Quantum Mechanics - I
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Lecture - 32
Central Potential: The Radial Equation

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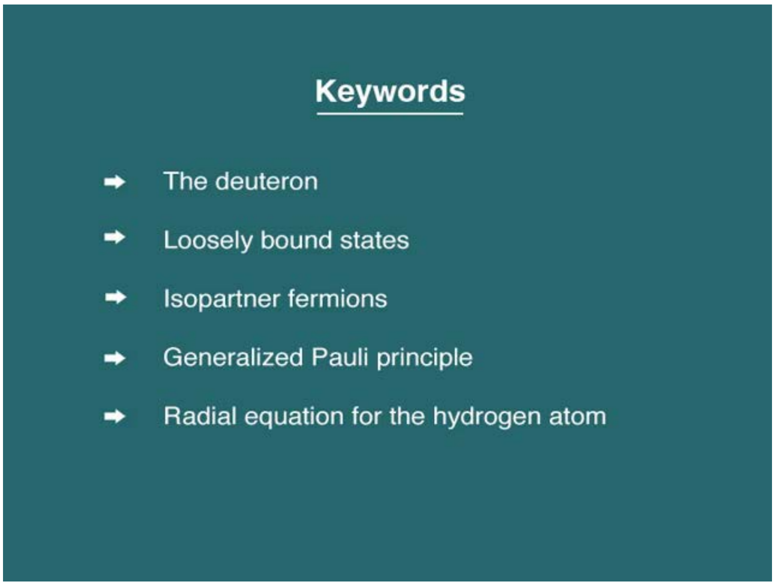

We were looking at the central potential problem and in the last lecture we have reached the point where we could write the radial equation.

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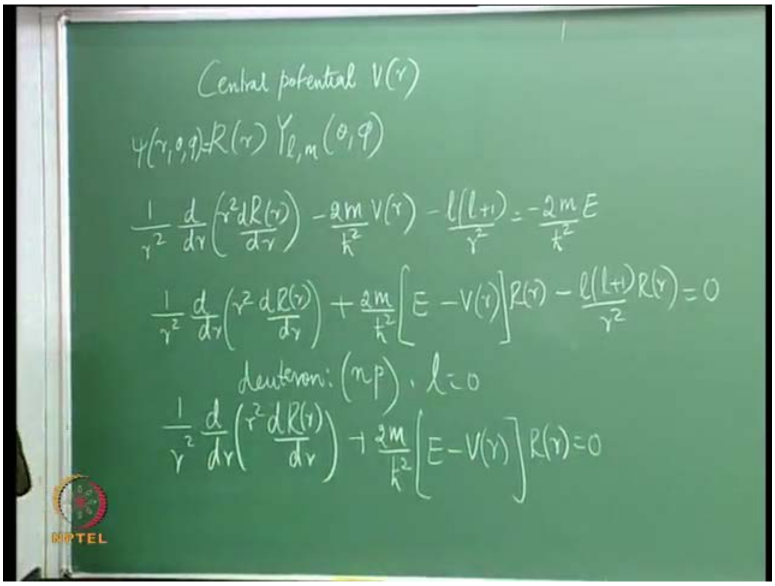

So let us begin with the radial equitation. So, here we have a central potential V of r working in spherical polar coordinates and so we will write the equation for R of r. The entire wave function was a function of r theta and phi and that was R of r y l m of theta phi. Now if I did not realise that the potential is an operator acting on R of r I would write a wrong equation like this, but I should remember that all terms there multiply R of r and so I have 1 by r square d by d R of r square d r by d r plus 2 m by h cross square E minus V R of r minus l times l plus 1 by r square R of r. This object is equal to 0.

Let us look at a simple problem. Let us look at a situation where we only concern ourselves with the ground state of say a nucleus. Since, we have just done the shell model of the nucleus we can look at a problem where we just look at the ground state of a nucleus and the specific nucleus that I would like to consider is the deuteron. This is a neutron proton bound state there is 1 neutron 1 proton. Nobody has seen a deuteron in the excited state. We now know that the deuteron exists only in the ground state that means in the l equals to 0 state. So, as far as the deuteron problem is concerned the radial equation simply becomes 1 by r square d by d r of r square d R by d r plus 2 m by h cross square E minus V of r R of r equals 0. What is it that we are trying to look for?

Now, we will do a very rough calculation. Use an effective model and see if we can explain that for a generic potential that means without assuming any specific properties for the potential more than is necessary without going into the details of the potential we will see if the deuteron is a loosely bound state. By a loosely bound state we mean the following: that if you take the deuteron and give it a very small perturbation, a small kick then the amount of energy that is needed to go to a possible excited state is much more than what is needed to separate them.

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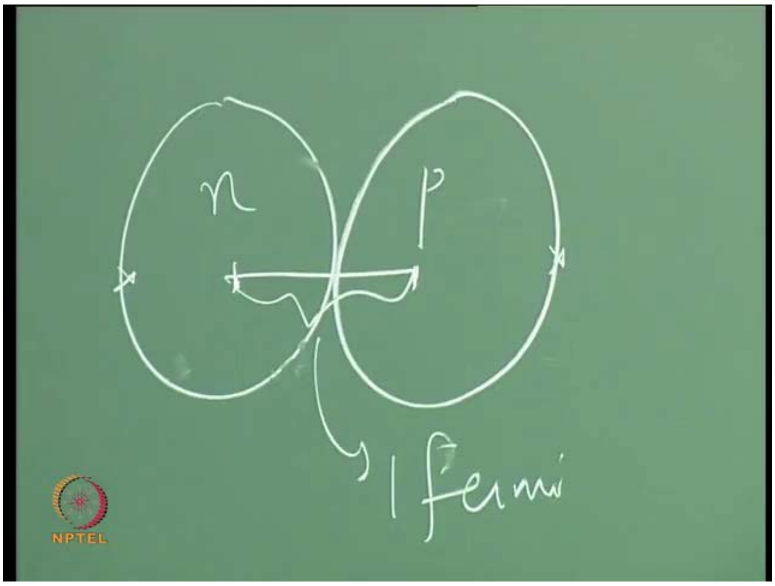

In other words, in a classical picture if you think of the neutron and proton as hard spheres that would be a tightly bound state in a classical picture and since the typical size of the nucleus is 1 Fermi the centre to centre distance would be 1 Fermi. This is a true picture, but it should do the job. Now, a loosely bound state is one where you do not expect a situation like this where they are as close as possible to each other. So, you would expect the root mean square size of the deuteron to be much more than a Fermi. And you would expect therefore, that the entire distance from there is more than 2 Fermi and then you would say it is loosely bound.

The idea is to try to explain why the deuteron cannot be seen in an excited state. So, if it so loosely bound even a small perturbation, a small kick to the deuteron, a small supply of energy is enough to dissociate the neutron from the proton and separates the nucleus into the neutron and the proton separately, not keeping them as a bound state. Whereas, the amount of energy that is needed to kick it to a higher excited state is much more. And therefore, since even a small perturbation would separate the deuteron into a free neutron and proton that would explain: Why the deuteron is in a loosely bound state? Why the deuteron does not exist in the excited state?

