in Lx Ly or Lz. So all these are right, I am writing because we want to find the maximal compatible set of operators.

So since Lz and L squarer commute they can form a simultaneous eigenket. Similarly, here you have seen that these Lz and the Hamiltonian operator commutes so they can form all simultaneous eigenket. However, Lx and Ly or any of these Li and Lj they do not commute so one cannot obtain simultaneous eigenket for these operators. However, when you obtain Lx when you operate Lx with L square or Ly with L square or Lx with L square you can have a simultaneous eigenket because these Ly's with L square commute.

So the maximal compatible, maximal compatible group or set of operators are L square, okay at that is Lz and H. You can very well write here Lz instead of Lz you can also have or you can have Lz and Ly; you can have a compatible set of L, Lx, H or L, Ly and H. So these form the compatible set of operators. And these operators can be such that when you pair them you can have you can form a simultaneous eigenket for these operators.

And we have seen in the tutorial 5 some example wherein you had two operators which commute so the eigenket obtained by operator one operator say B was the simultaneous eigenket of operator A. In the previous problems we have seen such examples. So this was problem 4. Problem 5, I think part of it was done in the class that is one needs to know how to derive this Schrodinger equation in polar coordinates.

It is very interesting to get the result which is given in the question that you can try by writing the Cartesian coordinates in terms of polar coordinates. And when you rewrite in polar coordinates you obtain this Schrodinger equation which is a function of R capital R, capital Theta and capital Phi.

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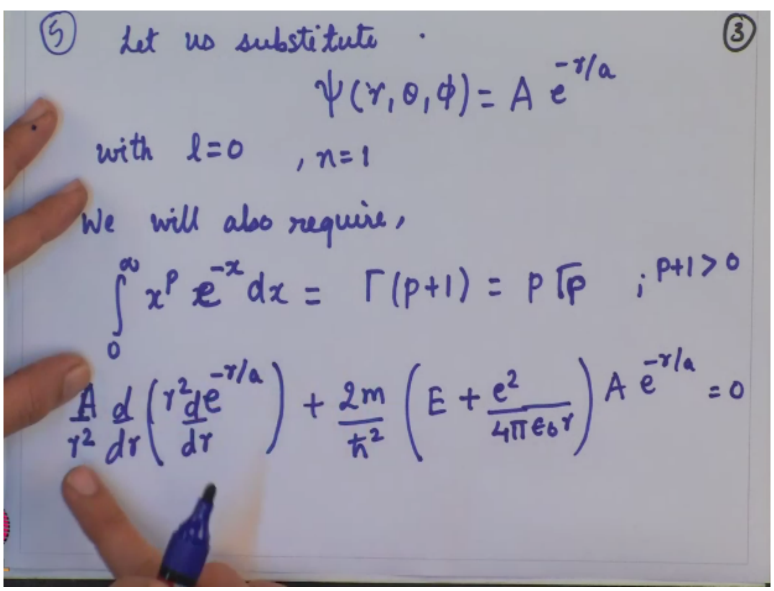

So if give wave function, in the radial part let us substitute let us substitute Psi we are given R theta and Pi as e raise to –r/a this is given with we will assume that n is 0. So let us simplify that L is 0. So when L is 0 n can take value 0 to 1 so n, we assume n=1, okay. And now we also we will also require this Gamma function integral. So you will be using this which is nothing but P gamma of P. And P+1 > 0. So this is y we are going to use. So we will try to evaluate or substitute the wave function for the ground state.

So when you substitute the wave function in the radial part of the equation you have the first term is 1/r square, d/dr of r square. And in the wave function you have A, e raise to –r/a, so e raise to –r/a okay; r square d/dr so r square this is the first term; the second term is cross square e + e square upon 2pi epsilon0 r. So this term will remain untouched. So I have A e raise to –r/a 0. So this you can easily do you have to take the derivative with respect to r, this will give me –A and I will have derivative with respect to r square.

