Quantum Mechanics– I
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Lecture -31
The Spherical Harmonics

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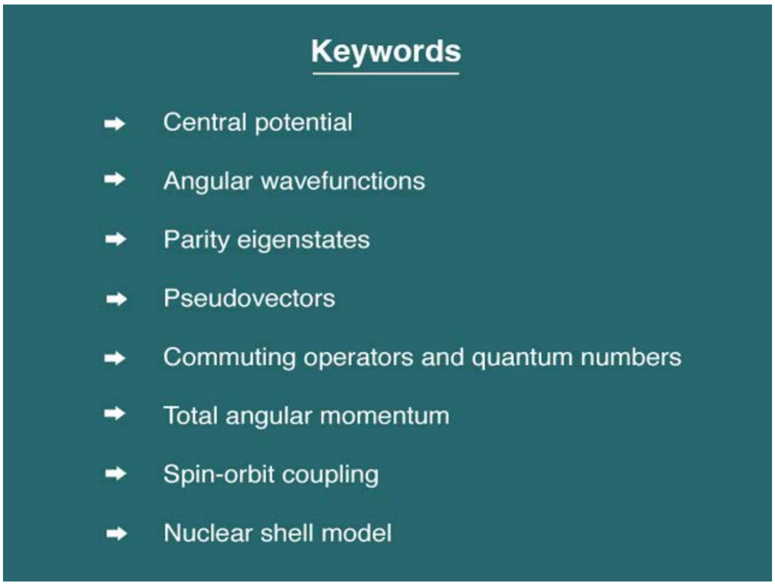

Keywords

- Central potential
- Angular wavefunctions
- Parity eigenstates
- Pseudovectors
- Commuting operators and quantum numbers
- Total angular momentum
- Spin-orbit coupling
- Nuclear shell model

In the last lecture, we had looked at the Eigenfunctions of L squared and L z.

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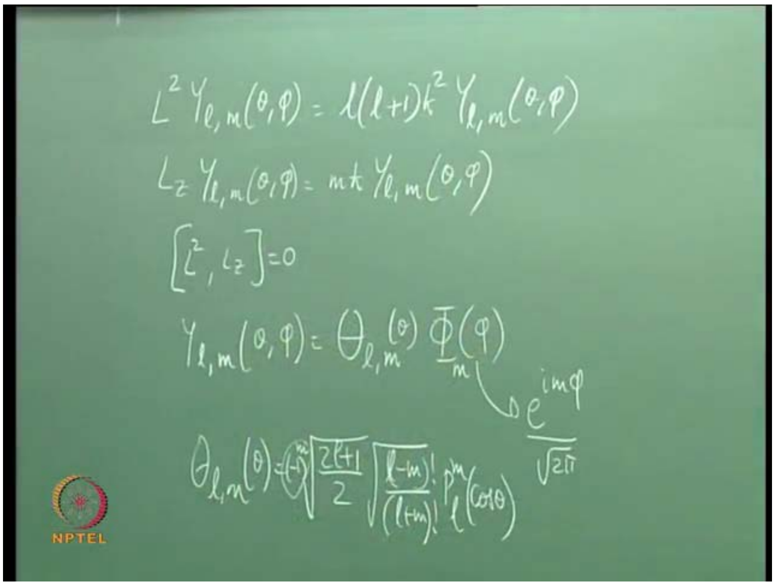

$$L^2 Y_{l,m}(\theta,\varphi) = l(l+1)\hbar^2 Y_{l,m}(\theta,\varphi)$$

$$L_z Y_{l,m}(\theta,\varphi) = m\hbar Y_{l,m}(\theta,\varphi)$$

$$[L^2, L_z] = 0$$

$$Y_{l,m}(\theta,\varphi) = \Theta_{l,m}(\theta)\, \Phi_m(\varphi) \qquad \Phi_m(\varphi) \rightarrow \frac{e^{im\varphi}}{\sqrt{2\pi}}$$

$$\Theta_{l,m}(\theta) = \boxed{(-1)^m} \sqrt{\frac{2l+1}{2}} \sqrt{\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)$$

These are the spherical harmonics and we had the following: L squared acting on Y l m of theta phi. Gave me l times l plus 1 h cross squared Y l m of theta phi. And L z acting on Y l m of theta phi, whose m h cross Y l m of theta phi. Just a quick recapitulation as to what exactly happened. We were looking at common Eigenstates of L squared and L z since, they commute with each other. This was all in the context of the 3 dimensional problems where we had separated the wavefunction into r of r just depending upon the radial component and Y l m of theta phi which is the angular wavefunction.

Now, really in my notation this was some theta l m of theta phi of phi. So, this is the way the wavefunction separated and actually we should write phi sub m of phi, because this object is e to the i m phi. You normalize it by putting root 2 pi down stairs there and theta l m of theta was related to the associated Legendre polynomials and this was 2 l plus 1 by 2 root of l minus m factorial by l plus m factorial p l m of cos theta. Except that sometimes by way of a sign convention, one could put a minus 1 to the m out there. That is merely a sign convention which goes with the general angular momentum framework so this is a convention.

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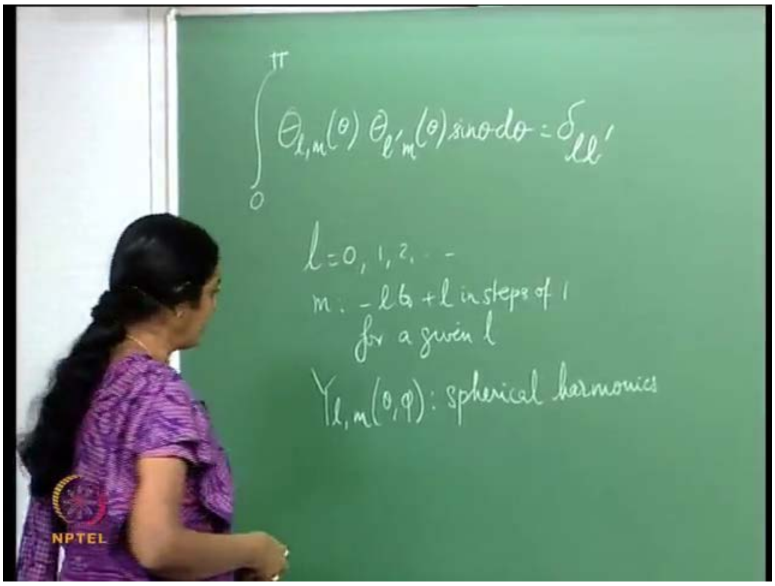

$$\int_0^\pi \Theta_{l,m}(\theta)\,\Theta_{l',m}(\theta)\sin\theta\, d\theta = \delta_{ll'}$$

$l = 0, 1, 2, \ldots$

m : $-l$ to $+l$ in steps of 1 for a given l

$Y_{l,m}(\theta,\varphi)$: spherical harmonics

Now, with these normalizations you can easily check that theta l m of theta is normalized. In other words, integral theta goes from 0 to pi theta l m of theta theta l prime m of theta sin theta d theta is delta l l prime. So, that is the way the wavefunction gets normalized. So, what we have really seen is this, that in a problem where the potential is a central potential so merely a function of r and not a function of theta and phi you could work in spherical polar coordinates and separate variables get the angular wave function (Refer Slide Time: 00:23) which is really an Eigenfunction, a common Eigenfunction of L square and L z. In fact, this is a complete set of Eigenfunctions not just one, because l can take various values and correspondingly m takes different values, l takes values 0, 1, 2 and so on and m takes values minus l to plus l in steps of one for a given l. And therefore, (Refer Slide Time: 00:23) this is a complete set of wave functions that you have and these are the various values that l and m can take.

