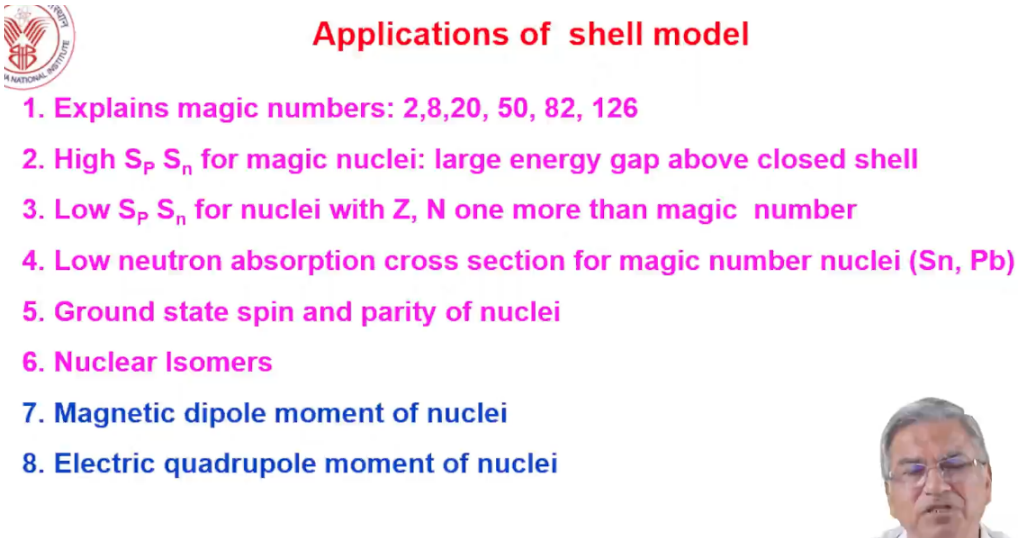
Applications of shell model

B.S.Tomar

Homi Bhabha National Institute

Lecture-5, module-2

Hello everyone. In the previous lecture, we discussed about the shell model. And in the shell model, we discussed the nucleons orbiting in their individual orbitals. So, it is sort of a weak interaction among the nucleons, though the nuclear force is a strong force. But the nucleons in their individual orbitals do not interact with the other nucleons in other orbitals. And by solving the Schrodinger equation of a nucleon using the potential, the potential though it is non-central, we assume that it is central potential offered by other nucleons to the particular nucleon. We get the energy states of the nucleons and whereby you populate those levels to get the configuration of the nucleons in the nucleus. And the shell model could explain the magic number. So, that will be the application of the shell model. What are the different applications, what are the limitations we discussed in terms of liquid drop model, we can now try to see how this shell model scheme explains those things.