So, the idea is to use a generic potential and see if indeed the average size of the deuteron is much more than 2 Fermi. Then we have some handle on this problem and that is what

I would try to do right now. (Refer Slide Time: 00:24) Now, having set l equals 0 I need to assume some form for the potential.

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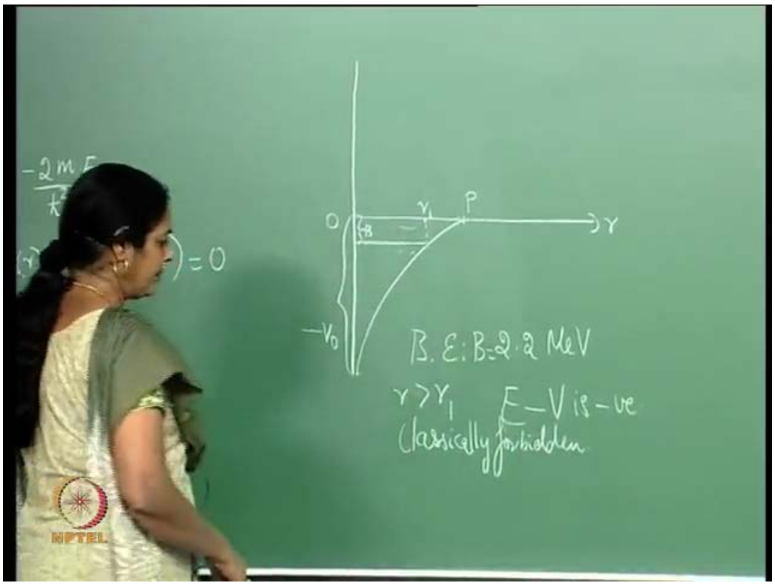

As I said we should be able to see this without going into great details of the potential. I know it is a bound state and therefore, it is an attractive potential. So, let us say that it goes from minus V naught, but the nuclear force is a short ranged force and therefore, it drops off to 0 at some point, let me say P. So, this should roughly be of about a Fermi. I am not assuming anything more about this potential. It is a short ranged force and it is an attractive potential. (Refer Slide Time: 00:24)

Now, what is the energy? The energy is really the binding energy of the deuteron and that is the energy that binds the neutron and the proton together. And it is known from experiments that the binding energy is about 2.2 Million electron Volts for the deuteron. And therefore, this is minus 2. 2 Million Electron Volts. I am just going to call this binding energy B equals 2.2 M e V. I am not so concerned about what happens in this region so somewhere here is minus B if you wish and that is about 2.2 M e V. The point is the following.

Here in this region it is clear that V naught is greater than V

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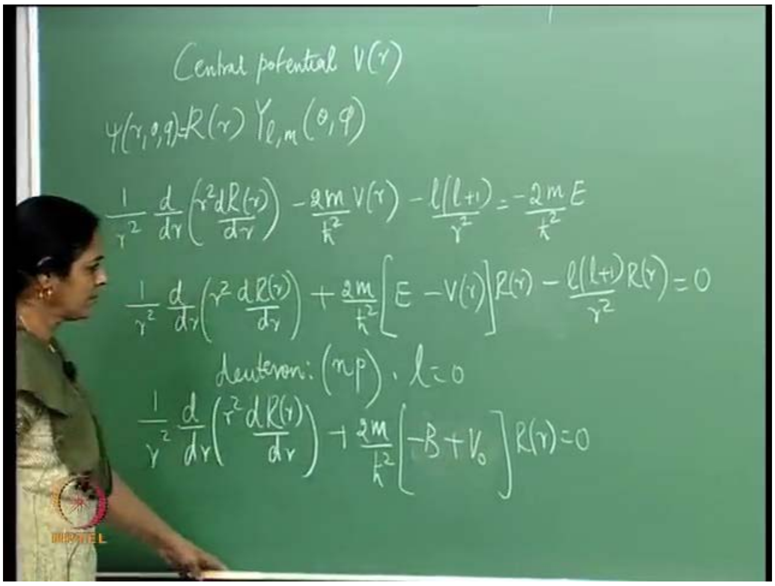

And therefore, this equation would just become minus B plus V naught. Let me imagine that it is not a function of r. Let me imagine that all over this place V naught is a constant and it is greater than b and then of course, here V naught is equal to B so it some kind of decreasing function or a constant function which gets cut off at that point and becomes equals to B.

I am not assuming any details of the potential. Just using the fact that up to this point V naught is greater than B. And therefore, this is a positive quantity, and that is okay. (Refer Slide Time: 05:56) But then out here beyond r 1 for r greater than r 1 you can see that E minus V is negative because V abruptly goes off to 0 pretty fast actually. It is a short range potential and this object is negative. So, e minus v is negative in this region and therefore, it is a classically forbidden region beyond r 1 because the kinetic energy is negative. So, it is this region that I am really interested in because in tight approximation that is where the neutron and the proton are like spheres which are touching each other the end to end distance is 2 Fermi.

Now, I am really interested in how much penetration is there, in this quantum mechanical problem, into the classically forbidden region? But that is the region where the potential is 0 so basically I am looking at things here. As you can see this is proved calculation. Because, I am not really worrying about the actual form of the potential. On the other hand, if I can show even with these minimal assumptions that the size of the deuteron is much larger than 2 Fermi then indeed it is a loosely bound state and one has as I said an explanation of why the deuteron does not go to the excited state?

So, what is the equation in this region? So I am only concerned with the radial equation in the region r greater than r 1. (Refer Slide Time: 00:24) So this is 0 let us look at this equation in any case and try to write it in a better form.

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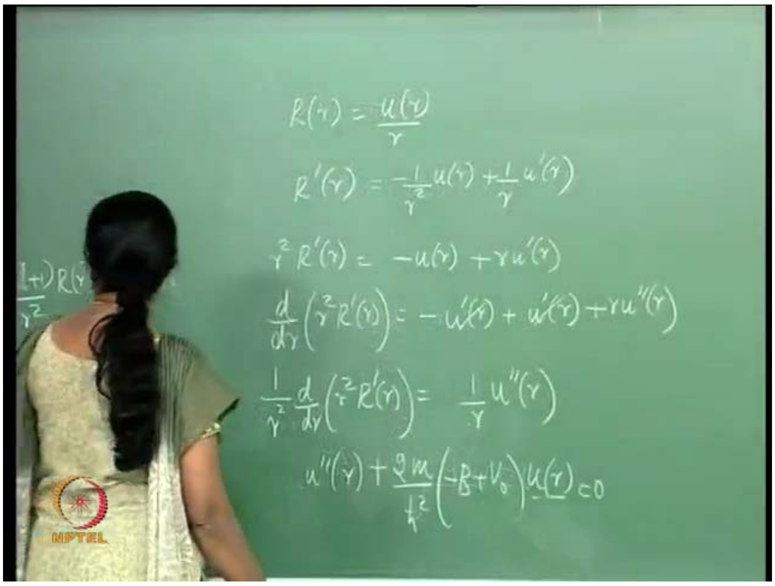

Let me write R of r as sum u of r by r. Then R prime of r, prime means differentiation with respect to r is minus 1 by r square u of r plus 1 by r u prime of r. And r square R prime of r is minus u of r plus r u prime of r. I have d by d r of r square R prime of r and that is minus u prime of r plus u prime of r plus r u double prime of r. So 1 by r square d by d r of r square R prime of r. The u prime cancels out and I just have a plus 1 by r u double prime of r so the first term is just u double prime of r by r because I should remember when I write R of r as u of r by r I should worry about what happens when r goes to 0 and when r goes to infinity. Clearly, u of r has to behave reasonably for r going to 0 and r going to infinity because I want things not to blow up.