So, Y l m of theta phi is a very important angular set away functions. They are called the spherical harmonics and they arise whenever the potential is taken to be a central potential. This is the angular part of the wave function. There is a radial part of the wave function and one writes the radial differential equation. That part of the equation which depends upon the radial coordinate r solves for that to get r of r, the radial wave function

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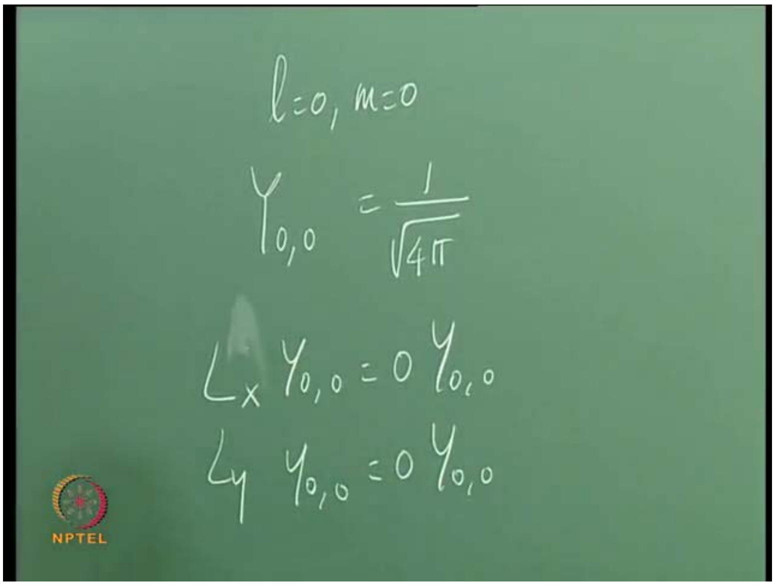

$l=0,\ m=0$

$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$

$L_x Y_{0,0} = 0\, Y_{0,0}$

$L_y Y_{0,0} = 0\, Y_{0,0}$

Just to give a flavor of what Y l m of theta phi is when l is 0 m can only take the value 0 so you have Y 0, 0 and that turns out to be a constant 1 by root 4 pi. You see (Refer Slide Time: 00:23) that just gives me a 1 and this gives me a 1 by root 2, nothing out here. This is p 0 0 of cos theta and that is our 1 by root 2 pi and therefore, I have 1 by root 4 pi out here. This is interesting since, this it is just a constant, it is an Eigenfunction of L x, L y and L z.

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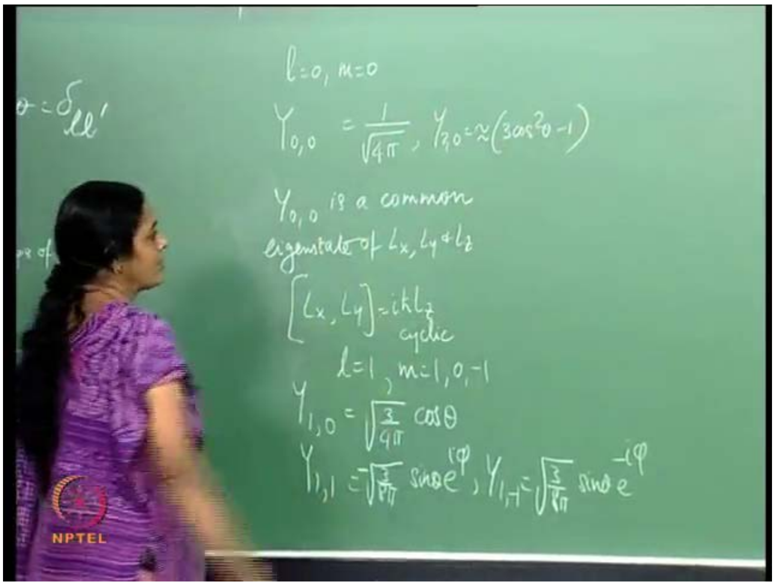

So, there is nothing to say there because this does not even act on it.

So, there is nothing to say there because this does not even act on it and therefore, Y 0, 0 is a common Eigenstate of L x, L y and L z. This is a good thing to note because you will recall that L x, L y do not commute with each other. There is a cyclic relation commutator L x, L y is i h cross L z and that is a cyclic relation. But that does not prevent three objects which do not commute with each other from having a single common Eigenstate.

So, the statement is really this: “If 2 operators do not commute with each other they cannot have a complete set of common Eigenstates”. On the other hand, nothing prevents them from having a common Eigenstate and Y 0, 0 is an example. You cannot find a complete set of common Eigenstates of 2 operators which do not commute with each other. So, the word complete is to be emphasized. Now, if you look at l is equal to 1 then you can have m equals 1, 0, minus 1 so you can have y 1, 0 and that turns out to be root of 3 by 4 pi cos theta.

And Y 1, 1 of theta phi is root of 3 by 8 pi sin theta with the minus sign e to the i phi. If you look at Y 1minus 1, that is root of 3 by 8 pi sin theta e to the minus i phi, if you look at Y 2, 0 clearly that would be related to (Refer Slide Time: 00:23) P 2, 0 of cos theta, which is 3 cos squared theta minus 1 apart from some factors. So, Y 2, 0 let me write that, here is essentially 3 cos squared theta minus 1, apart from some constants. So the Y l m’s have a definite parity. So, we need to understand, what we mean by the parity operator here in this context.

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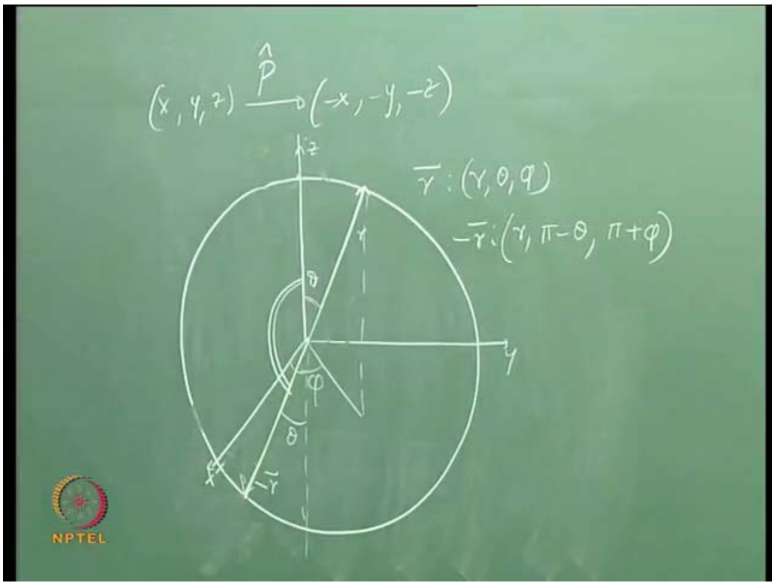

As you know, parity operation takes x, y, z to minus x, minus y, minus z under parity, that is an operator. So, construct the circle and this is the x, y plane and that is the z axis. I have a vector r here, which means the radial coordinate is r and the angles r, theta and phi here once I make a projection on to the x, y plane.

So, this is the continuation of the z axis. So, when x goes to minus x, y goes to minus y and z goes to minus z. Let us do this a little bit better that is x so this phi, r just goes to minus r which is this object here, which I show in yellow. So, where as the vector r was given by the coordinates r, theta and phi minus r will also have a modulus r and what about theta itself? Theta is this angle; the angle which it makes with the z axis and since vertically opposite angles are equal, this is theta and what you have here is pi minus theta. Similarly, you can find out what has happened to phi? Phi goes to pi plus phi.

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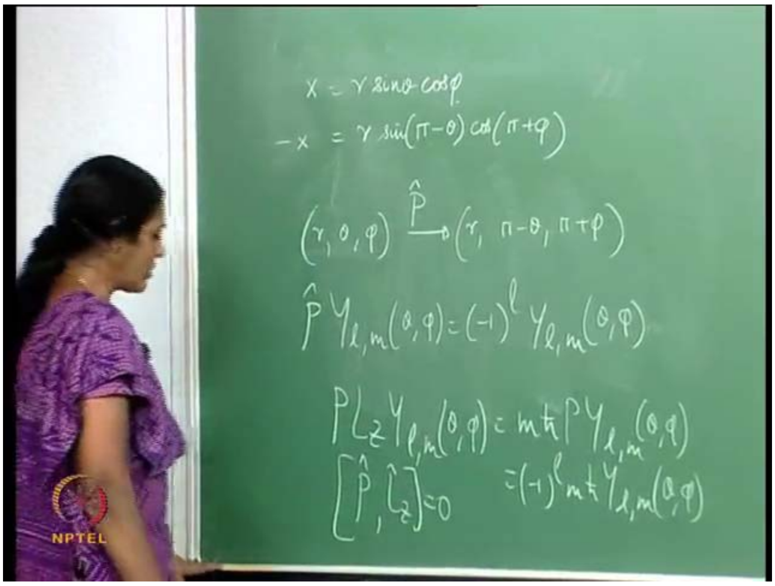

You can look at it this way, x is r sin theta cos phi and minus x under parity r theta goes to pi minus theta and phi goes to pi plus phi and its consistent similarly, y and z. So, under parity r theta phi go to r, pi minus theta and pi plus phi. This is what happens under parity. So, what happens to the Y l m's under parity (Refer Slide Time: 06:04) Y 0, 0 is a number. So, the fact that theta changes to pi minus theta and phi changes to pi plus phi do not affect Y 0, 0. Now, if you look at Y 1, 0 cos theta out here, under parity it becomes minus of itself.