Applications of shell model

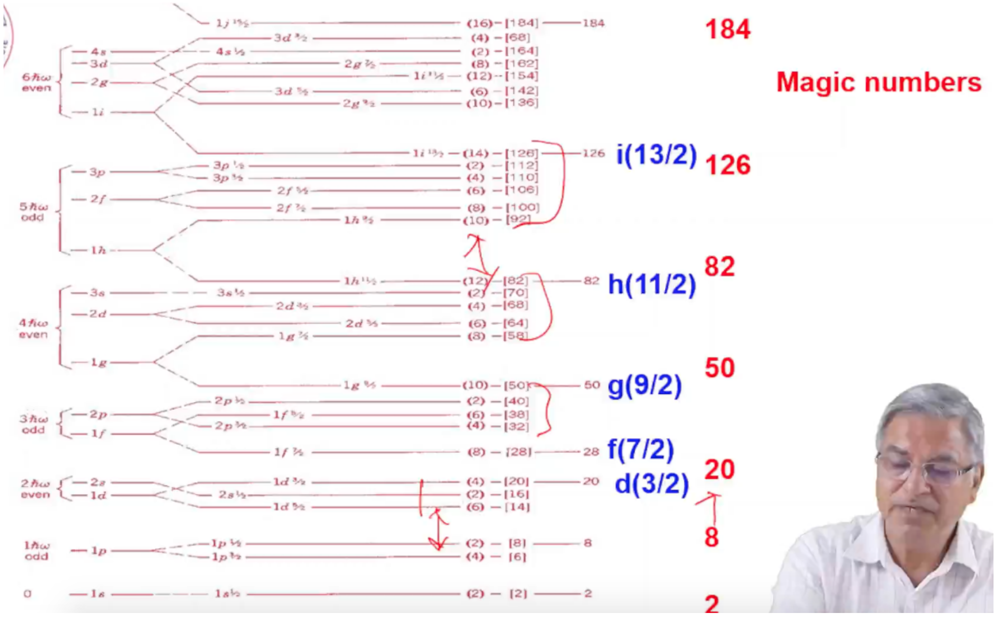
1. Explains magic numbers: 2,8,20, 50, 82, 126
2. High S_P S_n for magic nuclei: large energy gap above closed shell
3. Low S_P S_n for nuclei with Z, N one more than magic number
4. Low neutron absorption cross section for magic number nuclei (Sn, Pb)
5. Ground state spin and parity of nuclei
6. Nuclear Isomers
7. Magnetic dipole moment of nuclei
8. Electric quadrupole moment of nuclei

So, the shell model explains the magic numbers. we saw in the previous lecture, that by introduction of the spin orbit coupling between the l and s, we could reproduce the magic numbers. Essentially, because of the strong spin orbit coupling, the l+1/2 state is lowered and the l-1/2 is raised. And the gap between l+1/2 and l-1/2 increases as the l value increases.

Now, the high value of separation energy of protons and neutrons for magic number of magic nuclei, those nuclei which have magic number of nucleons, can be explained by large energy gap above the closed shell. So that is like tightly bound nucleons in the closed shell are tightly bound to remove any individual nucleon on that tightly bound shell requires extra energy and that is why the separation energy is higher. If you have a neutron more than or a proton more than the magic number, then again, it is easy to remove that particular neutron or proton from the nucleus. The absorption cross section for the such nuclei which have magic number of protons and neutrons again is very low, because again, the large energy gap above the closed shell.

The ground state spin now, this is important now, the shell model can explain the ground state spin and parity of the nuclei. In fact, the liquid drop model could not explain the spin and parity of nuclei in their ground state. Also, the liquid drop model could not explain the nuclear isomers and by using shell model, we can explain the existence of isomeric states. The nuclear isomers are nothing but excited states of nuclei, which are having metastability means having higher half-life. So, they do not come down by gamma decay immediately. Normally, you know, gamma decay will take place in picoseconds time, but the isomers will take about maybe it could be milliseconds, seconds or minutes, hours and so on.

