# Basic Quantum Mechanics

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**Module No. # 06**
**Hydrogen Atom and other Two Body Problem**
**Lecture No. # 05**
**3D Oscillator and Dirac's Bra and Ket Algebra**

In my last lecture, we had, at the end of the last lecture, we were considering the solution of the Schrodinger equation, for the 3 dimensional isotropic oscillator. We will, in this lecture continue our discussion on that and make a few comments about the 2 dimensional oscillator, which is also a problem of great interest in quantum mechanics particularly in the theory of magnetism.

And then, we will hopefully start on the Bra Ket algebra formulation of quantum mechanics, so we continue our discussions where we left off in the first in the previous lecture.

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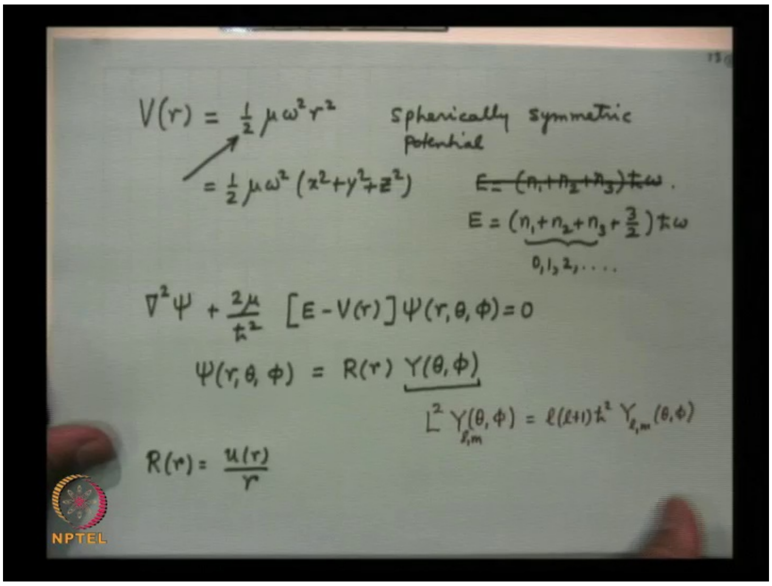

We were considering a spherically symmetric potential which is half mu omega square r square, it is a spherically symmetric potential it is a spherically symmetric potential. In my previous lecture, I wrote this as half mu omega square x square plus y square plus z square; and solved the Schrodinger equation in Cartesian coordinate and obtain the Eigen values as E is equal to n 1 plus n 2 plus n 3 h cross omega sorry I am sorry, I am sorry, this we had obtained as E is equal to n 1 plus n 2 plus n 3 plus 3 by 2 plus 3 by 2 h cross omega.

Where each of these integers n 1, n 2, n 3 can take values 0, 1, 2, 3 etcetera. Now, if I use this equation, then we can as we had shown earlier, we can solve this equation 2 mu by h cross square E minus V of r psi and we will we can use the method, we can use this spherical polar coordinates, r theta phi to solve this equation.

Since, the potential energy function depends only on the r coordinate, we can write the solution as psi of r theta phi as R of r times Y theta phi, where Y theta phi are the Eigen functions of the operator L square as we had seen that that y theta phi are the spherical harmonics. Which are L square Y theta phi was equal to l into l plus 1 h cross square Y l m, sorry this is also Y l m theta phi, these are the spherical harmonies (Refer Slide Time: 03:55).

So, if I substitute this, in this equation then you will get the radial part of the Schrodinger equation, and if I define a function R of r u of r such that, R of r is equal to u of r by r then u of r satisfies the following equations.

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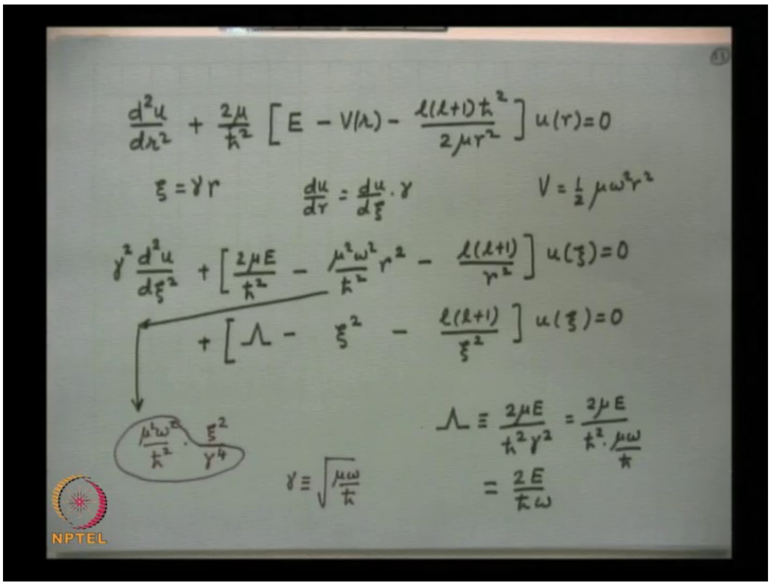


This is the d 2 u by d r square plus 2 mu by h cross square E minus V of r minus V of r minus l into l plus 1 h cross square by 2 mu r square u of r is equal to 0, this is the radial part of the Schrodinger equation. This is one of the forms of the radial part of the Schrodinger equation, and this simplification this simplification is always possible as long as the potential energy function is spherically symmetric.

So, now we assume that V of r is half mu omega square r square, and then we write down as we have done for the harmonic oscillator that xi is equal to gamma r gamma r, so this becomes d u by d r becomes d u by d xi into d xi by d r which is gamma. If I differentiate this again, so you get d 2 u by d xi square multiplied by gamma square, so I want to put this down in the denominator, so plus please see this, 2 mu E by h (()) let me write this down here, then I will do it again.