Similarly, Y 1, 1 change to minus of itself and Y 1, minus 1 also does whereas, Y 2, 0 does not change. So, the parity of Y l m of theta phi by inspection I have written it is minus 1 to the l and it is an Eigenstate of parity. So, these angular wave functions have definite parity and it is given by minus 1 to the l. So, when l is equal to 0 ,its parity plus 1, l is equal to 1, 3 and so on minus 1, l is 2, 4 plus 1 and so on. So, these are definite parity states.

Now, what happens if I work with P on L z. P L z Y l m theta phi is m h cross P Y l m theta phi, which is minus 1 to the l m h cross Y l m theta phi. Now, suppose I had started with L z P, it would have been the same thing. I would have picked up a minus 1 to the l, L z acting on Y l m of theta phi which gives me the same answer. So, P and L z commute with each other. Just put hats on it to remind you that, these are operators. Now, any operator which commutes with the parity operator.

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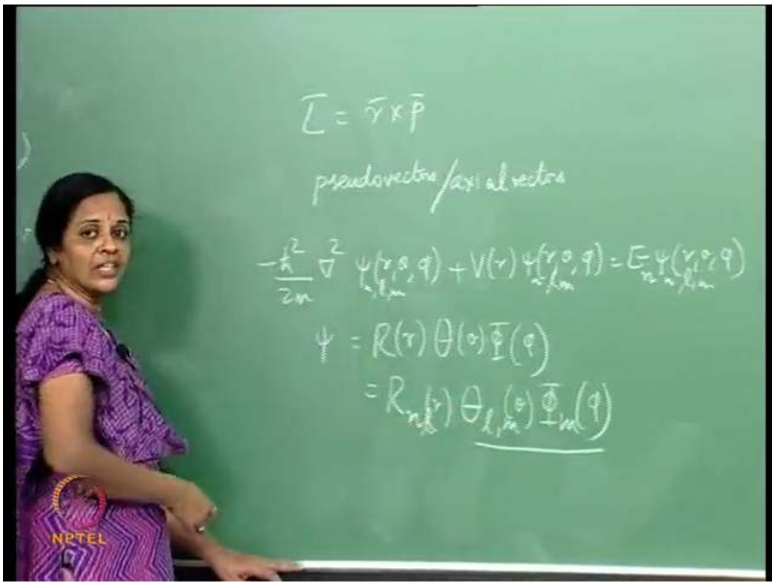

So, in general look at L the orbital angular momentum vector, L r cross p. So, under parity r goes to minus r and p goes to minus p. This is the linear momentum and therefore, L does not change sign. So, under parity L remains invariant.

Now, vectors which commute with the parity are called pseudovectors or axial vectors. And it is that you see here, (Refer Slide Time: 11:25) P commutes with L z so much for Y l m of theta phi, what we need to remember is the following. That in a problem like this, since L squared and L z commute with each other, there are 2 quantum numbers m and l and while the fact that the wavefunction satisfies certain very important properties like single valuedness, vanishing at space boundaries and so on. While these tell us what are the admissible solutions and what are the non-admissible solutions. It also fixes m in terms of l so the quantum numbers get related to each other.

Now of course, if you were doing a problem where you put in the full Schrodinger equation and say minus h cross squared by 2 m del squared psi of r theta phi plus V of r psi of r theta phi equals e psi of r theta phi. Since, this problem has a central potential the Hamiltonian also commutes with L squared and L z and that would provide another quantum number n and n gets quantized. So, in fact you will have psi n out here. Not just psi n, you would have psi n, l, m, because already we have the angular part of the wave function providing us with 2 quantum numbers l and m.

And if I wrote psi as R of r, theta of theta, phi of phi in fact, it would be R n of r, theta l m of theta, R n l of r, theta l m of theta, phi m of phi and this is the part that we have already looked at and we need to worry about what the radial equation is. But on the other hand, even as n and l has got related, l and n will get related once we solve the radial equation.

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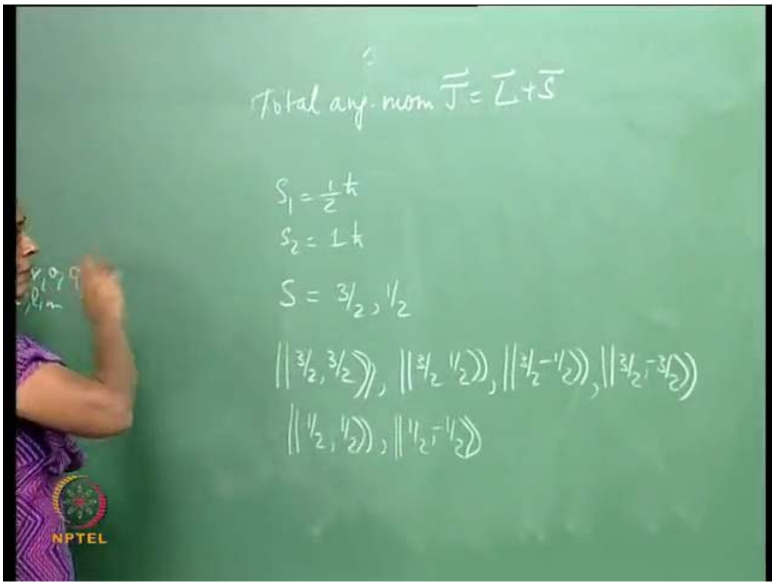

Total ang. mom $\vec{J} = \vec{L} + \vec{S}$

$S_1 = \frac{1}{2}\hbar$

$S_2 = 1\hbar$

$S = 3/2, 1/2$

$||3/2, 3/2\rangle\rangle, ||3/2, 1/2\rangle\rangle, ||3/2, -1/2\rangle\rangle, ||3/2, -3/2\rangle\rangle$

$||1/2, 1/2\rangle\rangle, ||1/2, -1/2\rangle\rangle$

This leads us to a very important and interesting application right away. First of all, the total angular momentum, J is the vector sum of the orbital plus spin. Addition of angular momentum follows the same rules that we have discussed earlier when we spoke about spin. For instance, when you had S 1 as half h cross and S 2 as say 1 h cross, where S 1 and S 2 are 2 spins. S could take values 3 by 2 and half in units of h cross. Therefore, coupled state of spin in my notation would have S taking values 3 by 2, 3 by 2. This is my notation double braces 3 by 2 half, 3 by 2 minus half and 3 by 2 minus 3 by 2 this was the spin quartet.

And of course, there was a spin doublet which was half, half and half, minus half. You will recall this from earlier lectures on angular momentum. The same rules of addition apply here, except that l, the orbital angular momentum quantum number can only take 0 or positive integers in units of h cross.