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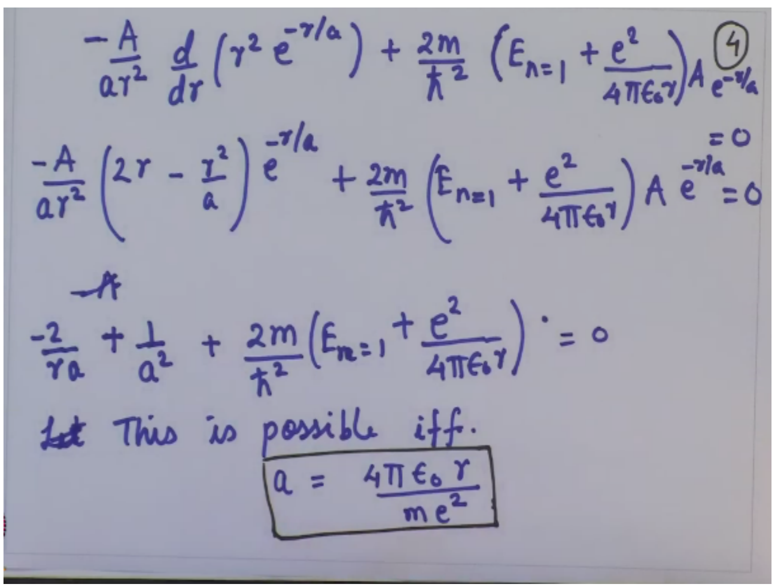

Here you will have –A okay upon; in the previous term we had a upon r square so let me write a upon r square and derivative of e raised to –r/a I will have a A term so I will have a – sign then I have d/dr okay. First term I have r square e raise to –r/a, okay. So again this is A/r square derivative of e raised to –r/a will give me -1/a. So I write here -1/a and I have derivative with respect to r square and e raise to –r/a.

So this we have to evaluate + 2m upon h cross square into e where e is for the ground state n=1+ e square upon 4pi epsilon0 r times the wave function. The wave function is nothing but A e raise to –r/a, so this will be A e raise to –r/a; I will write right downstairs. This entire thing is equal to

0. So I have here –A a/r square derivative of this I will have two term, so I have here 2r; I will have e raise to –r/a - minus r square/a times e raise to –r/a + 2m upon h cross square; this term will remain as it is; it will come down because there is nothing to operate on.

This is e+ e square upon 4pi epsilon0 r times the wave function A e raise to –r/a which is 0. Now in the next step we can actually take these wave functions out. So I have A, I have to take A out so I will have 2- 2pi r first term times A then the next term will be +1/A square because r square r square will get cancelled so I have first two terms of the first term plus I will have 2m upon h cross square e=1+ e square upon 4pi epsilon0 r times the wave function. So this entire quantity is equal to 0. This coefficient is equal to 0.

So here what we do is we will try to simplify this further. So let us or rather this is possible only when if this term is going to 0 that is I can take h cross square upon 2m times this expression this goes to 0 this expression times this part, okay. So when you simplify this if and only if A okay; if and only if A is equal to 4pi epsilon0 r upon m e square. So this is possible only if A is 4pi epsilon0 r upon m e square.

So what we have done here is that if we have assumed that this quantity is nothing but 2/r, okay. This entire quantity is nothing but 2/a, okay. S we have got a relation with respect to of A in terms of e0, okay. So what we have assumed here that this quantity is equal to this term, okay. So with this we have A is 4pi epsilon0 upon r upon m e square. So from this if we substitute for A we will be able to obtain the value of energy the ground state energy. So we have to substitute. So after substituting again this is nothing but Bhor radius, okay.

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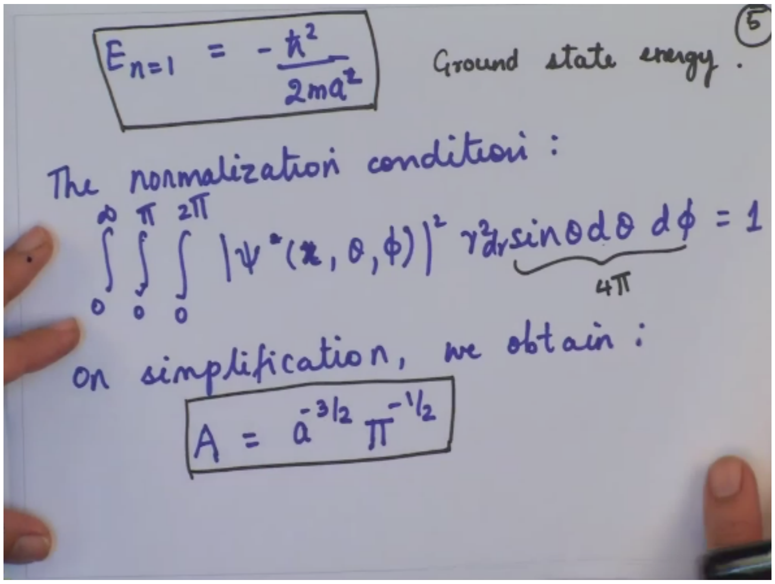

Now we will get the value of the ground state energy is given by; from the previous expression we can get this as 2ma square, okay. So this will be the expression for the ground state energy, fine. Now we have obtained the ground state energy; we have obtained the value of small a; we have to obtain the value of capital A. So capital A we can obtain by taking by get; A is a normalization factor capital A.