And this is half, my potential energy is half mu omega square r square, so half into 2 cancel out, so you get mu square omega square by h cross square r square, if I take 2 mu by h cross square out inside, so you get minus l into l plus 1 r square u of xi equal to 0. So, I divide by gamma square, so I get plus 2 mu E by h cross square gamma square, so I write this as capital lambda, where capital lambda is defined to be equal to 2 mu E by h cross square gamma square and this becomes please see, r square is xi square by gamma square.

So, this term becomes this term becomes mu square omega square by h cross square r square is xi square by gamma square and there is one gamma square coming from here, so this will become gamma to the power of 4 (Refer Slide Time: 07:26). Now, I choose my gamma, so that this factor is 1, I have not yet this is the same method that we had used in solving the harmonic oscillator problem, so I choose gamma, so that this is equal to under root of mu omega by h cross.

If I choose this value of gamma, then this coefficient becomes 1 and this becomes minus xi square, and the last term l into l plus 1 gamma square r square, so that is xi square; so minus l into l plus 1 gamma square r square, so that is xi square u of xi is equal to 0. So, gamma square, so from here gamma square is mu omega by h cross, so this becomes 2 mu by E by h cross square mu omega by h cross, so mu mu cancels out, so you get 2 E by h cross.

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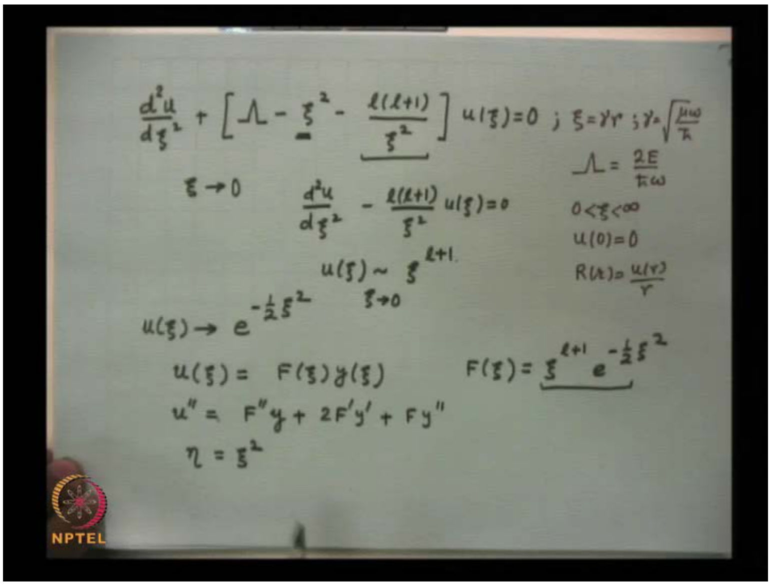


So, the Schrodinger equation simplifies to simplifies to the radial part of the Schrodinger equation, simplifies to d 2 u by d xi square plus lambda minus xi square minus l into l plus 1 by xi square u of xi is equal to 0, where xi is equal to gamma r gamma r, gamma is equal to under root of mu omega by h cross. Now, lambda is now the Eigen value, so lambda is equal to 2 E by h cross omega, you must remember that xi now goes from 0 to infinity and of course, u of 0 will be 0, because at the origin you have R of r is equal to u of r by r.

So, at r equal to 0, so u u of 0 will be 0, these are the boundary conditions and u of infinity is 0, now we use the same trick, same methodology as we (()) used in the hydrogen atom problem, as xi tends to 0 this term dominates and you will you can the solution of this term is d 2 u by d xi square minus l into l plus 1 by xi square u xi. This will be u of xi will be xi to the power of l plus 1; because if you differentiate this twice it will be l plus 1 into l xi to the power of l minus 2 l minus 1, so that is what it (()), so as xi tends to 0 it behaves like this.

As xi tends to infinity it is this term which dominate, we had experienced this term in the harmonic oscillator problem, so the the if you recollect that, so u of xi as xi tends to infinity behaves as e to the power of minus half xi square. So, we this suggest that we try out a solution just as we did in our hydrogen atom problem F of xi y of xi, where F of xi is equal to xi to the power of l plus 1 e to the power of minus half xi square.

So, as you recall that we had u double prime is equal to F double prime y plus 2 F prime y prime plus F y double prime, and we can calculate F prime from here, F double prime from here and we have to make one more. These are rigorously correct solutions rigorously correct solutions, we make another transformation that we define a new variable eta is equal to xi square as we had done in the harmonic oscillator problem. If I substitute this for F of xi and then make a transformation eta is equal to xi square.

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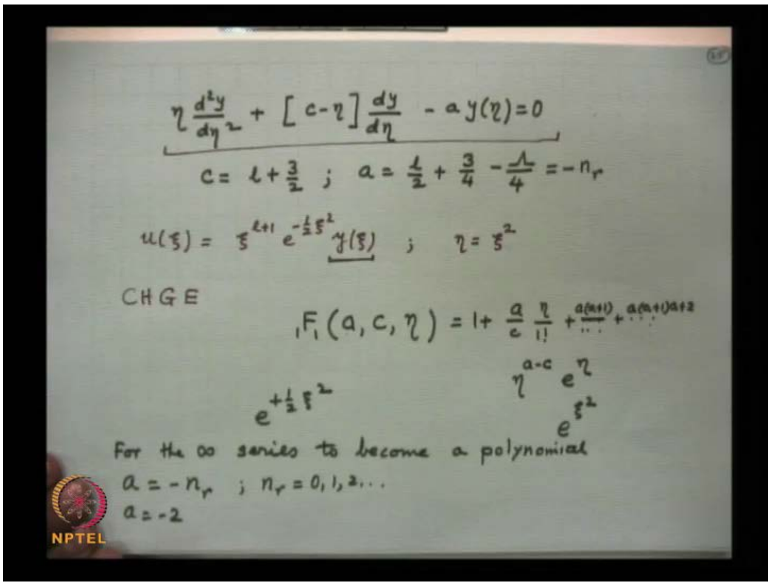

Then the y satisfies this equation, eta d 2 y by d eta square plus c minus eta d y, I leave that as an exercise to show this minus a y eta is equal to 0, where c will and we shown to be equal to l plus 3 by 2 and a is equal to l by 2 plus 3 by 4 minus lambda by 4. So, once again what I have done is that that u of xi, I have written as xi to the power of l plus 1 e to the power of minus half xi square into y of xi and then obtained an equation for y of xi.