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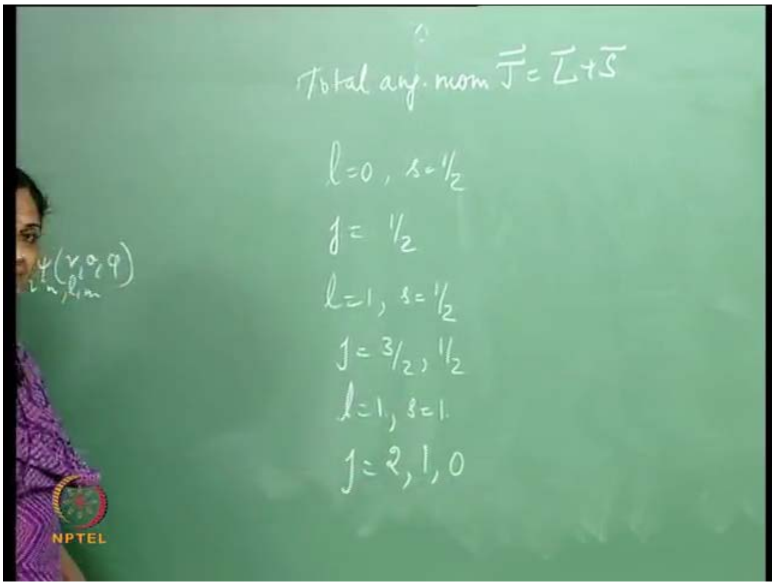

So, for instance if we look at an example l equals 0 and s equals half, j is l plus s which is half. If l is 1 and s is half, j is 3 by 2 or half and so on. If l is 1 and s is 1, j can take values 2, 1, 0 because it goes from 1 plus 1 to 1 minus 1 in steps of 1.So, the addition rules are the same as when 2 spins add. Except that l is constrained to take only integer values and not half integer values.

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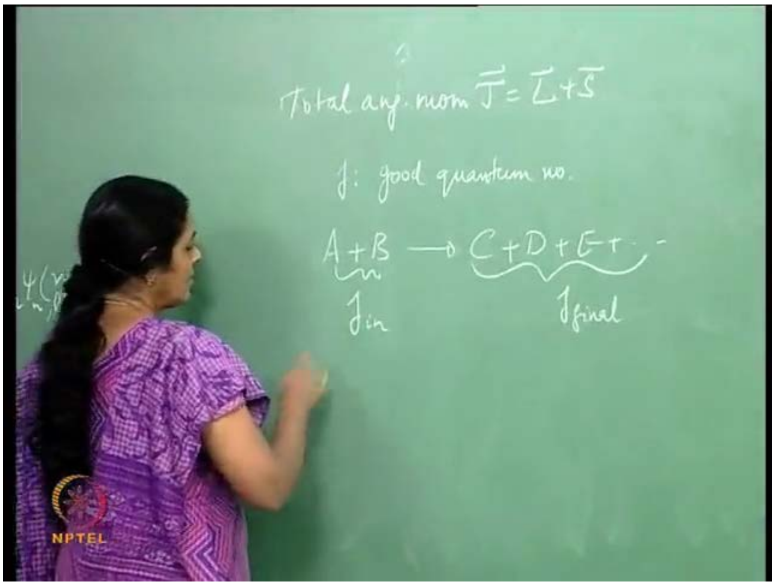

Now, j is a good quantum number. What do you mean by a good quantum number? Well, in a very popular sense of the term, it simply means the following that j is what is conserved in any process. Suppose, I have 2 particles interacting with each other to produce a final state of particles: could be electrons interacting with protons, protons interacting with neutrons, pions interacting with sigma anything. The total angular momentum here which I will call j initial should be conserved. In other words, it should be equal to j final. So, what one does is do pair wise addition. So, you do l plus s finds various possibilities for j.

So, if l was 1 and s was half, there are 2 possible values of j, just 3 by 2 and half. The final j should be 3 by 2 or half or perhaps both. But if the initial value for j is half, the final value should be half, if the initial value is 3 by 2, the final value should be 3 by 2. If j final is not 3 by 2 or half in this example, the process cannot go through. So, total angular momentum must be conserved. In other words, the total angular momentum in the initial state must be equal to the total angular momentum in the final state. And how do I find the total angular momentum? By the kind of addition rules that I prescribed when I add 2 spins or when I add 2 orbital angular momenta or when I add an orbital angular momentum with spin. It goes from l plus s to modulus of l minus s in steps of 1.

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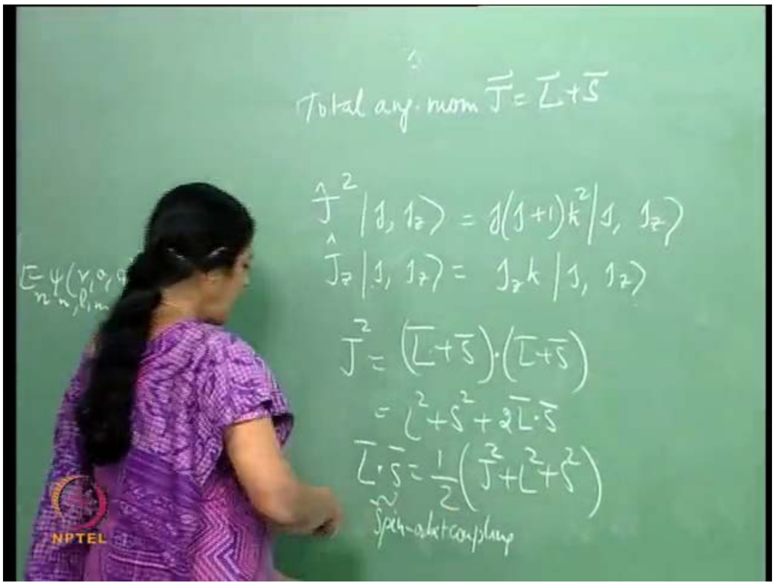

So, this is how you get j. Then you can write Eigenstates of j squared. So, j squared if you do not want to use the word m, let us call the J z, is j times j plus 1 h cross squared j, j z. I used to call the 3rd component m, do not want to do that because you do not want to confuse it with the orbital angular momentum quantum number. J z acting on j j z these are operators gives me j z h cross j j z. So, j squared is a very important operator particularly, because j is what is conserved in processes. In all processes be the strong, weak electromagnetic, you name it. The total angular momentum of the initial state should be equal to the total angular momentum of the final state. Orbital angular momentum need not be conserved separately. If it happens, it happens, but it is not necessary in general.

Similarly, the initial spin need not be equal to the final state spin in general, but j yes j initial should be equal to j final. But J squared is clearly L plus S dotted with L plus S. These are vectors under notations so that is L squared plus S squared plus 2 L dot S and therefore, L dot S is half of J squared plus L squared plus S squared. This is a very important term. The whole business of working with J square involves what is called the spin-orbit coupling. The spin-orbit coupling that means, the L dot S term has remarkable physical significance, accounts for many many things which go unaccounted for, if you do not take into consideration the spin-orbit coupling.

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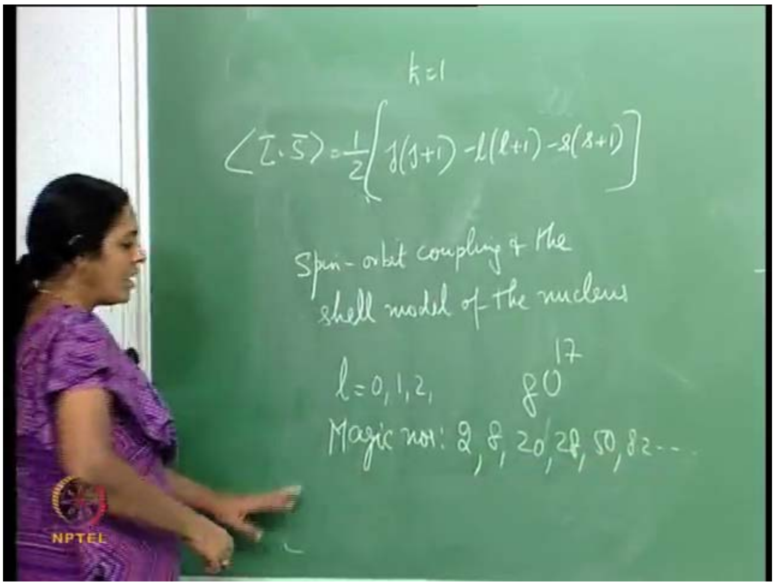

So, how do I find the value of L dot S, this is the way I will do it. So, the value of L dot S is half, the Eigenvalue of j squared. We are working with Eigenfunctions of these objects j times j plus 1 so I have set h cross equals 1