So, for instance when r goes to 0, I would expect u of r to at least go as r and so on. In any case, writing down this equation in terms of u double prime of r. I basically have 1 by r u double prime of r plus 2 m by h cross square B plus V naught u of r by r equals 0 and therefore, I have a simple equation like this. I have u double prime of r plus 2 m by h cross square minus b plus V naught u of r equals 0. So, in the region r greater than r 1 so let me just write it here.

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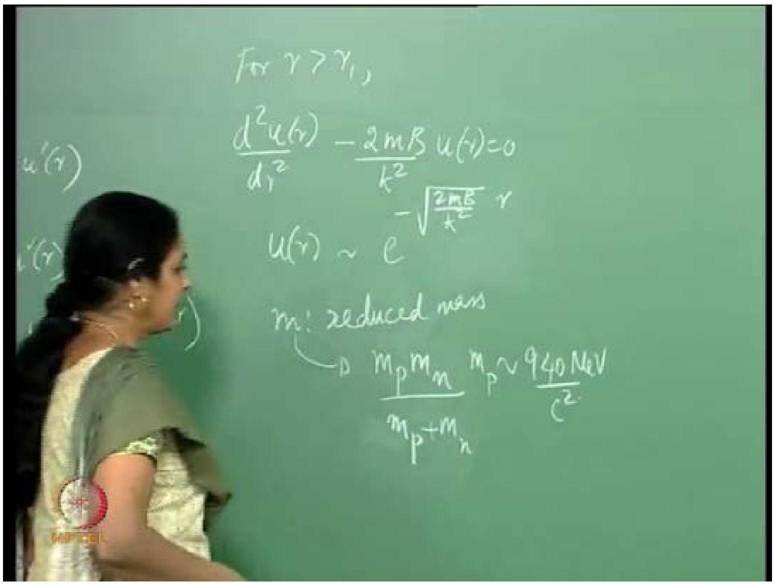

For r greater than r 1 my equation is d 2 u by d r square minus 2 m B by h cross square u of r equals 0. So, the solution is simple u of r is e to the minus root of 2 m B by h cross square r. The m here is clearly the effective mass or the reduced mass. In this problem it is m p, m n by m p plus m n. Mass of the proton is approximately equal to the mass of the neutron so its m p is approximately 940 M e V by C square and that is a same as the mass of the neutron. For purposes of this calculation we can substitute m p equals m n.

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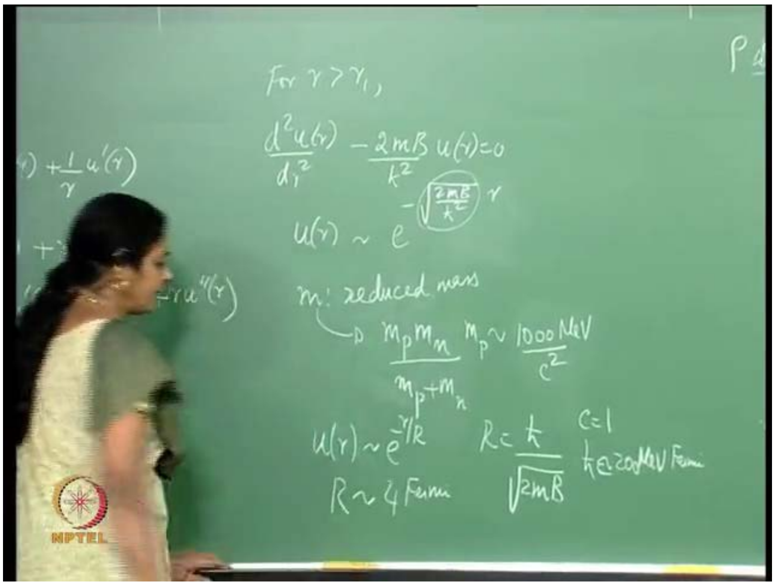

I would even just say this is roughly a 1000 M e V by C square should do. That is a same as m n. So, you see the length scale in this problem is given here so u of r goes as e to the minus r by R where R is h cross by root of 2 m B. B is the binding energy it is an experimental input that is 2.2 M e V, m we know is just 1000 by 2 because this is twice m p and that is an m p square. So I can put that there and I can substitute for these numbers, substitute for the Planck's constant and find out what is happening and if I just put in these numbers and remember that if I said c equals 1 then h cross is about 200 M e V Fermi .

So if I put in these numbers I find that r which is really the length scale in my problem and that is why the deuteron has a bound state. This r is somewhere between 3 and 4 Fermi. So, that is 4 Fermi.

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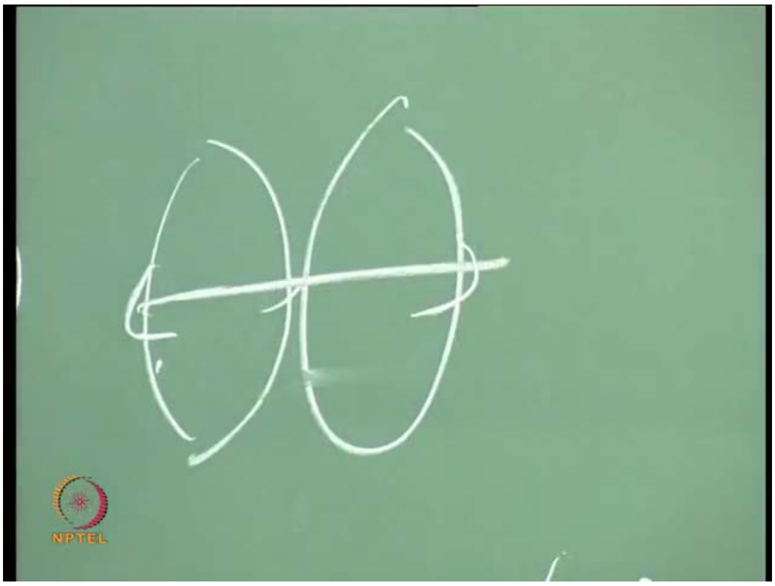

What should have been 2 Fermi if I think of them as hard spheres? What should have been 2 Fermi across this distance that is 1 Fermi typically. It is really 4 Fermi and therefore, I know that this classical picture is no longer true and in fact there is a lot of penetration into the classically forbidden region and the deuteron is a loosely bound state. It is therefore, easy to envisage a situation where the smallest perturbation separates the deuteron into a free neutron and a free proton.