And then we have since, there is a xi square term here, we substituted a variable transform, we used a transformation eta is equal to xi square then this function y of eta satisfies this equation. As we all know, this is the familiar confluent hyper geometric equation, this is the confluent hyper geometric equation, and the solutions are the solutions, the well behaved solutions are F 1 1 a, c eta and as you know this is 1 plus a by c eta by factorial 1 plus a into a plus 1 and so on.

If this series is not terminated then for large values of eta it behaves as a, e to the power of plus eta, so this infinite series once again is convergent. But, if it is not terminated, if it is an infinite series, then for large values of eta it will behave as e to the power of eta, that is e to the power of xi square.

So, e to the power of xi square times e to the power of minus (()) xi square becomes e to the power of plus half xi square and therefore, the function will (()). We cannot let that happen and so therefore, a must be therefore, this must be a polynomial and since, in the numerator you have a into a plus 1, then a into a plus 1 into a plus 2.

So, a must be integer, negative integer, so we must have for the infinite series to become a polynomial polynomial, a must be equal to minus n r, where n r can be 0, 1, 2, 3. Because, if (()) let us suppose a is equal to minus 2 then the first term will be a into a plus 1, the second term divided by something.

Then it will be a into a plus 1 into a plus 2, so that will become 0 not only that term, but all subsequent terms will become 0 and the series will become a polynomial. So, for the series to become a polynomial, a must be a negative integer and therefore, this must be minus n r. So I obtain so I obtain that that a must be a negative integer, so l by 2 plus 3 by 4 minus lambda by 4.

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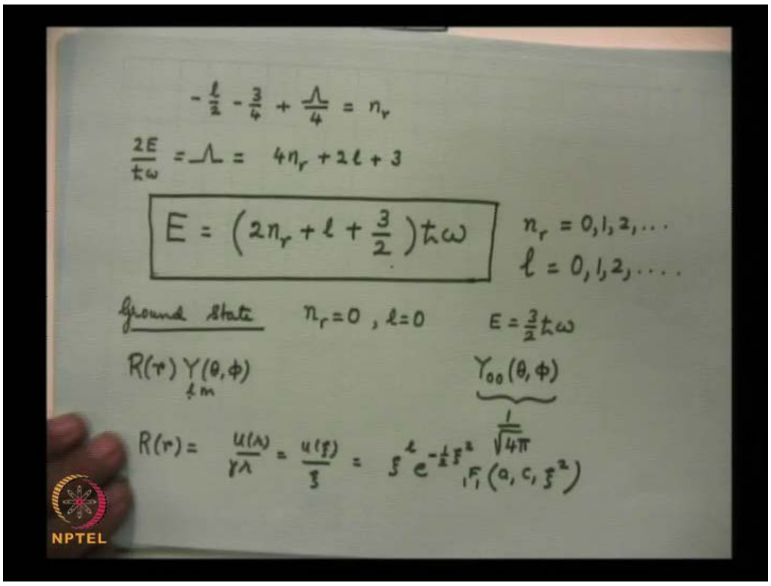


So, if I multiply this by minus 1, so you get minus l by 2 minus 3 by 4 plus lambda by 4 is equal to n r, I take this to that side and I multiply by 4, so I get lambda is equal to 4 n r plus 2 l 2 2 l plus 3. If you recollect that lambda of we had put equal to lambda was equal to 2 E by h cross omega, so this is equal to 2 E by h cross omega 2 E by h cross omega and therefore, we will have E is equal to if I divide by 2. So, 2 n r plus l plus 3 by 2 h cross omega, so these are the rigorously correct energy Eigen values, where n r and l both takes the values 0, 1, 2, 3 l also take the value 0, 1, 2, 3 etcetera.

So, as in the previous case where we had used Cartesian system of (()) we of course, must be at the same Eigen values, so you will have you will have the ground state the ground state will be n r equal to 0 and l equal to 0 and so therefore, E will be equal to 3 by 2 h cross omega. And what will be the wave function, the wave functions we had denoted that since l is equal to 0, so m will be equal to 0, so my angular part will be Y 0 0 theta phi, so this will be just a 1 over under root of 4 pi.

So, this will be the angular part and because my wave function is R of r times Y theta phi y l m theta phi, l is 0 then m will be also 0 and and the, and R of r R of r will be u of r by r, if I divide by, so this is the same as so. If I multiply by gamma, so u of xi by xi and this will be with normalization constant, this will be xi to the power of l e to the power of minus half xi square F 1 1 a, c, xi square.

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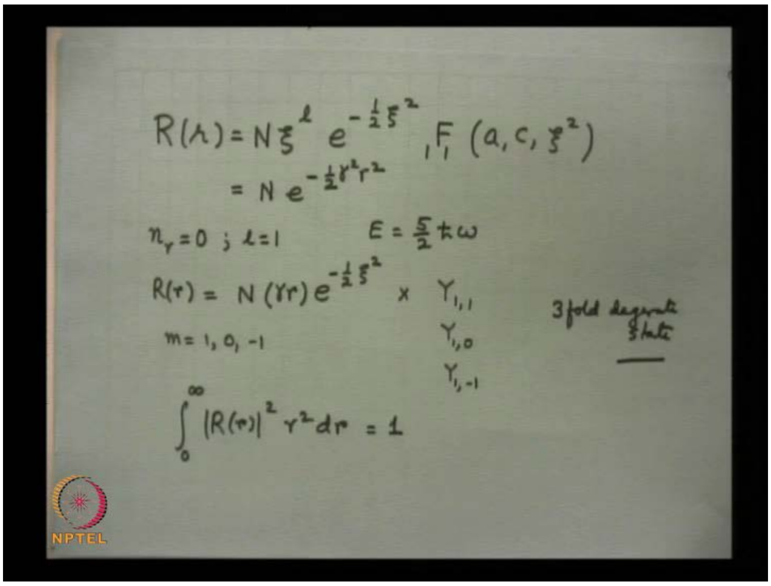