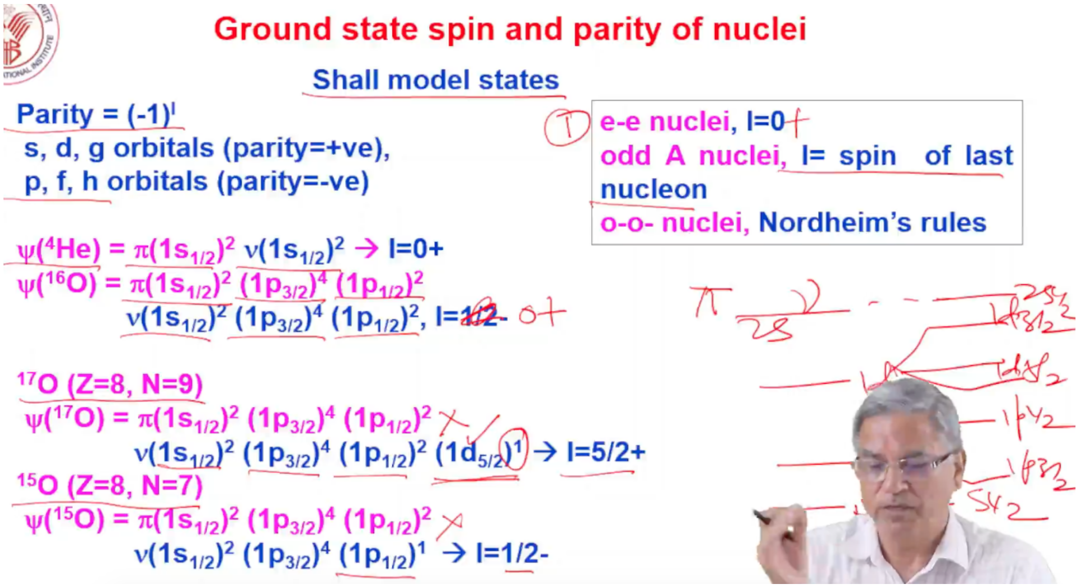
In addition to these properties, there are other properties of nuclei, the magnetic dipole moment of the nuclei and the electric quadrupole moment of nuclei also can be explained using the shell model, but I will not discuss these two points in this particular course.



Now, let us see how we can explain the magic numbers. Just now we discussed this, that the magic numbers arise whenever there is a large gap between, in fact, this is called the shell essentially the concept of shell has come because that we have a shell like after this 8 and 20, there is a large gap. So, this is one shell, let us say shell 1, say second shell, third shell, like this, this is third shell and then you have the fourth shell. So, this is actually a shell, you know, and so there is a gap between two shells. So, the different levels have bunched together and in fact, you can see the nucleons can occupy the states, the energy of these orbitals are very close. And the result of that close energy between the different orbitals, we will discuss subsequently in explaining the properties of nuclei, such as the ground state spin parity. So, the concept of shell has come because after that close configuration, there is a large energy gap. And so, the nucleus will try to attain that configuration. So, if there is a neutron extra over this close shell configuration, it will be easily able to give that nucleon to form the close shell configuration.

And that is what is the concept behind this shell. So, the spin orbit coupling we introduced to explain the magic numbers, the high separation energy of the nuclei having magic number of protons or neutron can be explained by the large energy gap here. So, this is a very compact nucleus. And similarly, the low separation energy for the nuclei with nucleon number 1 above the magic number, again, because of the magic number configuration, above the magic number, there is one nucleon, it can be easily removed. So, energy required to remove a nucleon over the magic number is much less.

Again, suppose you have a nucleus having 82 protons, then it has got a low neutron absorption cross section because it would not like to take a neutron to become a one nucleon more than the magic number. So, this is how properties , particularly with regard to the magic number can be explained.



Ground state spin and parity of nuclei

Shall model states

Parity = $(-1)^l$

s, d, g orbitals (parity=+ve),

p, f, h orbitals (parity=-ve)

e-e nuclei, I=0+

odd A nuclei, I= spin of last nucleon

o-o- nuclei, Nordheim's rules

$\psi(^4He) = \pi(1s_{1/2})^2\ \nu(1s_{1/2})^2 \rightarrow I=0+$

$\psi(^{16}O) = \pi(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2$

$\nu(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2$, I=~~1/2~~- 0+

^{17}O (Z=8, N=9)

$\psi(^{17}O) = \pi(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2$

$\nu(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2\ (1d_{5/2})^1 \rightarrow I=5/2+$

^{15}O (Z=8, N=7)

$\psi(^{15}O) = \pi(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2$

$\nu(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^1 \rightarrow I=1/2-$

Now, let us see how can explain the ground state spin and parity of nuclei, the bulk of this lecture we will spend more on this one. So, we will construct the shell model states for nuclei using the filling of the nucleons in the shell model states. What is parity? it is nothing but (-i) to the power l, that is the l state.