So this is one situation where I have used the radial equation and try to explain at a very simple level why an object is seen only in the ground state? And we have not used any particular form for the potential and so on. Needless to say that this can be improved in fact, you can use a potential which is perhaps in its details more realistic.

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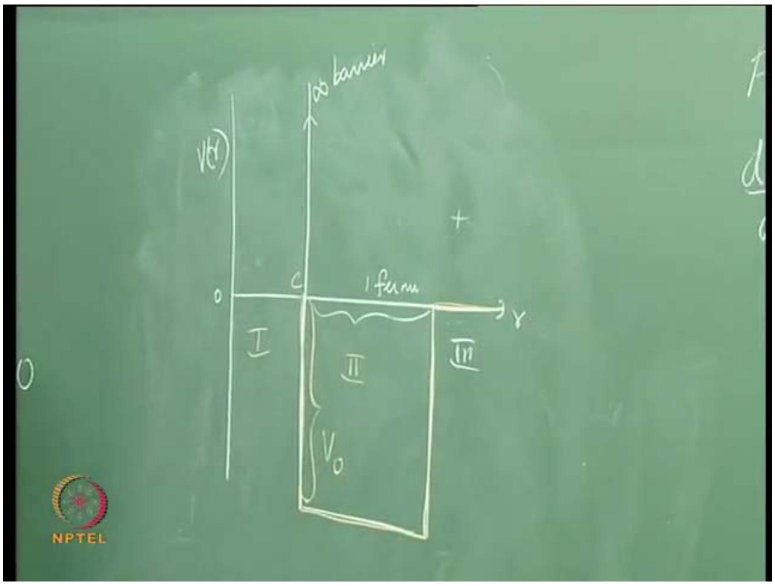

You could use a potential like this. A hard core which means no penetration here so that is an infinite barrier this is V of r and then there is a square well here extending over a certain range typically say 1 Fermi and then 0 here. So this is region 3 and a potential is not even there because it is a short range potential and then there is a region 2 where we can use a square well and this is region 1 we call it the hard core because there is no penetration here.

And of course, you could write down the Schrodinger equation in the 3 regions like you were used to doing and then when you match the wave functions here remember that this wave function in region 2 should vanish at r equals c because there is no penetration onto this side, psi 1 is 0 the wave function in this region vanishes. And then here you could match the wave function and the derivatives between psi 2 and psi 3 the 1st derivative. Go through all the details and you could fit a typical V which would tell you that it is a loosely bound state.

So, the root mean square size is much more than 2 Fermi. So, you can improve upon this simple model that I started off with. But even with this very simple model an important feature emerges and that is perhaps the strong point of such a simple model. No need to go into details to see a very important fact that you can verify experimentally. So, that is the deuteron problem and then by way of a comment in one of my earlier lectures I had spoken about the generalised Pauli principle.

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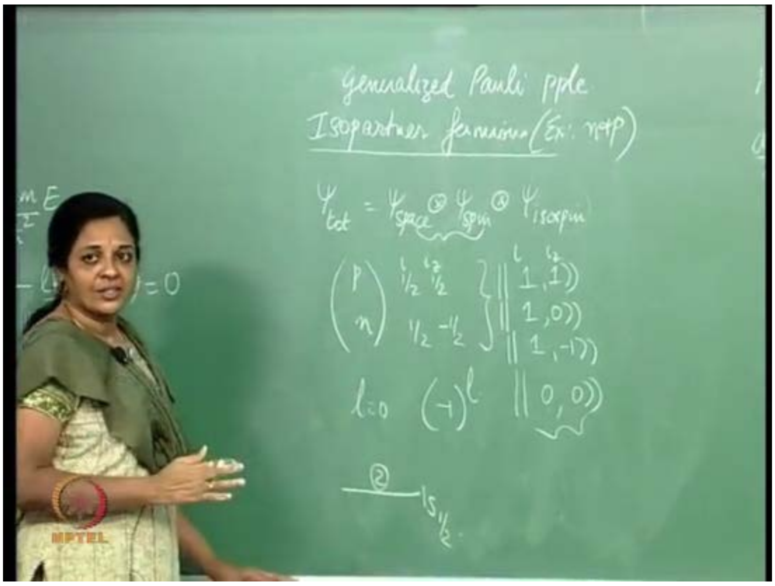

That I had said that isopartner fermions this is the generalised Pauli principle which I did talk about in one of my earlier lectures isopartner fermions example neutron and proton they form an isodoublet. Consider isopartner fermions the total wave function has a space part, a spin part and an isospin part and I said that under interchange of the space spin and isospin labels the total wave function must be antisymmetric. If you are considering fermions which are isopartners of each other you will recall that the proton and the neutron form an isodoublet. This is i equals half and i 3 equals half and the neutron has i equals half and i 3 minus half.

Now, let us look at the deuteron. Since l is equal to 0 the space parity as you have now learnt is given by minus 1 to the l it is in the ground state. And therefore, the space wave function is symmetric because the Eigen value of the parity operator. Remember that the angular wave function is the spherical harmonic y 0 0 so the space parity is plus 1. So the space wave function is symmetric. Now, if you look at the spin wave function yesterday we had looked at a very simple shell model for the nucleus.

So, you know that the ground state the 1 s state can be filled with 2 nucleons and since there is only 1 neutron and 1 proton they occupy only the s state. This is the 1 s half j is equal to half in this state. Experimentally you find that the spin wave function is also symmetric so psi space psi spin is symmetric that is what you get from here. So, if the spin wave function is symmetric and the space wave function is symmetric and the total wave function must be antisymmetric, psi isospin should be antisymmetric and since these are isopartners the coupled states that you can have are 1 1 1 0 and 1 minus 1.

The first is the isospin and the second is i z and 0, 0 and you will recall that these are symmetric wave functions, symmetric under interchange of the i z labels. So, if you interchange the i z labels of the proton and the neutron the isospin wave function is symmetric whereas, this is the antisymmetric wave function. And therefore, by this token, by this fact that the generalised Pauli principle holds here the deuteron has isospin 0 which means it has no isopartner.

So, that is a bit of prediction that one can make. The fact that the spin of the deuteron is 1 and the fact that it exists only in the ground state and therefore, the space wave function is symmetric would imply by the generalised Pauli principle that the isospin wave function is antisymmetric, which means that because each of this is an i equals half state the proton and the neutron it exists in the iso singlet state, the deuteron exists in the iso singlet state. So, it is a consequence of the generalised Pauli principle we now infer that the deuteron exists in the iso singlet state. There is no isopartner for the deuteron. So, so much for the deuteron problem.