So, I write this down once again once again R of r will be xi to the power of l e to the power of minus half xi square F 1 1 a, c, xi square, if a is 0 this is a normalization constant, a is 0, so this is 1 and l is 0, so this is, so this is just n into e to the power of minus half r square gamma square r square, this is my wave function. Let me do one more case and then we will end there, the second Eigen function will be n r equal to 0 first excited states.

And l is equal to 1, if l is equal to 1 the Eigen values will be 5 by 2 h cross omega, so your radial part of the wave function, the radial part of the wave function will be n xi to the power of l, that is r to the power of l, so that is r gamma r to the power of 1 a is 0. And n r is 0, so a is 0, so this is one so e to the power of minus half xi square, but since Y l is 1, so m can take values 1, 0 minus 1.

So, we will have this multiplied by Y 1 1 Y 1 0 and Y 1 and minus 1, so this will be as we had obtained earlier 3 fold degenerate state, so what we have tried to show you is that for the 3 dimensional oscillator problem, isotropic oscillator problem. One can solve the radial part of the Schrodinger equation, in terms of the confluent hyper geometric function.

And one you give me the value of a and c, that is you give me the values of n r and l, and I will be able to immediately give you a is equal to minus n r and c is equal to l by, so a is equal to minus n r and c is equal to l plus 3 by 2.

So, if you give me the values of a and c, I can immediately write down the polynomial and I can write down the corresponding wave function, so it is really very straight forward you give me any value of a, you give me any value of N r any value of N r and any value of l, I can immediately write down the wave function, within a normalization within a normalization factor.

And that can be easily calculated by using the normalization condition, that 0 to infinity R of r mod square r square d r, from r equal to 0 to infinity this must be equal to 1. So, finally, we consider the last problem in the series and that is the 2 dimensional harmonic oscillators.

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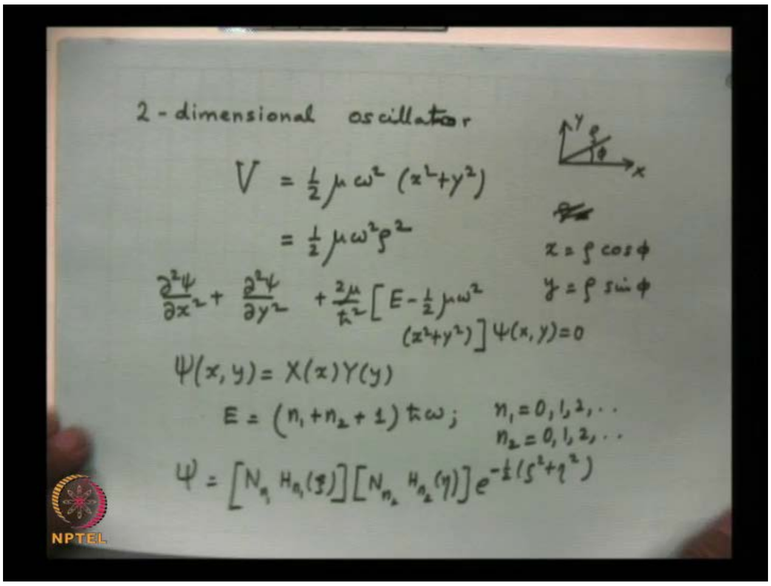


Now, if I have the 2 dimensional, we conclude this lecture by considering the 2 dimensional oscillators, and in which we will have the V as half of mu omega square x square plus y square. So, we have to solve the 2 dimensional Schrodinger equation in terms of x and y or in terms of rho and phi, were rho phi are circular are the are the (()) coordinates like this rho x is equal to rho cos phi and y is equal to rho sin phi.

So, you have here x, y 2 dimensional and this is my rho and this is the angle phi, these are known as the circular coordinates. So, in this if I take rho and phi as my coordinate system, then I can write this down as my coordinate system, then I can write this down as half mu omega square rho square.

So, the Schrodinger equation is in 2 dimension either I can write this down as delta 2 psi by delta x square plus delta 2 psi by delta y square plus 2 mu by h crosses square E minus half mu omega square multiplied by x square plus y square psi of x, y is equal to 0, and I leave this an exercise, you again use the method of separation of variables.

You write this down as psi x, y as X of x Y of y you will obtain Hermite-Gauss function and the energy Eigen values will be n 1 plus half plus n 2 plus half, so n 1 plus n 2 plus 1 h cross omega; these will be the Eigen values n 1 is equal to 0, 1, 2, 3, n 2 will also be equal to 0, 1, 2, 3 etcetera.

And the corresponding wave functions would be N of n 1 H n 1 of xi multiplied by N of n 2 H of n 2 eta e to the power of minus half xi square plus eta square. So, these are the Hermite-Gauss function, but since I can use also the cylindrical coordinates.