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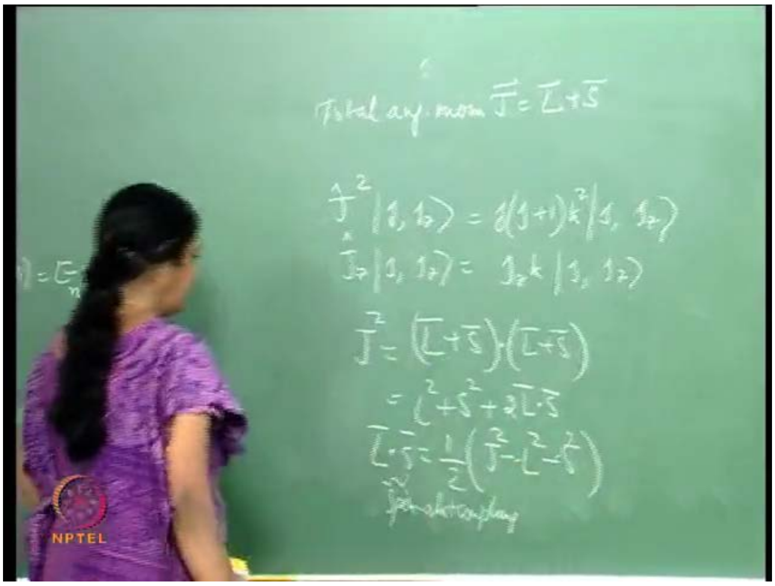

It is j squared minus l squared, minus s squared out here. Minus l times l plus 1 minus s times s plus 1 so this is going to be the value. Now, I remember this and I will look at an application. Specifically, I look at the shell model of the nucleus where the importance of the spin orbit coupling comes into the lime light. So, look at this, the spin orbit coupling and the shell model of the nucleus. This is an example, the shell model of the nucleus is an example, where the spin orbit coupling becomes very important. There are certain nuclei which were seen, which were stable.

Now, the idea is that the nucleus which is of course, made up of protons and neutrons and you distinguish between the protons and neutrons. They are different particles. Put the protons in various shell, that means various orbital angular momentum quantum numbers, l is equal to 0 corresponds to a shell, l is equal to 1 corresponds to another shell, l is equal to 2 to another shell and so on. So, you fill up these shells in a certain order starting from l is equal to 0. Fill up protons in the various shells that means in the l is equal to 0 state and the l is equal to 1 state, 2 state and so on, as many protons that are there in that particular nucleus, that we consider. For instance, if you take the nucleus 8 o 17 so you fill up these protons in the l is equal to 0 state, 1 state, 2 state and so on so that you have to find out how many protons can occupy the various levels, the various shells.

So, we will do a simple calculation to see that. Similarly, fill up the neutrons and see if you can account for the fact that certain nuclei are very stable. These are the nuclei with closed shells that means, there are as many protons in the outer most shell as are allowed and as many neutrons as are allowed in the outer most shell in which you have filled up the neutrons. So for instance, there these things called magic numbers: 2, 8, 20, 28, 50 and 82 and so on. And nuclei which have these number of nucleons are found to be stable nuclei and therefore, these numbers are called magic numbers. The spin-orbit coupling becomes very important in trying to explain the stability of the nucleus.

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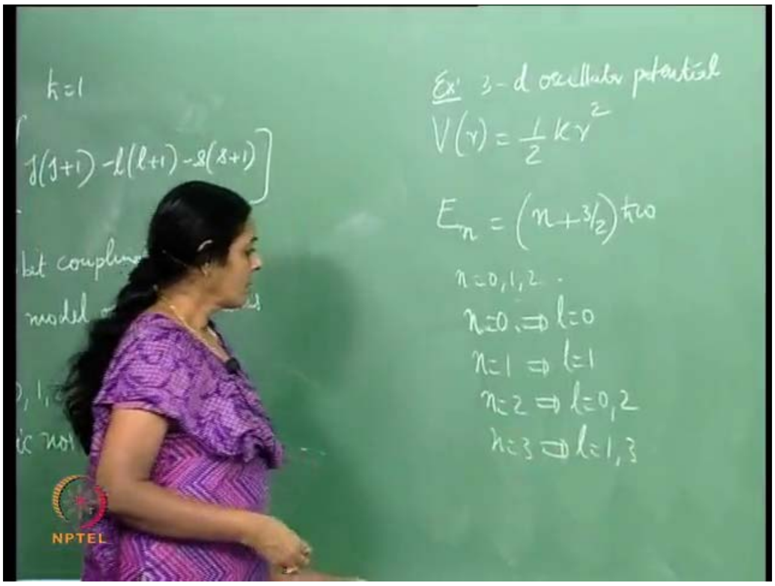

So, let us see how that works. Let me start with this belief: I have to build a model, because I cannot possibly take particularly in the case of heavy nuclei, a whole lot of protons and a whole lot of neutrons write a complicated messy equation involving all their wave functions. Instead, I would use an effective model where I say that the entire nucleus is subject, is influenced by its own potential, an effective potential. And I would like to choose for example, the harmonic oscillator potential it is a 3 dimensional problem. So, I write half k r squared, where r squared is x squared plus y squared plus z squared. And therefore, it is clear what the energy Eigenvalues would be. It is an n plus half h cross omega for x, for y and for z each. So, it is n plus 3 by 2 h cross omega.

So, these are the various energy levels and n itself takes values: 0, 1, 2, 3. Now, as I said earlier even as m got constrained, m and l got related to each other when we solved the angular momentum problem, once you solve the radial equation you will find that n and l are related to each other. It turns out that for a given value of n in the problem of the 3 dimensional oscillator potential. In this problem, l takes values if n is even for instance, n is 0 then l takes value only 0, if n is 1 it takes value 1, if n is 2 it takes values 0 and 2, if n is 3 it takes values 1 and 3 and so on.

So, basically if n is even it takes all even values from 0 up to n and if n is odd it takes all odd values. So, this would be the constraint between n and l in the 3 dimensional oscillator potential problem. I have not proved this, but ((Refer Time: 30:03)) let us just take this for granted for the moment, because I want to use this to demonstrate the importance of the spin orbit coupling. And here we see the following: what is the degeneracy? n and l are related but m, the 3rd component does not play a role at all in this picture.

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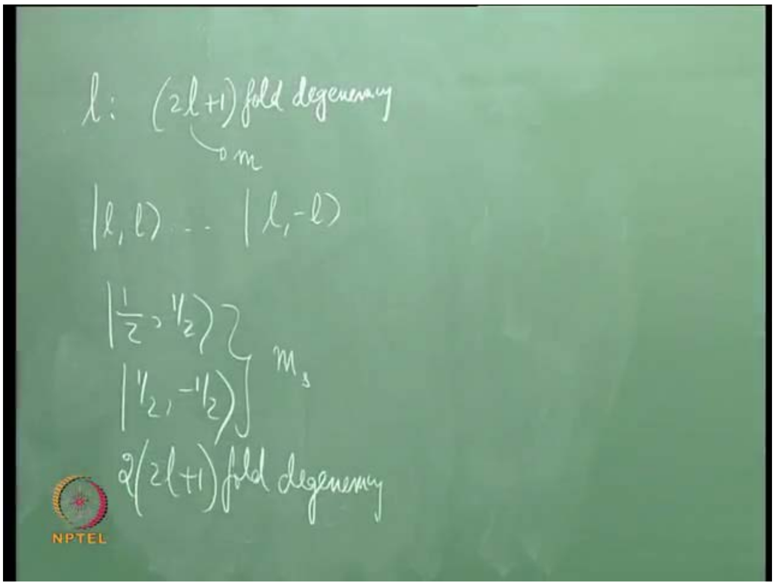

l: $(2l+1)$ fold degeneracy $\to m$

$|l, l\rangle \ldots |l, -l\rangle$

$\left.\begin{array}{l} |\frac{1}{2}, \frac{1}{2}\rangle \\ |\frac{1}{2}, -\frac{1}{2}\rangle \end{array}\right\} m_s$

$2(2l+1)$ fold degeneracy

Therefore, for a given value of l there is a 2 l plus 1 fold degeneracy because of m. So, for a given value of l there are 2 l plus 1 states ranging from l, l to l, minus l in steps of 1. And all of them would correspond to the (Refer Slide Time: 28:09) same value of l and n. There is also a further degeneracy because of spin, because the proton and the neutron each have spin half objects and therefore, I could have used them in the spin up state or in the spin down state which means the second component s z could be half or minus half and it wouldn’t make a difference.