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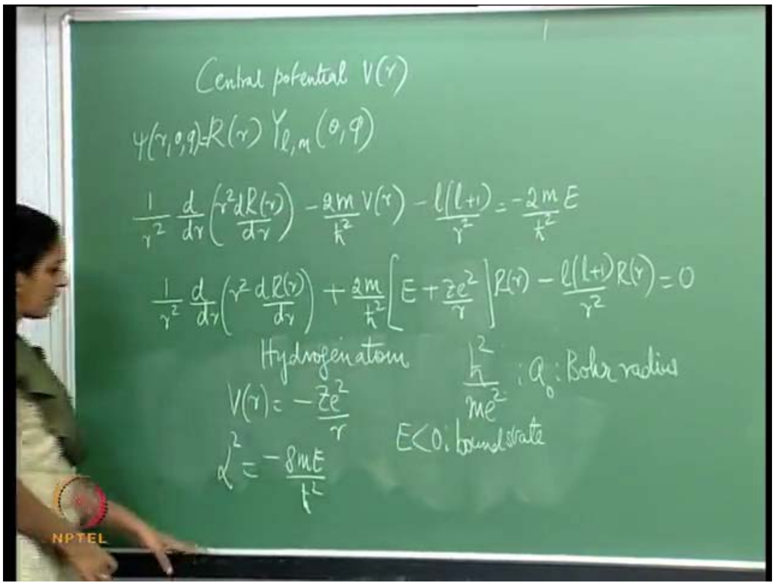

Now, let me consider the radial equation in the more general context that means where I do not set l equals 0. So, the problem that I would now like to look at is a hydrogen atom. So, let us forget this and we will look at the hydrogen atom problem. Of course, the angular wave function is y l m of theta phi because V of r is minus z e square by r. In general for a hydrogen like atom the z would tell you the number of protons. So, I will just write it as minus z e square by r in general and it is attractive so there is a negative sign out there m is of course, the reduced mass between the nucleus and the electrons because we are looking at an atom here.

And therefore, retaining this as well I can substitute here in this equation as plus z e square by r. This is what I have. Now, in order to go to dimensionless variables which is the way I do these problems. 1st of all identify a length scale h cross square by m e square provides me with a length scale I will call that a naught or call it as the Bohr radius. So, that is going to give me a length scale in this problem. I will look for a bound state. There is some point in looking for a bound state now and then let me define an object alpha square as minus 8 m E by h cross square because E is negative, E is less than 0 because we are looking at a bound state and therefore, alpha square is positive.

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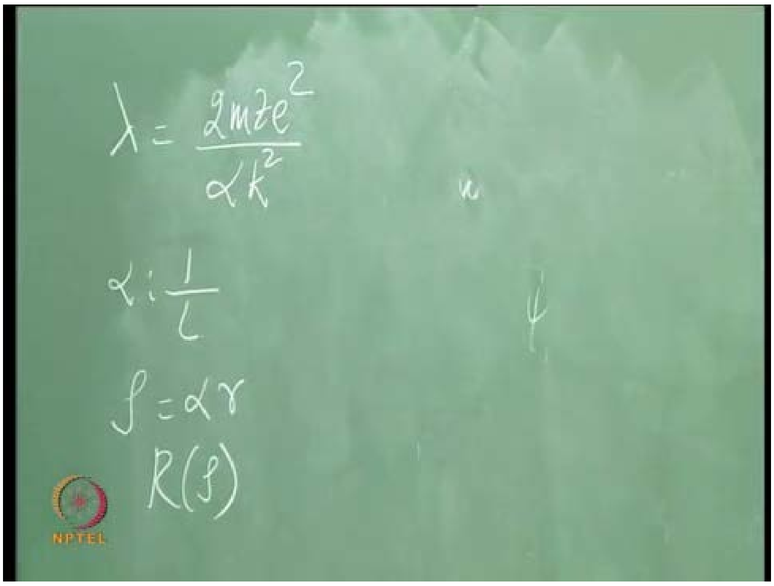

So, if I put alpha square is minus 8 m E by h cross square and I define an object lambda of course, this as you know would have dimensions in terms of length. So now, I define a lambda which is 2 m z E square by alpha h cross square. Alpha has dimensions of 1 by length and lambda itself is dimensionless h cross square by m e square has dimensions of length and therefore, lambda is dimensionless.

(Refer Slide Time: 24:57) So, in terms of lambda and alpha I can just rewrite this equation. Let me also do the following substitution that rho is alpha r and rho is dimensionless. So, this differential equation is going to be written for R of rho and how does this equation look?

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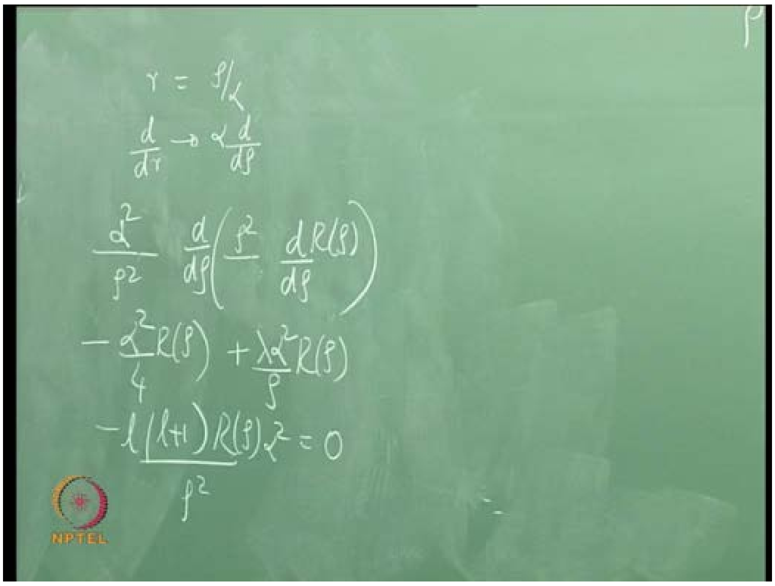

So r is equal to rho by alpha and therefore, d by d r goes to d by d rho times alpha and therefore, this equation just becomes 1 by rho square. There is an alpha square on the top d by d r becomes alpha d by d rho r square is rho square by alpha square d r by d rho that is again an alpha d by d rho r of rho. That is the first term and as you can see the alpha square here is cancel out I have an overall alpha square there and that is how there is in the 1st term.

(Refer Slide Time: 24:57) The 2nd term is plus 2 m E by h cross square and that means it is minus alpha square by 4 r of rho that is this term. 2 m z e square by h cross square alpha is lambda therefore, I have lambda alpha by r that gives me another alpha out there. So, it is lambda alpha square by rho minus l times l plus 1 r of rho by r square which gives me a rho square alpha square. This is equal to 0 or let us write this neatly.