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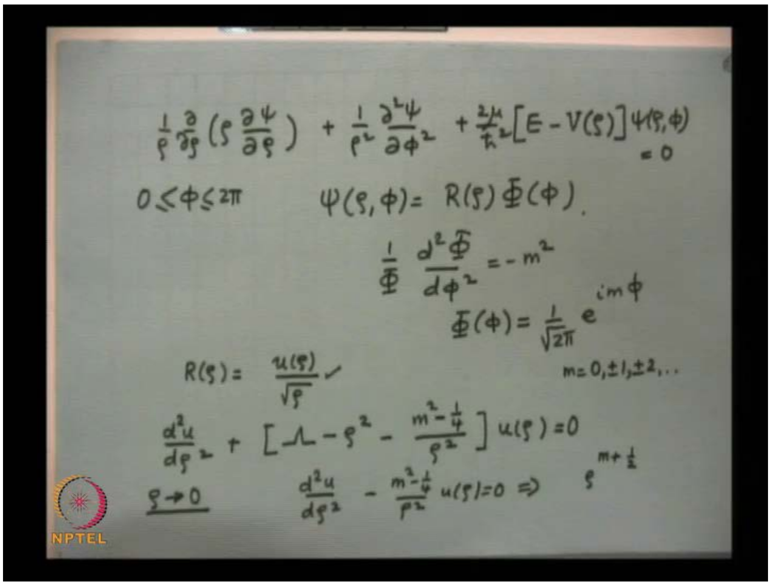


And we will obtain 1 over rho 1 over rho delta by delta rho rho delta psi by delta rho plus 1 over rho square delta 2 psi by delta phi square plus 2 mu by h crosses square E minus V of rho, V depends only on the rho coordinates psi of rho phi. I can again use the method of separation of variables and phi goes from 0 to 2 pi, so the phi variables, so I can write this down as psi of rho, phi is equal to the radial part times the phi part.

And one will obtain a term like this, so if I I will obtain a term like this 1 over phi d 2 phi by d phi square as we had obtained in the angular momentum case problem, we will set this equal to minus m square and we will get phi of phi is equal to the normalized E root 2 pi e to the power of I m phi, where m is equal to 0 plus minus 1 plus minus 2 etcetera.

So, we will have a equation which will involve only the rho term and and I leave it as an exercise for you, if you define any function which is such that, R of rho is equal to u of rho by square root of rho. Then u of rho will be, will satisfy the following equation, d 2 u by d rho square plus lambda minus rho square minus m square minus 1 by 4 by rho square u of rho is equal to 0.

So, the phi part will separate out and you make a substitution like this, it is fairly straight forward and one will obtain in equation like this, once again we look at the limiting form of rho tending to 0. So, this term will dominate and you will have d 2 u by d rho square minus m square minus 1 by 4 by rho square u of rho and the solution of this equation will be will be rho to the power of m plus 1. So, it will come out to be rho to the power of m plus half, so if I differentiate it once, so it will become m plus half times m minus half, so that will be m square minus 1 by 4.

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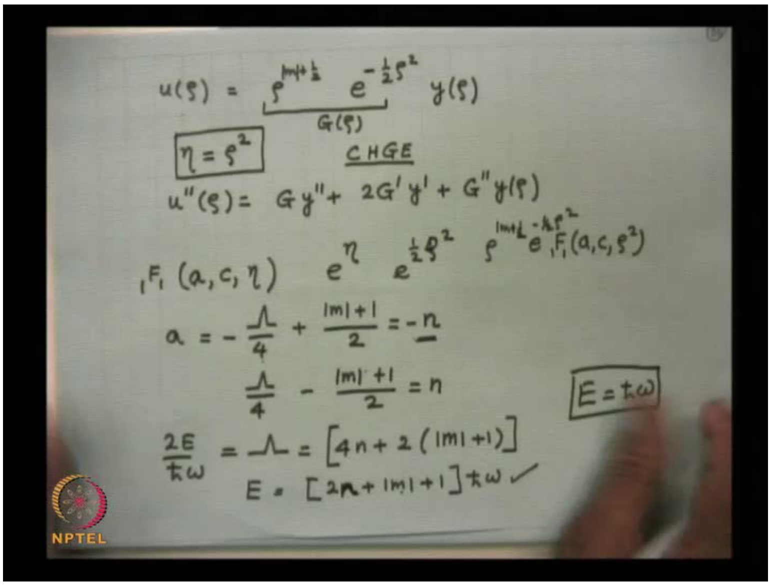


So, therefore, the the the small rho behavior will be u rho, the same methodology will be rho to the power of m plus half actually mod m mod m, because here m square appears, times the large wave behavior will be again e to the power of minus half rho square and multiplied by y of rho.

Then because of this term you introduce another variable which is eta is equal to rho square and this we take G of rho and we can write down just as we did for u double prime of rho will be equal to G times y double prime plus 2 G prime y prime plus G double prime y of rho, but the primes do not differentiation.

And if you use this transformation, that eta is equal to rho square, and then you will find that the solution is again can be written down in terms of confluent hyper geometric equation. And for the confluent hyper geometric equation to get terminated, the solution will be F 1 1 a, c, eta and a will be equal to minus lambda by 4 plus m plus 1 by 2 is equal to minus n.

For this to terminate a must be equal to a negative integer, so if you multiplied by negative sign, so you get lambda by 4 minus m plus 1 by 2 is equal to n, so lambda will be equal to, this is equal to 2 E by h cross omega, so this will be 4 n plus 2 modulus m plus 1. So, E will be, if I divide by 2, so this will be 2 n 2 n plus m plus 1 h cross omega, so if n is 0 m is 0 then you have the ground state the ground state energy Eigen value as we had obtained earlier.

But, these solutions are of extreme importance in considering the effect of the magnetic field and so, what we have done is that we have to summarize, that we have to consider a 2 dimensional oscillator. We can solve this by using the method of separation of variables and then or we can use the circular coordinates, where x is equal to rho cos phi and y is equal to rho sine phi. If we do that the corresponding del square operator in 2 dimensional becomes this.

We can use the method of separation of variables, so this becomes d 2 phi by so, this term will separate out, if you multiply this equation by rho square, and then divide this equation by R times phi it you will have a term which depends only on phi and the remaining terms will depend on rho.

So, this phi term we set equal to this constant and the phi solution will become as we have obtained in the angular momentum case, 1 over root 2 pi e to the power I m phi; so with that, we obtain we make a transformation something like this.