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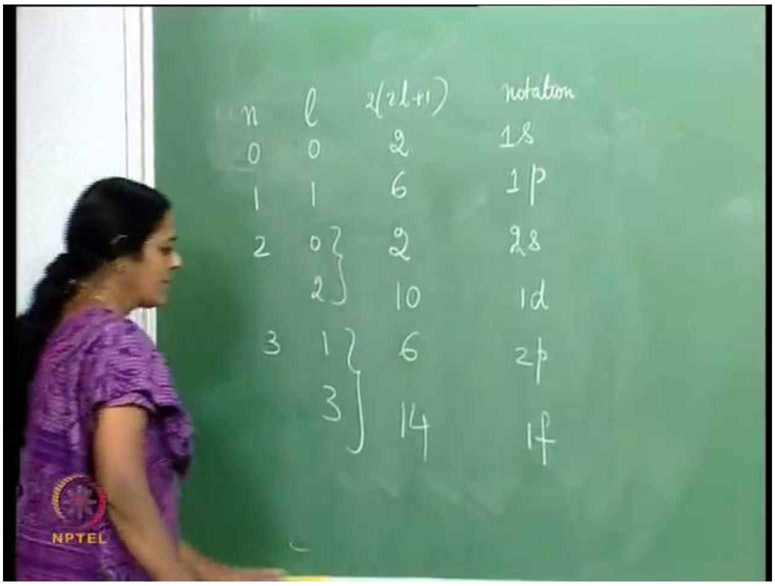

n	l	2(2l+1)	notation
0	0	2	1s
1	1	6	1p
2	0	2	2s
	2	10	1d
3	1	6	2p
	3	14	1f

So, there is twofold degeneracy because of spin and therefore, the total degeneracy is twice 2 l plus 1. Now, let us do this calculation. I have not put in the spin-orbit coupling term at all. I am just working with the oscillator. So let us start with n, n equals 0 so l takes value 0, the degeneracy which means the number of particles, number of protons for instance, which I can put in this level. It is twice 2 l plus 1 which means I can put in 2 protons. The neutrons are filled separately so I could put in 2 neutrons, that is a separate filling and my nomenclature notation. If l is equal to 0, it is called an s state and this is the first of the s states.

Then when n is equal to 1, l takes value 1. So, again I can put in 6 particles now, in this state and l is equal to 1, the nomenclature it is the p state and this is the first of the p states. When n is equal to 2, l can take values 0 and 2 of course, if it takes a value 0 only 2 particles can be put in, but this is the second of the s states. This is a certain notation that is being used.

You will find that atomic physicists use a different spectroscopic notation all together. But in this context you understand this notation as the first of the s shells, the 2nd of the s shells and so on. Now, when l is equal to 2 I can put in 10 particles and l is equal to 2 is called the d state and that is the first of the d states. When l is equal to 3, l can take values 1 and 3 and here of course, you can put 6 particles, l is 1 which means it is the second of the p states. Take care to understand this notation; this is not the atomic physicist's notation at all. When l is equal to 3, you can put in 14 particles that is the degeneracy in this state and l equals 3 is called the f state. So, that is the 1st of the f states and so on.

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So, now if we draw a neat diagram to see what exactly happens. We have used the oscillator potential. So, there is a state with l equals 0 that (Refer Slide Time: 31:59) is a 1st of the s states that has 2 particles and that could be a magic number. Because if there are only 2 protons available or 2 neutrons available I have filled that shell, it can take a total of 2 particles and I have put in both the particles. That is a closed shell, there is no way I can put in more particles in this level. Then of course, (Refer Slide Time: 31:59) I go to the 1 p state and here I can put in 6 particles.

So, there is a total of 8 particles now. So, suppose I started with 8 protons I will put 2 in the 1 s state, the l is equal to the 0 state and 6 in the 1 p state. The outer most shell now is the p state and there is no space to put in more particles that is it. It is a closed shell. It is such nuclei that are considered to be stable, because these are the magic numbers. It is a closed shell if you had only 2 and this is a closed shell, if you had 8 because you fill 2 here, you fill 6 there and that is it. There is no more a nucleon available for filing.

So, the magic number 2 and 8 are explained very simply even using the 3 dimensional oscillator potential. Now, let us go to the 2 s state. (Refer Slide Time: 31:59) Now, if you did that there are two ways of doing this. One is the 2 s state out here and then the 1 d state also. The 1 d state takes 10 particles, the 2 s state take 2 particles and then that takes care of things, because now that is an 8 here, and this is a 12, 20 is another magic number.

So, the harmonic oscillator potential is able to explain the fact that if there were 20 nucleons they fill closed shells, the outer most shell is complete, it is closed. But now let us see what happens? After 1 d comes 2 p and 2 p has 6 particles and then comes 1 f, 1 f has 14 particles, 26 is not a magic number, 28 is and even if this were suppressed compare to that, that is a 34 and 34 is not a magic number either. So, the harmonic oscillator potential fails even to explain: why 28 is a magic number? So, the potential has to be modified. This does not seem to be a good way of explaining things, because not 26 and not 14, none of these are magic numbers, 34 is also not a magic number.

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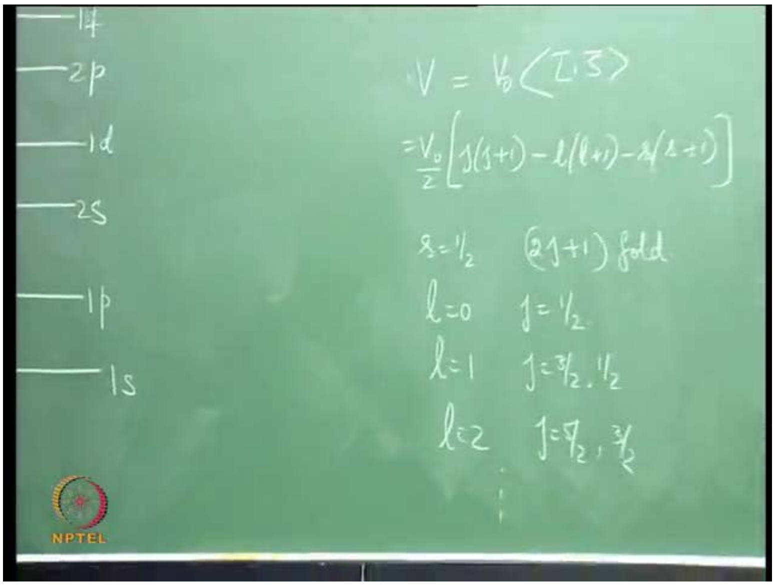

So, now let us look at the spin orbit coupling. Let us put that in. Suppose, the potential had an extra term, I will just write the extra term here, it is some V naught, average value of L dot S and that is obviously V naught times half j times j plus 1 minus l times l plus 1 minus s times s plus 1 as we have discussed earlier. Now, the spin of the particle is always half. Let us start with l is equal to 0, the ground state. If l is equal to 0, j just takes the value half. If l is equal to 1, j takes the value 3 by 2 and half. If l takes the value 2, j takes the value 2 plus half and 2 minus half and so on.

So, we only work in terms of j. For a given value of j, the degeneracy is 2 j plus 1 fold. So, for a given value of j I can fit in 2 j plus 1 nucleons in that state. We no longer consider l and s and therefore, the 2 l plus 1 times 2 fold degeneracy. The good quantum number is j and everything is translated in terms of j. So, let us see what happens now. Because we have put in the spin-orbit coupling here, things are written in terms of j. The notation is in terms of j and this is going to be the value of the potential.