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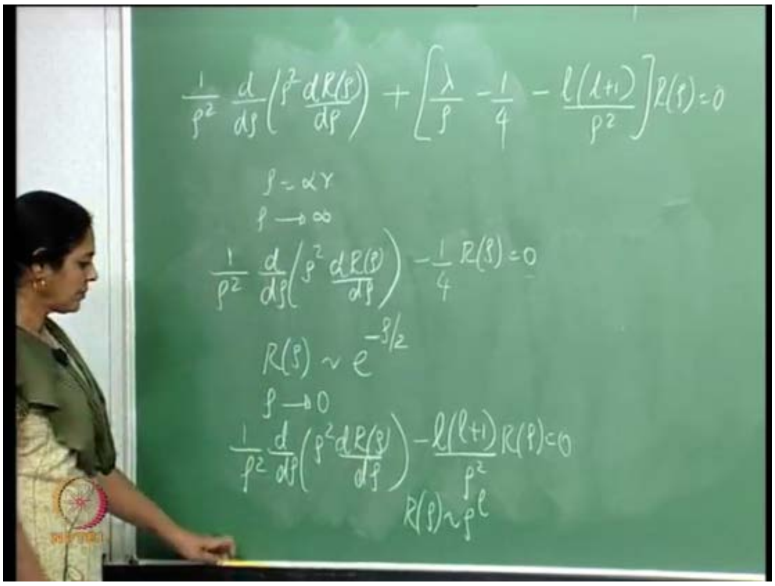

It is clear that the alpha square can be cancelled out in every term and then I have the following: 1 by rho square d by d rho of rho square d R of rho by d rho. That is the first term plus lambda by rho minus quarter minus l times l plus 1 by rho square R of rho equals 0. So, this is the equation that I have. As always this is in terms of the dimensionless object rho and as always I would like to look at the asymptotic form and see if it is well behaved.

So, let us see what happens for large rho. Recall that rho is alpha r and rho therefore, goes from 0 to infinity now, for large rho what survives in this equation is this: 1 by rho square d by d rho d square d R of rho by d rho minus quarter r of rho equals 0. And then you can see that R of rho is essentially e to the minus rho by 2, because it pulls out a minus half in the differentiation and then once more that gives me a plus quarter and that is what it is going to cancel with this. Quite apart from this 2 rho here and there is a rho square there so it is a simple matter to check that R of rho goes as e to the minus rho by 2.

Now, look at what happens as rho goes to 0. If a rho going to 0, 1 by rho square d by d rho of rho square d R of rho by d rho. That term has to be put in here minus l times l plus 1 by rho square R of rho equals 0. Now, this tells me that R goes like rho to the l.

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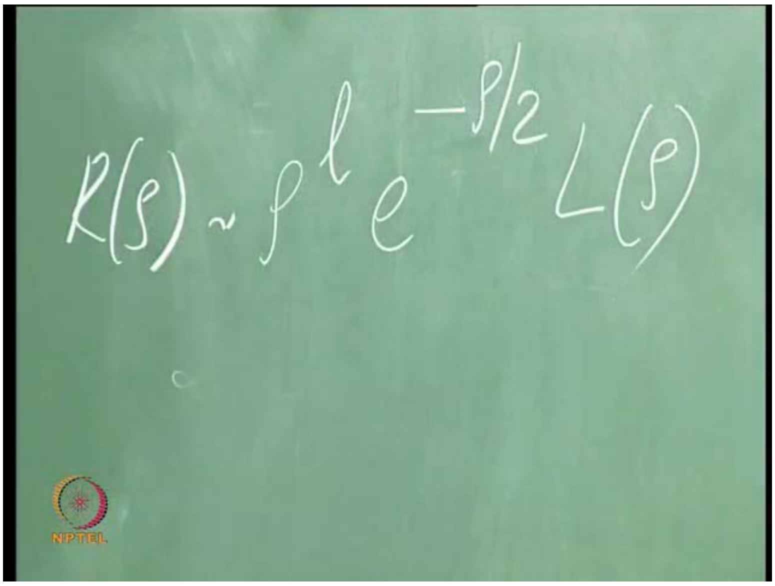

I will leave this to you as an exercise for small rho, this is for rho going to 0 and therefore, I have a particular form for r of rho that is rho to the l that comes out of looking at rho going to 0, e to the minus rho by 2 and that is there because when rho goes to infinity should be well behaved. Some l of rho. (Refer Slide Time: 30:14) So, basically as always I should recast this equation this equation and write it in terms of an equation for l of rho. I should just change, I should substitute for R of rho as rho to the l e to the minus rho by 2 l of rho and get a differential equation for l of rho. I will leave it to you as an exercise.

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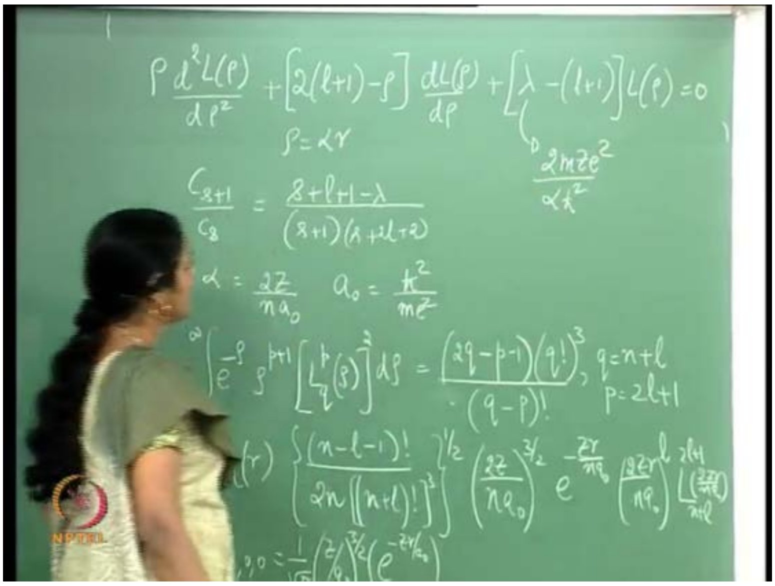

You will get an equation like this you get rho d 2 l of rho by d rho square plus twice l plus 1 minus rho d l by d rho plus lambda and this lambda you will recall is 2 m z e square by alpha h cross square. Rho itself is alpha r minus l plus 1 l of rho is 0. So, this is the equation that you will get. I will leave this to you as an exercise it is a simple straightforward substitution.

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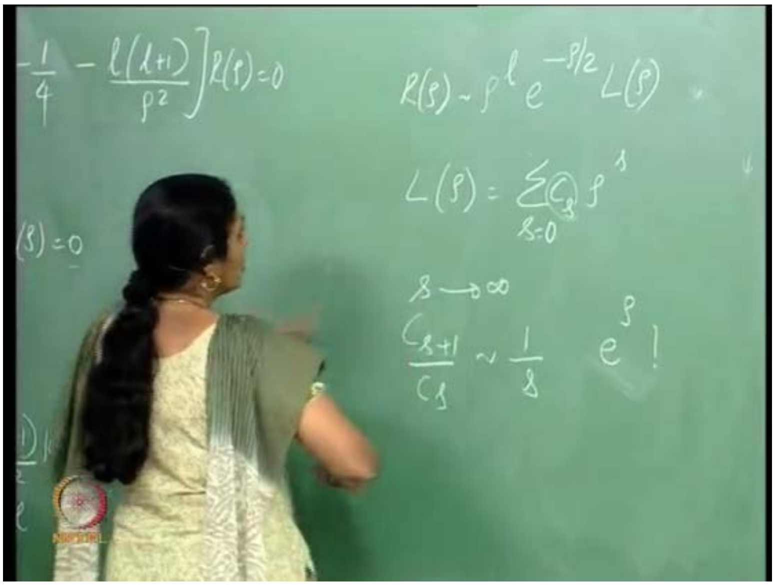

Of course, we know by now that the next step is to use a series solution for l of rho. So, you would write a series solution of the form l of rho is summation over s c s rho to the s.