We look at the small rho behavior small rho behavior will be rho to the power m plus half, large rho behavior will be dominated by this term, so this will be e to the power of half rho square and therefore, we will try out the solution like this. And then we will substitute eta is equal to rho square; we will I leave it as an exercise, it is a very simple exercise, and you will get the confluent hyper geometric equation. And that confluent hyper geometric equation the equation the function must be terminated otherwise, it would behave if it is, if this series is not terminated at large values of eta, it will behave as e to the power of eta.

So, therefore, this would behave as e to the power of rho square, because eta is equal to rho square rho square, if you multiply this here it will become e to the power of half rho square, so the wave function will diverge at rho equal to infinity, we cannot let that happen. And therefore, a must be a negative integer and therefore, which is given by minus lambda by 4 plus m plus 1 by 2 must be a negative integer.

And so therefore, if I these are the Eigen values of the problem and the Eigen functions can be written down in terms of the confluent hyper geometric function a, c rho square times e to the power of minus half rho square, times rho to the power of n plus half, let me write it down carefully.

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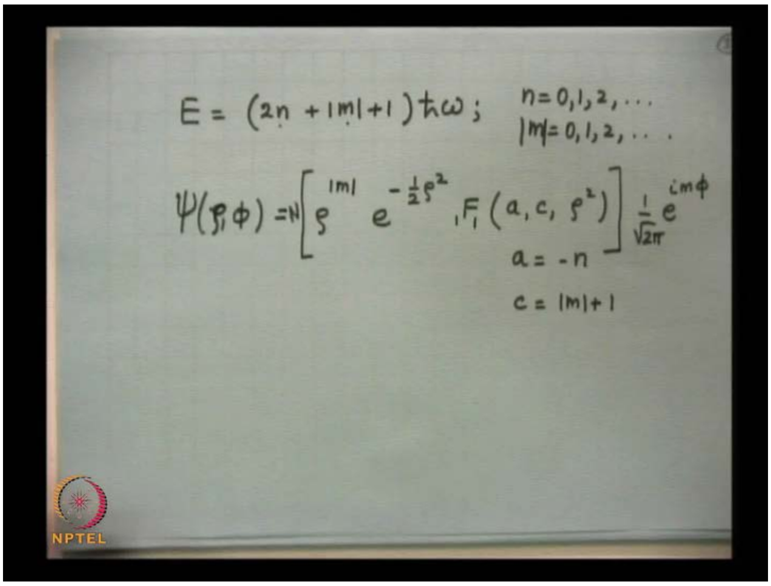


So, the wave functions, so the final energy Eigen values will be E is equal to 2 n plus m plus 1 h cross omega where n is equal to 0, 1, 2, 3 m is equal to mod m 0, 1, 2, 3 etcetera. And the wave functions will be psi of r phi or rho phi will be rho to the power of m plus half, so the if I divide by square root of r then half goes away E to the power of minus half rho square F 1 1 a, c, rho square where a is equal to minus of n. And so and c is equal to mod m plus 1, so this are the and the phi dependence of course, there is a normalization constant here, and phi dependence will be 1 over root 2 phi to the power of i m phi, this is the phi dependence, this is the rho dependence. These are the rigorously correct solutions for the harmonic oscillator, for the 2 dimensional oscillator problem and as I told you that the ground state corresponds to n equal to 0 and m equal to 0, so this is equal to 1.

So, this completes this completes the solutions of the 1 dimensional Schrodinger equation and sometimes the 2 dimensional Schrodinger equation and of course, the 3 dimensional Schrodinger equation. We have solved the hydrogen atom problem the 3 dimensional oscillator problem, the diatomic molecule problem, the linear harmonic oscillator problem.

And also we have considered tunneling through a barrier and things like that, so this is one aspect of the very important aspect of quantum mechanics, that we have considered, we also considered the free particle problem and propagation of wave packets. In the following few lectures, we will consider yet another formulation of quantum mechanics it is it is by Dirac in and it is for understanding this, one must be very familiar with the rules of matrix algebra.

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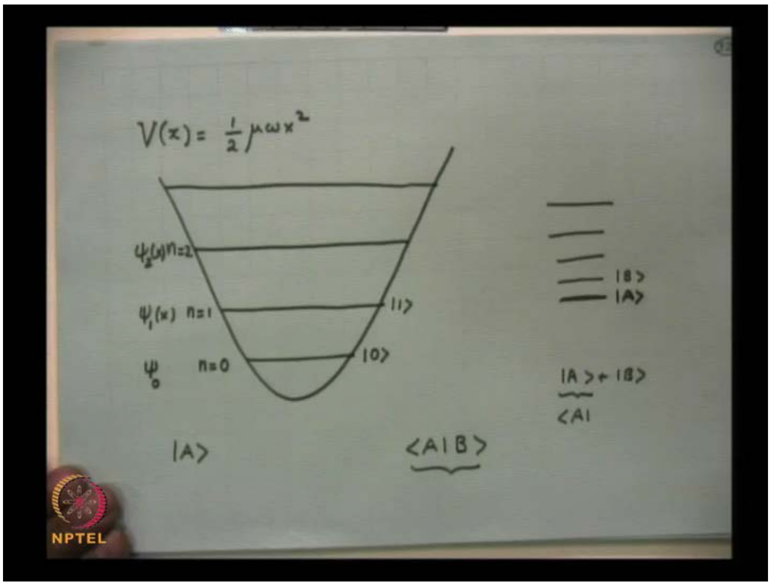

So, we will carry along, so we will try to tell you all these steps for example, let us consider the harmonic oscillator problem, V of x linear harmonic oscillator problem and we have the potential energy distributions like this. So, we have a parabolic index potential and we had obtained that these are the Eigen, these are the discreet Eigen (Refer Slide Time: 42:36).

So, this corresponds to n equal to 0 n equal to 1 and this is equal to n equal to 2 and similarly, n equal to 3 this was denoted by the wave function this psi 0 of x, psi 1 of x, psi 2 of x and so on. Now, we consider this linear harmonic oscillator, these are the different state of the oscillator.