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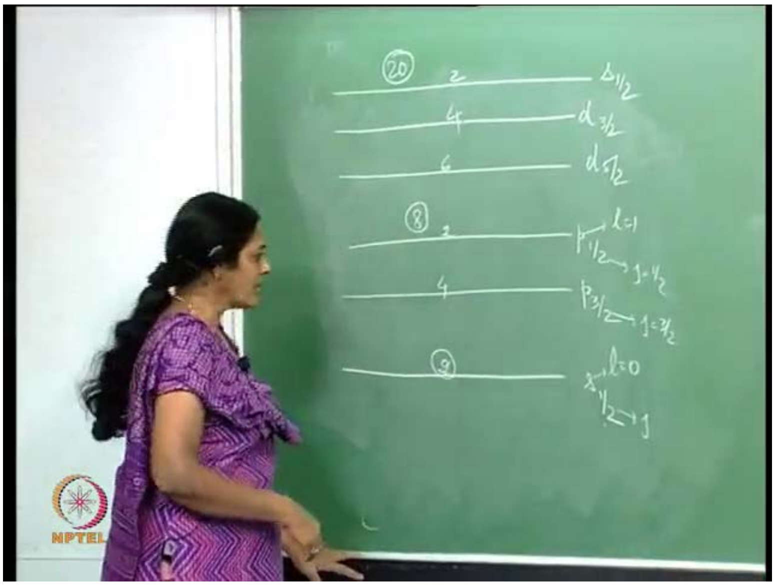

So, let us start with l is equal to 0. In my notation that is the first of the s states, (Refer Slide Time: 37:53) the first of the s states has j equals half. So, the suffix here is a value of j, s means l is equal to 0 and this is the value of j. Now, in this state I can put 2 j plus 1 particles that means 2 particles.

So, I have already accounted for the magic number 2. Then look at the l is equal to 1 state, (Refer Slide Time: 37:53) j is 3 by 2 and j is half, but this is the p state. So, there are 2 levels, one is p 3 by 2 and the other is p half. I will forget this, p means l is equal to 1 and this is the value of j. This level can have 2 j plus 1 particles, which means 4 and this level can have 2 particles. So, that gives me a total of 8 particles. So, the magic number 8 has been explained. Let us proceed further. (Refer Slide Time: 37:53) So, look at l is equal 2, if l is equal 2 I have 2 levels that is d 5 by 2 and d 3 by 2. This state can accommodate 6 particles and this state can accommodate 4 particles. There are already 8 particles and then comes the next level, s level that means l is equal to 0 and that can take care of 2 particles.

So, that gives me a 6 plus 4, 10 plus 2, 12 plus 8 20. So, you see there are other levels creeping in here. There is an s half, the second of the l is equal to 0 states there. So, the shell crosses here and 20 is explained. Without going into further details, we can now go for l is equal to 3 (Refer Slide Time: 37:53) and that gives me various values of j. You can put that in and you will find that various levels like the s state coming in here after the d's. Such things also happen and because you have taken j to be a good quantum number, you find that you are able to explain magic numbers 2, 8, 20, 28. 28 also can be explained, because if you now look at l is equal to 2 (Refer Slide Time: 37:53) and look at this, this gives me 6 particles and then introduce another s state with 2 particles. So, that makes it 20 plus 8 which is 28 and so on.

So, you can explain various levels by using this procedure. The important thing is that j is equal to 5 by 2 gets suppressed compared to j is equal to 3 by 2 in energy. Similarly, j is 3 by 2 gets suppressed compared to j is equal to half, for a given value of l. So, this happens because I have invoked an extra term in the potential (Refer Slide Time: 37:53) and by choosing appropriate sign here, a negative sign for instance, clearly this would help in suppressing 1 level compared to the other. The negative sign will take care of it. Remember that there is a j times j plus 1 in that expectation value.

So, the shell model actually in this very simple form explains closed shells 2, 8, 20 and if you go beyond 28, all the way to 82, but then for very heavy nuclei it has its limitations and its troubles. And therefore, cannot be used, but what I have given you is a very basic shell model. It is called the extreme independent particle shell model. Now, there are whole books written on the shell model and much more sophisticated models, shell models of the nuclei have come into vogue. But, this is a very basic thing which tells you the importance of the spin-orbit coupling and why j should be taken as the important quantum number and not l or s, for that matter.

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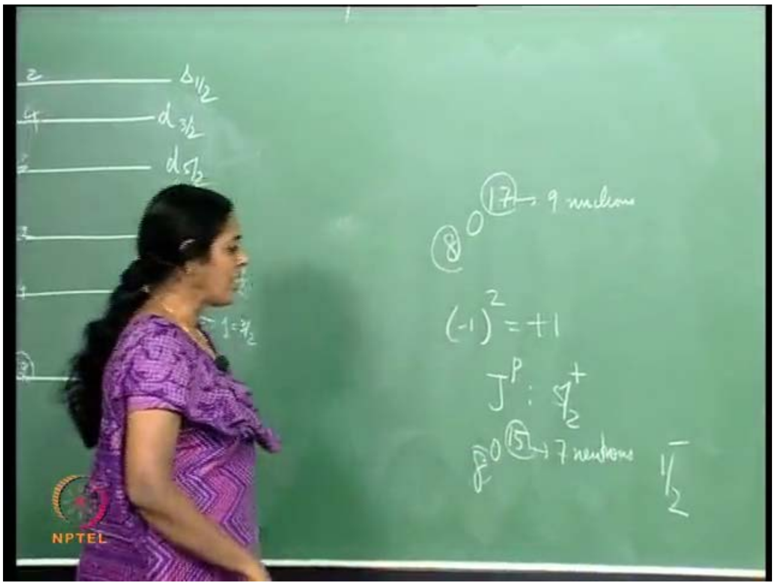

Since, the parity is minus 1 to the l. These are all problems, where there is a central potential and since the parity is minus 1 to the l. We always look for the outermost shell for instance, if it is 8 O 17, these 8 nucleons are already filled (Refer Slide Time: 39:47). It is a closed shell there and there is no question of it contributing to parity which is minus 1 to the l. But look at these, there are 9 nucleons here, because that is a total of 17. So, there are 9 nucleons and (Refer Slide Time: 39:47) if you use these to fill those 9 neutrons, the d shell is vacant, it can hold 6 particles, 6 neutrons but, you only have put 1. So, this is the outermost shell which is vacant and the parity is minus 1 to the power of l. (Refer Slide Time: 39:47) and what is l? s as l is equal to 0 and p as l equals 1 and d has l equals 2 so that is plus 1, the parity is plus 1. And this is the ground state we are discussing the ground state of the nucleus (Refer Slide Time: 39:47).

So, the ground state spin happens to be 5 by 2. So, the spin parity is 5 by 2 plus. So, merely if you look at 8 O 15 (Refer Slide Time: 39:47) these 8 protons have been filled up here, it is a closed shell. But there are 7 neutrons left here. I would have put 2 here and 4 there, but there is a vacant p shell and j is half and l is 1. So, the ground state spin parity is half minus. (Refer Slide Time: 39:47) Because l is 1 minus 1 to the l is a parity of y l m of theta 5. So, those are the angular wave functions and therefore, you have half minus. Now of course, this is for odd even nuclei.

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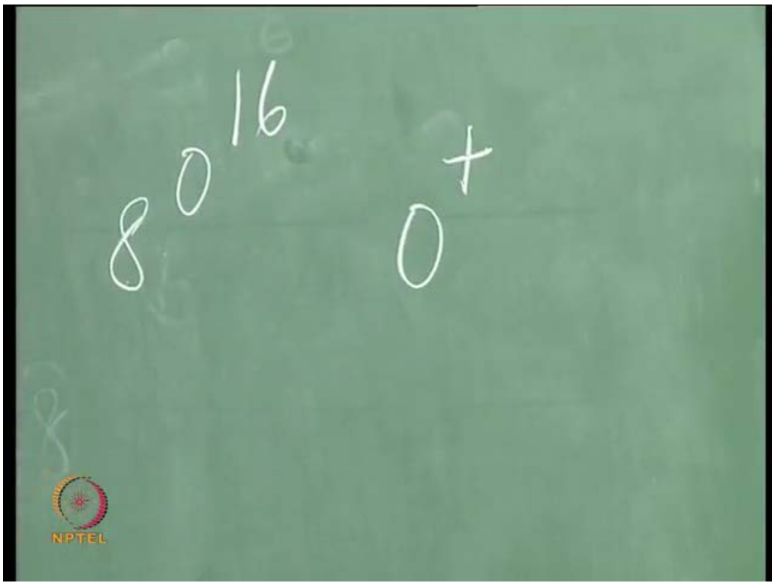

Now, suppose you had 8 O 16, 8 is an even number; no contributions. The remaining 8 is another even number; no contributions. So, the spin parity is taken to be 0 plus. The spin is 0 and the parity is plus and so on. As you can see, this is only a very rough model, it is not a very sophisticated model and several questions and issues can be raised regarding this model. (Refer Slide Time: 37:53) However, I merely wanted to give you a flavor for the importance of the spin orbit coupling and the fact that is related to the idea that j is a good quantum number and (Refer Slide Time: 39:47) the notation used is in terms of j and l.