But I know the following that when rho goes to 0, I know that r of rho should go as rho to the l. So, l of rho should go as some constant and therefore, s takes values 0 all the way up in principle to infinity unless the truncation of series is demanded. So, as if now I know that it starts with s equals 0 and goes all the way up.

(Refer Slide Time: 34:06) Substituting this in this equation I can find out the recursion relation and you see that c s plus 1 by c s turns out to be this quantity. So, these are the exercises that you need to do no new frills or fancies the same way in which we handled the harmonic oscillator problem or even the orbital angular momentum Eigen values and Eigen functions.

But look at this for s going to infinity for large s. C s plus 1 by C s goes as 1 by s that is an s there and there is an s square here, but that is precisely the ratio of coefficients in the series e to the rho. So, if you will expand the series e to the rho and look at the ratio of coefficients for large s. If you did this series expansion you will find that that goes as 1 by s and that is unfortunate because then it tells me that R of rho goes as rho to the l e to the plus rho by 2 and then for rho going to infinity it blows up and that is not what I want. As a result of that I will have to truncate this series. The series of course, gets truncated notice that s is an integer goes from 0 all the way up, l is an integer takes values 0, 1, 2, 3 it is the orbital angular momentum and there is a plus 1 here which is very crucial for further discussion.

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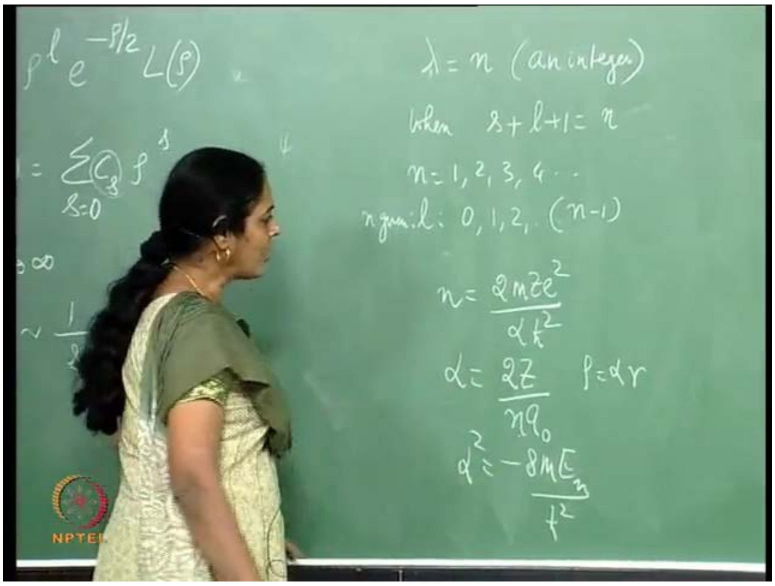

So, if lambda is an integer let us say lambda is equal to n an integer when s minus l plus 1 equals n or s plus l plus 1 equals n the series terminates and that is exactly what we want. So, after that the numerator is 0 in this recursion relation and therefore, you truncate the series when s plus l plus 1 equals n. Now, this is a very important matter because it also tells us the value of n, n can never be 0 because n is 1 plus something. So, n takes values 1, 2, 3, 4, up now, if n takes values 1, 2, 3, 4, up and there is already a 1 here the maximum value that l can take is n minus 1. Because let us assume that s is 0, but l is just n minus 1 so l can take value 0, 1, 2, 3, for a given n up to n minus 1, n is given. So, this is how l and n get related, n does not get directly related to n at all, but n can take these values and therefore, l takes those values.

Now, what does this mean for alpha? Lambda was 2 m z e square by alpha h cross square and alpha has taken the value n. Lambda has taken the value n. So, alpha is 2 z by n a 0 where a naught is the Bohr radius h cross square by m e square. So, one thing is clear now this means that since rho is alpha r, rho is independent and that is an important difference between the kind of problems that we have seen till now and what we see here. Rho itself becomes dependent on n.

Now, having said that what is the energy equal to? Energy is of course, quantized in units of n quantized with the quantum number n, because alpha square was minus 8 m E n by h cross square.

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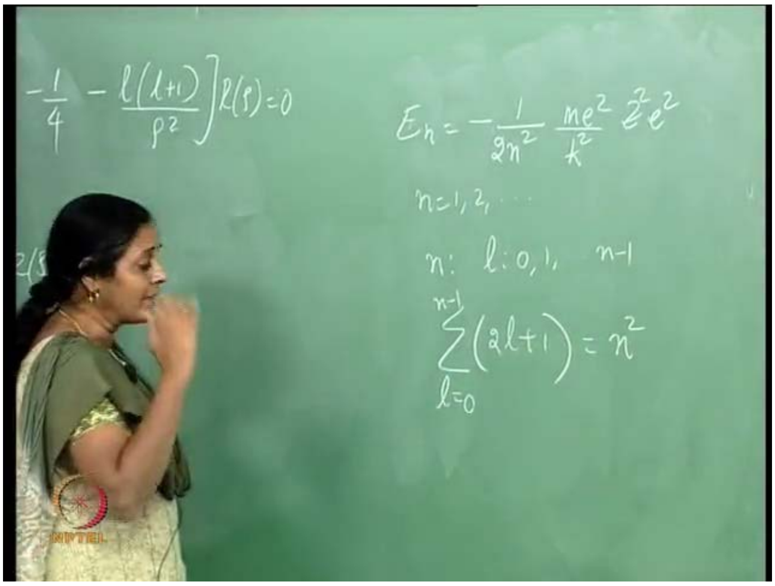

So, you can substitute for alpha square here and you find E n and what is E n? E n first of all it comes with a negative sign and that is good because it is a bound state and we do expect that. Alpha square has an m square so that goes as 1 by 2 n square and this is important times m e square by h cross square z square e square. So, this is the energy that you have, n is a reduced mass the energy spectrum here is not equally spaced n takes values: 1, 2, 3 that is a very important thing.

The energy spectrum is not at all equally spaced, but as we proceed to higher and higher values of n or large quantum numbers the levels get crowded and then for very large quantum numbers you find that it looks like a continuous energy spectrum. The discrete nature is no longer seen and if this is consistent with the fact that for large quantum numbers you go to the classical limit. Or the Rydberg atom can be treated classically that is when you work with atoms with which are in a highly excited state so that the energy is very large, sufficiently large for the level to look that it is part of the continuum and then you have approached the classical limit.

Now having said this look at the degeneracies. For a given value of n: l takes values 0, 1, 2 to n minus 1. So, basically there is a summation over l equals 0 to n minus 1, but then for a given l m can take 2 l plus 1 values. So, the degeneracy is this summation but that is n square and as you can see the degree of degeneracy does not depend upon m and that is a very interesting observation. It turns out that the degree of degeneracy comes only through accounting of l from 0 to n minus 1 and really n is related to l and not directly to m. What are the Eigen functions? So here are the Eigen values and we need to look at the Eigen functions. (Refer Slide Time: 34:06) So, let us go back to this equation and here we will substitute lambda equals n.