So, s, p, d, f, they have their parity, because essentially parity is the symmetry of a function. For example, if you take X to -X, and this function changes sign, we say it has odd parity. And if by changing X from X to - X, there is no change in the sign of the function, we say it has even parity. Like cosθ is an even function, sinθ is an odd function. Similarly, s orbital, d orbital, g orbital, l values are even. So, this has got, this has got even parity, because the l values are even. So, any even l value 0, 2, 4 has even parity and any odd l value 1, 3, and 5 have negative parity. So, depending upon the l value, the orbital state populated by a nucleon, we can straight away say what will be the parity of that nucleus.

Now, let us see what are the thumb rules for determining the spin and parity of the nuclei.

So, first is the even-even nuclei. It is very simple. Even-even nuclei, all the nucleons are paired up and therefore, the spin will be 0 and parity will be plus. So, the ground state spins of the even-even nuclei are always 0. So, any nucleus which is even-even, you can straight away say that spin will be 0.

When it comes to odd A nuclei, either the neutron will be odd or proton will be odd. So, the ground state spin of the nucleus will be the spin of the j value of the last occupied orbital. So, the nuclear spin (I) will be equal to j of the last occupied orbital and we will see subsequently how to do that.

There are odd-odd nuclei. In the case of odd-odd nuclei, there is an odd proton and there is a odd neutron. And so, the odd proton and odd neutron spins couple together to give you the spin of the nucleus and it is little complicated. So, there are rules which are called Nordheim's rules. By using Nordheim's rule, we will try to predict the ground state spin of odd-odd nuclei.

So, now let us see how to build the shell model states. I will give you some examples like helium-4. Now helium-4 has got two protons and two neutrons. So, when I say π, essentially it is the proton state and when I say ν, it is the neutron state.

The shell model is also called single particle model. Single particle means you take individual nucleon in a potential and generate the level scheme. So, sometimes shell models are also called single particle model. And for single particles, so the states are like proton state as π and neutron states as ν. So, what is the orbital occupied by that proton? You say $\pi(s_{1/2})$ and $\nu(s_{1/2})$.

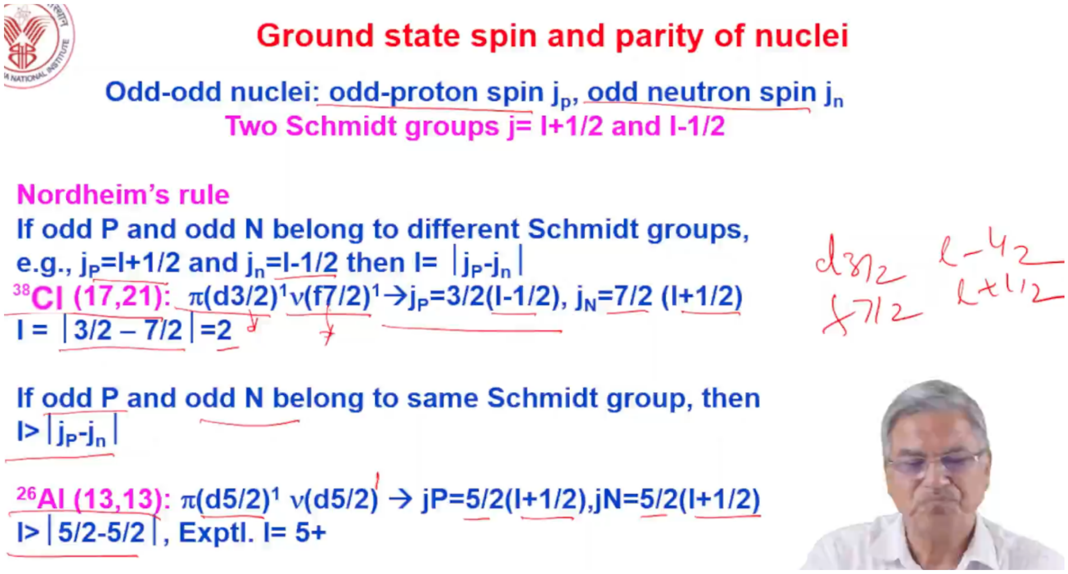
$$\psi\left(He^{4}\right) = \pi(1s_{\frac{1}{2}})^{2}\nu((1s_{\frac{1}{2}})^{2} \rightarrow l = 0$$