So by performing the normalization condition using the normalization condition that is integral over r theta and phi; r goes from 0 to infinity; theta goes from 0 to pi and phi goes from 0 to 2pi. So when you integrate r theta and phi that is Psi square r theta and phi okay this is square, r square sine theta, d theta, d phi and you have a dr also, okay. This should be equal to 1. So we know what is the value of the wave function given to us that is a square exponent of; so we will on simplification we obtain.

What do we obtain? Value of capital A as this you can check. It is not difficult and I have given you the hint you will just substitute for Psi square which is a square e raise to -2a 2r upon A. And then you integrate over r square, so integral over sine theta d theta will give you 4pi, so this integral will give you 4pi and the remaining integral is r square e raise to -2r upon A and you have to use the gamma function.

This will simplify A to this. So please check this, it is a simple integration. And in the next part we are asked to find out the mean distance, so again this B part is to find out; in the B part you have to find out the mean distance.

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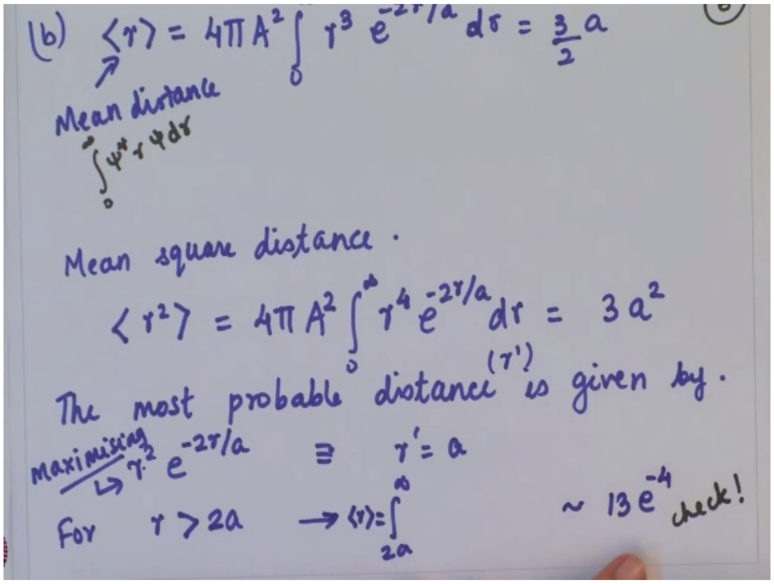

So the mean distance is the average which you can easily do is Psi* r Psi, very simple expression. So it will be 4pi A square 0 to infinity your; when you take Psi* Psi you obtain r cube e raise to -2r upon A which is into dr which is nothing but 3/2a. So this is the mean distance. So mean distance is one thing you have to evaluate; the root mean distance and the most probable distance these are the three quantities you have to evaluate for the electron in the nucleus with the ground state.

So this was the mean distance, this is the mean distance, okay which was obtained by; mean distance how I evaluated it, Psi* r Psi dr as simple as this 0 to infinity, okay. The next part is the mean square, mean square distance. This also you can evaluate mean square distance will be r square that is 4pi A square 0 to infinity. Now you have a r square so this becomes r raise to 4, e raise to -2r again you will use gamma function and get the result for this.

So this comes out to be 3a square, okay mean square distance comes out to be 3a square. And you can similarly calculate the most probable the most probable distance is given by; what we have to do is we have to maximize this quantity that is Psi*; r square Psi*Psi. So you have r square -2r upon A. So when you maximize this, this will lead to r equal to some or r prime equal to some A. And then you can obtain for that particular value of r or r prime we will have the most probable distance.

So the most probable distance let us call it as some r prime so that r prime is given by maximizing this quantity. When you maximize this quantity this will lead to r prime = A. So the most probable distance is equal to small a which is nothing but the Bohr's radius which we have evaluated. So with this end of this part third part is actually you have to calculate the classical and quantum mechanical probability for $r > 2a$. That is a easy check you can just do it for $r > 2a$.

So when you put the limits your limits will be from 2a to infinity; instead of 0 to infinity your limits would change for $r > 2a$ your limits of integration will be from 2a to infinity when you calculate the mean value, okay. So classically and quantum mechanically you have to evaluate for; for quantum mechanically you will integrate from2a to infinity for the expression and it is very simple. So this would come out to be something like 13 e raise to -4. So please check this if it is correct.

And with this we end this tutorial. And we will have more problems on harmonic oscillator or hydrogen atom. Based on these problems we will have further tutorials.