Now, what Dirac said was each state of a dynamical system is represented by A ket vector and we denote this by A ket like this. So this vector this state I denote by ket 0, this state by ket 1, I have hydrogen atom state also, we have solved the hydrogen atom problem each has a specific quantum number, a set of quantum numbers.

Now, each state of the hydrogen atom I represent by A ket vector, so let us suppose this state I represent by ket vector A, and another state by ket vector B. So, each state of a dynamical system is represented by A ket vector such that, any linear combination of these two vectors is also another vector in the same space. I will detail this little later, corresponding to each ket vector there is a bra vector A, such that we can form a scalar product which is bra A B and this quantity is a complex number.

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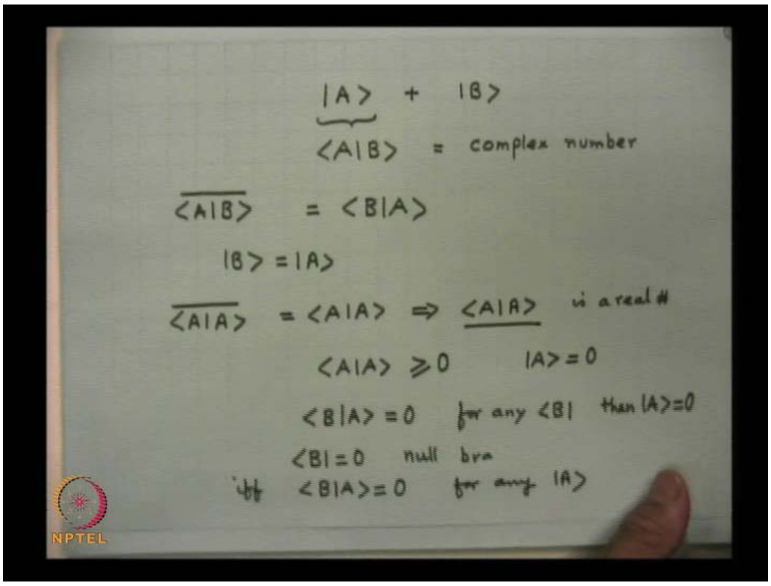

So that, we say that each state of a dynamical system, I represent by A ket vector there can be many ket vector associated with the state, one can take a linear combination of these two ket vectors. Corresponding to each states ket vector there is a bra vector A such that, we can form a scalar product A B, which is a complex number which is a complex number and a such that the complex conjugate of this number is denoted by B A it may appear a little abstract, but I will give you an example in a moment.

Now, let us suppose I put B is equal to A, so then this this tells me, this is an axiom then I have bra A ket A which is a number, so this is A times A. So, which tells us that the scalar product of A ket vector with its own bra is a real number, I further say that not only this is a real number, but this is always positive definite, that is this is greater than or equal to 0, unless A is a null ket.

Now, what is a null ket, a ket vector A is a null ket, when if pre multiplied by bra B, if this is 0 for any bra B, then ket A is said to be null ket sorry similarly, bra B is A null bra, if and only if bra B ket A is 0 for any ket A.

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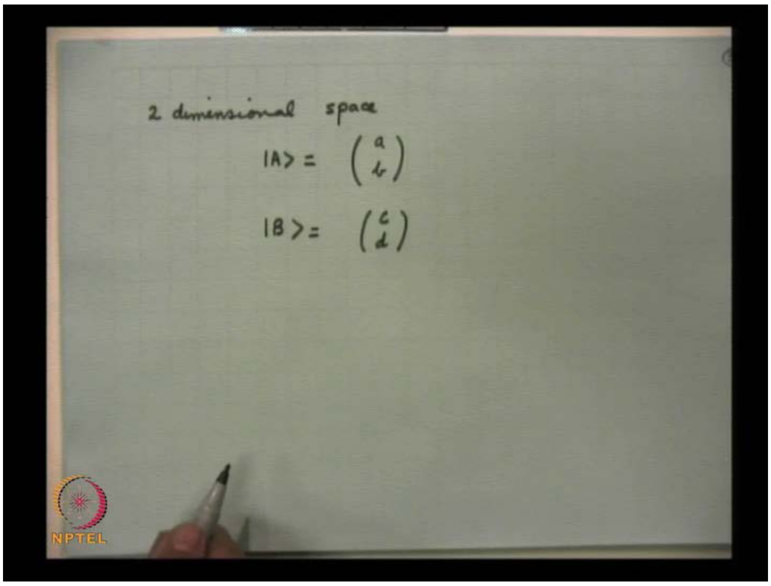


Let me make you, try to make you understand the concept that I have developed using matrices, now I consider a 2 dimensional space, so I have a column vector representing a vector a ket vector A, I represent this by say a b. Another vector B I represent this by c d I forgot to mention here, that if A B is 0, then A vector a ket A and ket B are said to be orthogonal to each other, this scalar product is said to be 0. If bra A ket A is 1, then we say that the ket vector is normalized (Refer Slide Time: 49:32).

So, let me let me go back to this 2 dimensional space, where a ket vector is represented by a, b 2 numbers and bra B also, ket B also belongs to the same same space 2 dimensional space.