So, two neutrons are paired in the ν(1s1/2) and two protons are paired up in this π(1s1/2). So, I=0+, very easy to construct. If you try to recollect the scheme, so I can see here that you have first this s orbital. So, it will be $s_{1/2}$. Then you have 1s 1p, 1p will split into $1p_{3/2}$, $1p_{1/2}$.

Then you have 1d will split into $1d_{5/2}$, $1d_{3/2}$ and you will have 2s, it will be $2s_{1/2}$. And like that, you can build up the scheme. So, for oxygen 16 again has 8 protons and 8 neutrons, so it should be 0+. For even, even nucleus (O-16), π [1s1/2 (2), 1p3/2(4) and 1p1/2 (2)], total 8 protons you occupy. And again, neutrons, ν[1s1/2(2), 1p3/2(4) and 1p1/2 (2), total 8 neutrons. Thus any even-even nucleus, will have the I equal to 0.

Let us come to the odd-A nuclei now. So, oxygen 17, 8 protons and 9 neutrons. So, lets find out which is the orbital occupied by the ninth neutron. The odd neutron that is the ninth one. So, you will have 9 neutrons you populate, 1s1/2(2), 1p3/2 (4), 1p1/2 (2), and you are left with one neutron that will go to 1d5/2. So, the spin, the j value of the last occupied orbital will be the spin of that particular nucleus. So, I=5/2. Since it is a d orbital, it is 5/2+. So, that is how we calculate the spin and parity of the ground state of a nucleus. For example, you have oxygen 15, N equal to 7, 7 neutrons. So, you will see again, proton states, we do not have to bother. the neutron states, you have now 1s1/2(2), 1p 3/2(4), and 1p1/2 (1). So, 1p1/2 is the last occupied orbital by the odd neutron. And accordingly, the spin I=1/2 and parity is p orbital is minus. So, this is how you can derive the spin and parity of the ground state of a nucleus by building up this shell model scheme and finding out what is the j value of the last occupied orbital.

Okay. So, we discussed the even-even nuclei, ground state spin is 0. We discussed the odd-A nuclei. Odd-A nuclei ground state spin is the j value of the last occupied orbital. And depending upon the orbital, the parity can be defined.



Ground state spin and parity of nuclei

Odd-odd nuclei: odd-proton spin j_p, odd neutron spin j_n

Two Schmidt groups j= l+1/2 and l-1/2

Nordheim's rule

If odd P and odd N belong to different Schmidt groups, e.g., j_P=l+1/2 and j_n=l-1/2 then I= $|j_P - j_n|$

^{38}Cl (17,21): $\pi(d3/2)^1 \nu(f7/2)^1 \rightarrow j_P$=3/2(l-1/2), j_N=7/2 (l+1/2)

I = |3/2 – 7/2| =2

d3/2 l-1/2

f7/2 l+1/2

If odd P and odd N belong to same Schmidt group, then I> $|j_P - j_n|$

^{26}Al (13,13): $\pi(d5/2)^1$ ν(d5/2)^1 → jP=5/2(l+1/2),jN=5/2(l+1/2)