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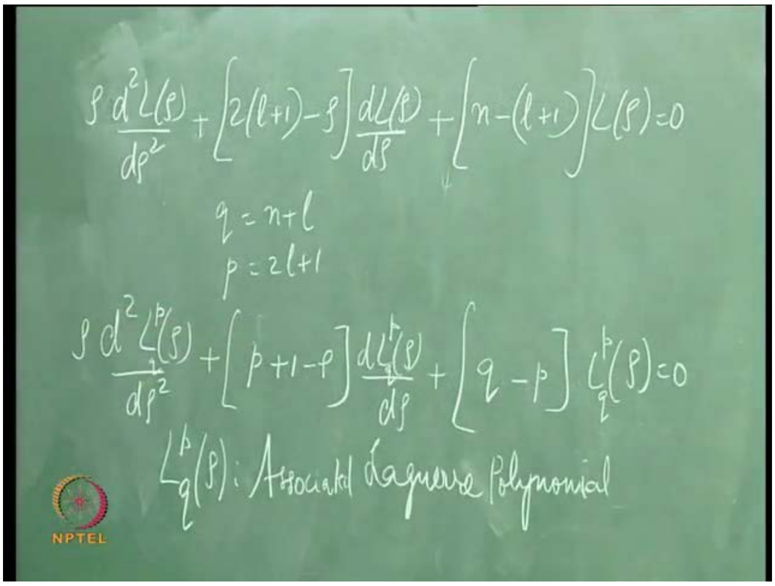

So, what we get is the following: rho d 2 L of rho by d rho square plus twice l plus 1 minus rho d L of rho by d rho plus n minus l plus 1 l of rho equals 0. Since, the series for l of rho is a finite series it has been truncated one would like to see if really this can be expanded or can be identified with one of the special functions, polynomial functions. In the case of the harmonic oscillator it was a Hermite polynomial and in the case of angular momentum we had the associated Legendre polynomials.

(Refer Slide Time: 34:06) So now, here I can do the following by inspection I can see that, if I write if I make this identification q is n plus l and p is 2 l plus 1 then the equation is d 2 L of rho by d rho square p plus 1 minus rho d L of rho by d rho plus q minus p l of rho equals 0. And indeed L q p of rho is the associated Laguerre polynomial which is really defined for rho going from 0 to infinity as in this case.

(Refer Slide Time: 34:06) So, actually in the hydrogen atom problem the radial equation turns out to be the associated Laguerre polynomial which satisfies the following orthonormality property. This is like psi star psi so it is L q p of rho square because it is real function of rho, but then there is an e to the minus rho, rho to the p plus 1 here integration from 0 to infinity and that turns out to be this object.

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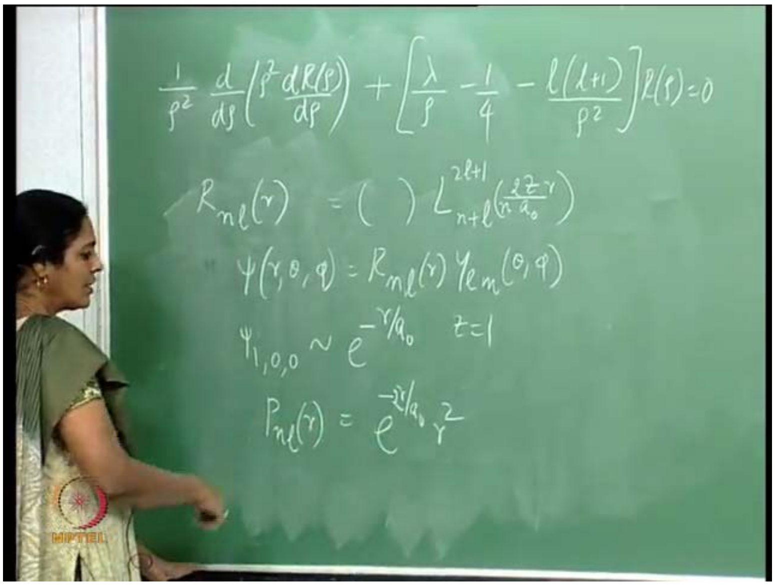

So, in fact when I now write down the wave function for the hydrogen atom the radial wave function there are 2 quantum numbers R n l of r. Because the polynomial itself is l with 2 numbers q and p associated with it and 2 l plus 1 is p and q is n plus l. (Refer Slide Time: 34:06) So, when I just put that in R n l of r is L q p of rho and rho is alpha r and alpha itself was 2 z by a naught r. So, that is what I have for rho 2 z by n. in so rho is alpha r that is 2 z m a naught r. But apart from this I would have some normalisation factors out here because of the orthonormality relation of the associated Laguerre polynomials.

So this is R n l of r and I have put down the expression here you can see that this is e to the minus rho r which takes care of the large rho behaviour. Then there is a rho to the power of l which is out here. So, that is an e to the minus rho r rho to the power of l and then you have the normalisation which comes from here substitute for q as n plus l and p as 2 l plus 1 and you will retrieve this q minus p factorial to the power of half because this is like psi star psi and therefore, there is a half.

You put these coefficients on top and that below and that is half of that and extras and then of course, the L q p of rho. So, this is the radial wave function of course, the total wave function is R n l of r Y l m of theta psi. So, basically psi of r theta phi in the case of the hydrogen atom this is R n l of r Y l m of theta phi; 2 special functions are involved here the associated Laguerre and there the associated Legendre.

Now, if you look specifically for the ground state has n equals 1 that is a lowest energy state and since l can only take value 0 to n minus 1, l takes a value 0 and therefore, m takes the value 0 so the ground state is psi 1, 0, 0, n l m. If you substitute those values there you find that apart from a constant it is e to the minus z r by a naught. Now, you see this feature is important for the following reasons. The ground state of the hydrogen atom it is essentially e to the minus r by a naught. I have said z e equals 1 for the electron, I am just looking at the hydrogen atom. So, z equals 1 and then what is the probability distribution of the radial position of the electron?

So that objects P n l of r and that that is simply e to the minus r by a naught so this is just the wave function. So, you looking at the probabilities so e to the minus 2 r by a naught r square and this is the probability distribution and you can see where it peaks up. This probability distribution is maximum at r equals a naught. So, in that sense we have connected up with something from the old quantum theory that the Bohr radius becomes very important and h cross square by m e square at that distance you have the maximum probability distribution of the radial position of the electron. And in that sense certainly we have connected up with some features of the old quantum theory those are the question of definite orbits and so on. The attitude in modern wave mechanics as we are seeing it here is very different from what there was in the old quantum theory.

So, I will stop here and we'll take it up from here in the next lecture and we will look at a different problem all together. The whole purpose of this exercise was to show the importance of various scales: length scales, mass scales and also the machinery of how exactly you solve for Eigen values and Eigen functions in function space and how special functions play a very important role in this context.