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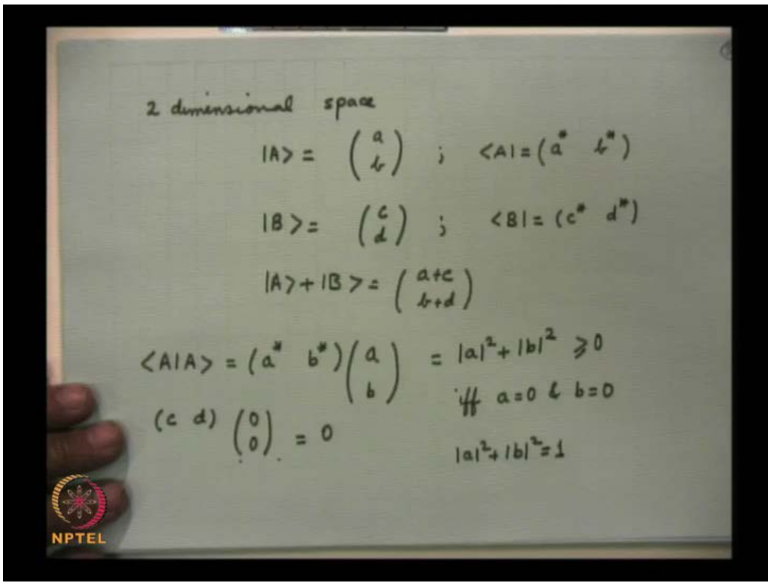


So, you can write down A plus B will be again in this another vector in the 2 dimensional space, so this is 1, 2, 3, 4, so this will be 4 plus 4 here and 5 here. Now, corresponding to this bra A corresponding to this the bra A will be the complex conjugate of this and this this is known as the dual vector space.

Corresponding to a column vector that is always a rho vector, and if I multiply these two bra A ket A it is a number, so you will have a star, b star, a, b, so this will be mod a square plus mod b square. So, this is always greater than 0, it can be 0 if and only if, a is 0 and b is 0, so then that is a null ket.

Because, if you have a null ket you can multiply this pre multiply by any bra and this will be 0, now here bra B is equal to c star d star and the same analysis I can do, now if I have bra A ket A. If this is 1, that is if mod a square plus mod b square is equal to 1, we say that the ket is normalized.

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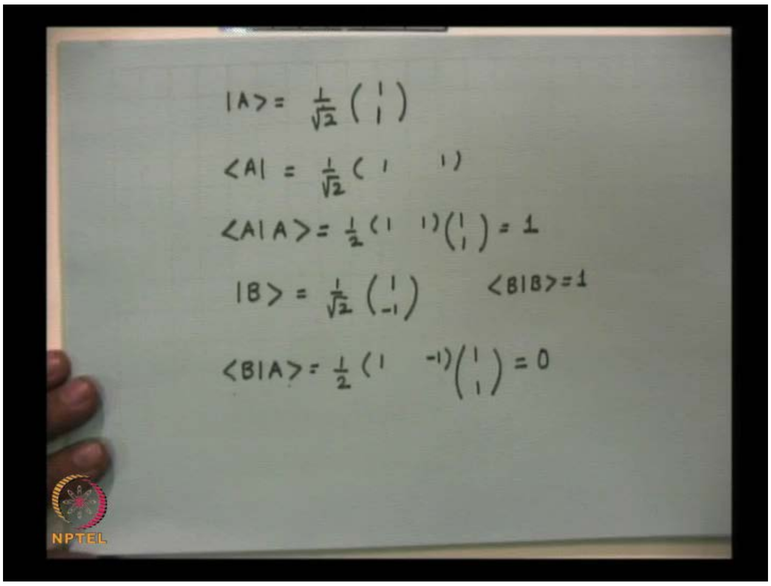


So, let me give you an example, so let me take a ket A which is given by (()) 2 dimensional space, 1 by root 2 1 by 1, 1 1, so these are both real numbers, so bra A is equal to 1 over root 2 1 1, so bra A ket A will be 1 over 2 1 1, 1 1, so that is 2 and that is 1. So, we say this is a normalized ket, now we again we take another ket B and we write down 1 over root 2 1 minus 1 as you can see, that this ket is also normalized.

However, if I now do B A then 1 over root 2 multiplied by 1 over root 2 is 1 over 2 and bra B is 1 minus 1 and ket A is 1 1, so this is 0, so we say that ket A and ket B are orthogonal to each other.

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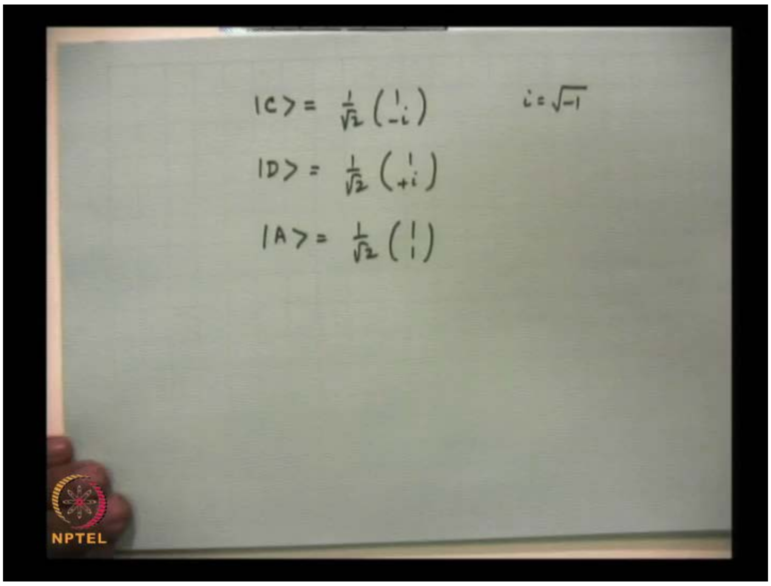


Let me give you another example, so let me write down there is another vector in the same space c, which is equal to 1 over root 2 1 minus i and I leave this is as an exercise, where I is equal to square root of minus 1, that this is a normalized ket. And if I take another ket D is equal to 1 over root 2 1 plus I then this and this arte orthogonal to each other, but if I take A ket A which is 1 over root 2 1 1 then that is not orthogonal to either of this vectors.

So, we will continue our discussion on bras and kets in our next lecture, but before that we will I will request all of you to brush up your matrix algebra, because the operator algebra that we will develop, it will be very easy to understand that; if we if we have a knowledge of the algebra involved with matrices, thank you.