I> |5/2-5/2|, Exptl. I= 5+

And now let us see for odd-odd nuclei, how we can calculate the ground state spin. So, for odd-odd nuclei, we have odd proton spin, jp and we have odd neutron spin jn. This jp and jn will couple together to give you the resultant spin of the nucleus. Now, in this case, there are some Nordheim's rules, which apply to what we call as the Schmidt groups. Now, what are the Schmidt groups? Actually, we are not discussing the magnetic dipole moment of the nuclei. But when we plot the magnetic dipole moment of the nuclei, last occupied orbital will be either in l+1/2 or l-1/2 state, what was found that the magnetic dipole moments for these two groups of nuclei, lie on two lines. And these two lines, l+1/2, having magnetic dipole moment in one way and the l-1/2 state magnetic dipole moment the other magnitude. So, there is a gap between the two groups. They have quite different magnetic dipole moment depending on the j value and they are called the Schmidt groups. So, a Schmidt group is actually the classification based on the magnitude of the magnetic dipole moment, that is l +1/2 or l-1/2. So, that same analogy we derived here, Nordheim proposed that if the odd neutron and odd proton, they belong to the different Schmidt groups. So, when we say different Schmidt group means one Schmidt group is l+1/2 lf, other Schmidt group is l-1/2. That is what we mean by Schmidt groups. So, if the odd proton and odd neutron belong to different Schmidt groups, that means one of them is l+1/2, other one is l-1/2 and vice versa. Then, $I = \left| j_p - j_n \right|$

the spin of the nucleus is the magnitude of $j_p - j_n$. Difference between the j_p and j_n, its absolute value will be the spin because the spin does not have negative sign, spin is always positive sign. So, $j_p - j_n$ will decide the spin of the nucleus.

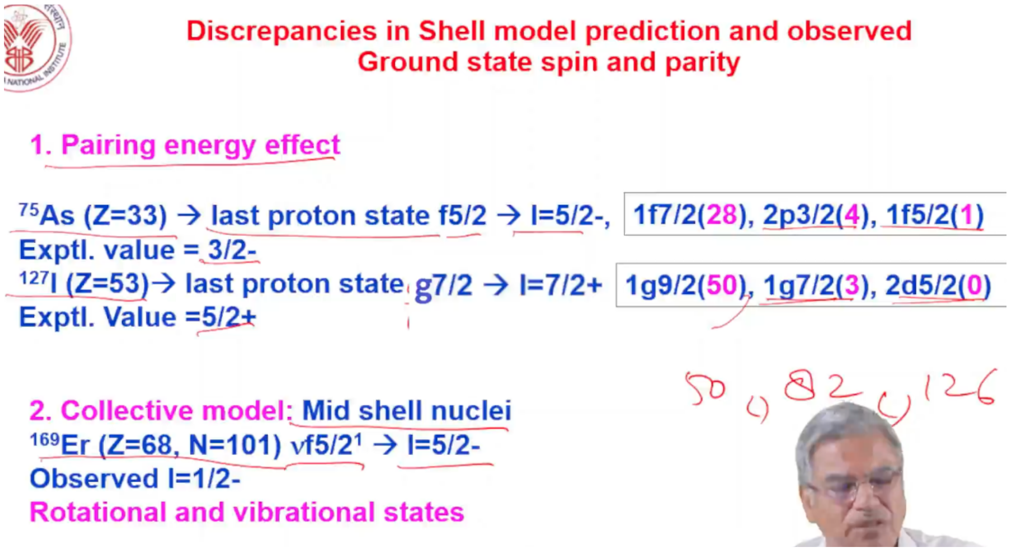
Just to give you an example, chlorine 38, chlorine 38, chlorine atomic number 17 and you have 17 protons and 21 neutrons. How you try to accommodate them? So, let us see how 17 protons you can occupy. You will see that the last proton will go to d3/2 state. Now, the 21st neutron will go to f 7/2 state. So, you can see here that d3/2 is l-1/2 and f 7/2 is l+1/2 because d 3/2 is l-1/2 and f 7/2 is l+1/2. So, they belong to the proton and neutron orbitals having different Schmidt groups. And so, j_p will be, 3/2, which is l-1/2, j_n is 7/2 is l+1/2. So, the nuclear spin of chlorine 38 will be difference between j_p and j_n and that is 3/2 -7/2 or 7/2 -3/2 which is the mod of that. So, that is equal to 2. And chlorine 38 ground state spin is indeed 2. So the Nordheim's rule very well explains the spin of the nucleus having an odd-odd configuration.