Now, as I said even in the case of the harmonic oscillator potential. The energy quantum number n, which should come from the radial equation is related to l. In other words, in the case of 3 dimensional oscillators, I mentioned that l takes values, even values of n is even all the way to n. And l takes odd values if n is odd, from one all the way to n.

So, in order to explain how exactly n and l are related let us go back to a simple problem, the hydrogen atom problem and while we solve the radial equation there, you will see how exactly n and l related.

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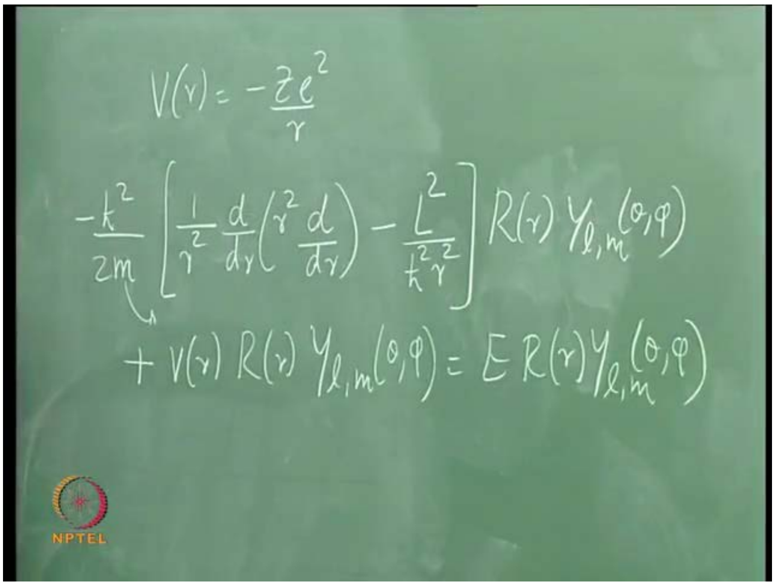

$$V(r) = -\frac{Ze^2}{r}$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{L^2}{\hbar^2 r^2}\right] R(r)\, Y_{l,m}(\theta,\varphi)$$

$$+ V(r)\, R(r)\, Y_{l,m}(\theta,\varphi) = E\, R(r)\, Y_{l,m}(\theta,\varphi)$$

So, in the hydrogen atom problem, the potential is minus Z e squared by r. And the Schrodinger equation is minus h cross squared by 2 m, where this is the reduced mass. We are working with the equivalent one body problem. Del squared is 1 by r squared d by d r of r squared d by d r minus L squared by h cross squared r squared. This is del squared psi of r theta phi, which I can write as R of r Y l, m of theta phi. So, we have minus h cross squared by 2 m del squared plus V of r R of r Y l, m of theta phi equals E R of r Y l m of theta phi.

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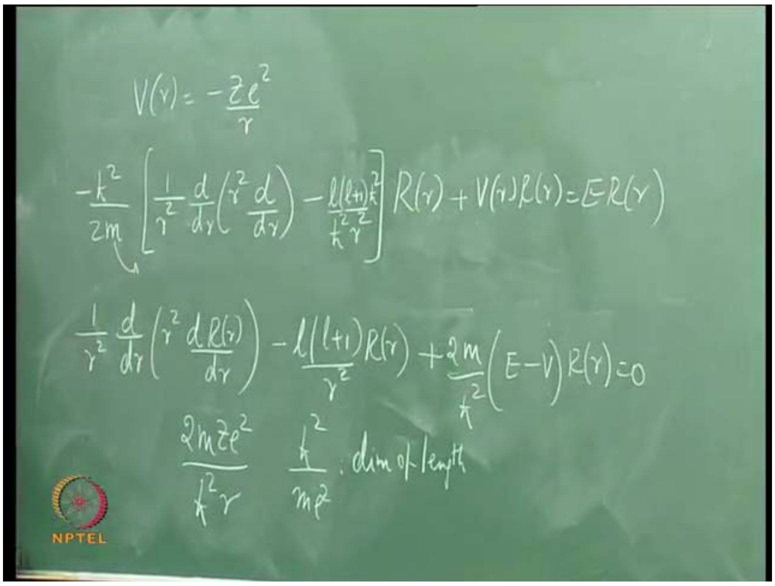

$$V(r) = -\frac{Ze^2}{r}$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) - \frac{l(l+1)\hbar^2}{\hbar^2 r^2}\right] R(r) + V(r)R(r) = E R(r)$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR(r)}{dr}\right) - \frac{l(l+1)}{r^2}R(r) + \frac{2m}{\hbar^2}\left(E-V\right)R(r) = 0$$

$$\frac{2mZe^2}{\hbar^2 r} \qquad \frac{\hbar^2}{me^2} : \text{dim of length}$$

So, this is the Eigenvalue equation that we have. It is clear that I can just remove Y l m of theta everywhere and l squared Y l, m of theta phi was minus l times l plus 1 h cross squared Y l, m theta phi. So, this is what I have. So, maybe I can just write it here plus V of r R of r is E R of r. So, this is what we have. Now, suppose I multiply the whole thing by 2 m by h cross squared so I have 1 by r squared d by d r of r squared d R of r by d r that is the first term, minus l times l plus 1 by r squared R of r that is the second term. Minus 2 m by h cross squared V of r equals minus 2 m by h cross squared E.

So, I can bring it to this side. There is an R of r here and an R of r there. So, I can just write this as plus 2 m by h cross squared E minus V R of r equals 0. Look at the potential term, the potential is minus Z e squared by r and therefore, I have 2 m Z e squared by h cross squared by r. That is the term that I have there. You can identify an object of the dimensions of length here, h cross squared by m e squared is an object with the dimensions of length. That is easy to see because h cross has dimensions energy time.

And e squared has dimensions energy times length because Z e squared by r has dimension of energy and there is a mass here. This is a very important point. We are going to look for a bound state. The hydrogen atom is a bound state, which means that there is a bound state size. There is a typical size for a bound state. How can you talk of a size of an object unless, there is an object with the dimensions of length which you can make with the parameters that are available in the problem like h cross, m e and so on.

So, you look at the radial equation. Look at the potential term. If there is no object with the dimensions of length associated with that potential comes usually as a coefficient of the potential. If there is no object with the dimensions of length, that you can identify with the constants that are available in your problem. There is no point in continuing to solve for the Eigenvalues and the Eigenfunctions because it will not support a bound state. Look back at the harmonic oscillator that was a parabolic potential. Of course, there was penetration into the classically forbidden regions, but then there was a certain length scale associated with it which was root of h cross by m omega.

Similarly, you look at the square well potential. The potential itself range from minus a to plus a. In my notation there was a size for the potential well, there was a width for the potential well. Therefore, there is a certain length scale associated with the problem. Similarly, here there is a length scale h cross squared by m e squared which has dimensions of length, you will find later that when we solve this radial equation the famous Bohr radius and the other distances that one talks about in this problem. The various energy levels, the length associated, the size associated with the various energy levels will be in terms of h cross squared by m e squared, could be some number times h cross squared by m e squared. The number is what you determine by solving the Eigenvalue equation.

But the moral of the story, the take home lesson is this. If you cannot find an object with the dimensions of length associated with the potential. An object that you can form with the fundamental constants or with the constants, that are available or the parameters that are available in your problem. Then there is no way you can have a bound state and there is no point trying to solve for the bound state. Come back for the next lecture and I will go ahead and solve the radial equation for the hydrogen atom.