The second aspect is that if the odd proton and odd neutron belong to the same Schmidt group. In fact, it is not that easy to predict the spin of this nuclei having odd proton, odd neutron in the same Schmidt group. But then we say that for such nuclei, the nuclear spin is more than $j_p - j_n$. So, it is not easy to just predict the exact spin value but it will be more than $j_p - j_n$. So, this is a very simple classification where then you have to see what value it is.

For example, the aluminum 26, aluminum 26 having 13 proton and 13 neutrons. So, the 13th proton will occupy d5/2 and the 13th neutron will also occupy d5/2, same value of proton and neutron numbers. So, j_p is 5/2, which is l+1/2, d5/2 is l+1/2, jn is also 5/2, l+1/2 state.

So, here is the case where both proton and neutron occupy the same Schmidt group, that is l+1/2. For such a nucleus, I is more than $j_p - j_n$, that is, it will be more than, 5/2 -5/2, that is, 0, it is more than 0. But experimentally, the value has been found to be 5. So, you can see here it has a range, it could be from 0 to 5, 5/2 +5 /2 is 5. So, it could be anywhere. And so, that is the kind of guess it gives that it is in that range. But you cannot exactly pinpoint what will be the value of the spin for such nuclei, when the odd proton and odd neutron belong to the same Schmidt group. Okay. So, now, in fact, the shell model, it is not completely successful in predicting the ground state.

Already we have seen in the odd-odd nuclei. So, there are a lot of cases where shell model cannot predict the spin exactly, it will give a range, okay, it will be more than this or it will be equal to this, depending upon in which Schmidt group they occupy. But for even-even nuclei it is very simple, it is 0. Odd A nuclei, by and large, the shell model can explain the ground state spin and parity.



Discrepancies in Shell model prediction and observed Ground state spin and parity

1. Pairing energy effect

^{75}As (Z=33) → last proton state f5/2 → I=5/2-, 1f7/2(28), 2p3/2(4), 1f5/2(1)
Exptl. value = 3/2-
^{127}I (Z=53)→ last proton state g7/2 → I=7/2+ 1g9/2(50), 1g7/2(3), 2d5/2(0)
Exptl. Value =5/2+

50 , 82 , 126

2. Collective model: Mid shell nuclei
^{169}Er (Z=68, N=101) $\nu f5/2^1$ → I=5/2-
Observed I=1/2-
Rotational and vibrational states

But there are some discrepancies. And the discrepancies we will discuss here. So, discrepancies in the shell model prediction and the observed ground state spin and parity. There are two important phenomena which in fact, will lead to these discrepancies. First is the paining energy. Now, what happens, you know, in odd-A nuclei, so there are cases in a particular shell, where there are different orbitals, which are close by in energy, the energy gap is very small. So, the thumb rule is that if a odd proton is there, and it happens to be occupying a high spin state, let us say G9/2, H11/2, then, and if there is a nearby low spin state, which is filled up, then what happens, there is a transition. That the paired nucleon will like to remain in the high spin state, because there will be a gain in the pairing energy. So, the pairing energy depends upon the l value. So, as we discussed, the higher the l value, the gap between the two states, l+1/2, l-1/2 is higher. So, if there is a one odd proton or odd neutron, it will jump to a low spin state. And so, the pair will go to the high spin state. And that would lead to discrepancies in the shell model prediction. So, whatever you predict based on the shell model, the spins are different from the prediction.

That I have to explain using this slide. So, arsenic 75 atomic number is 33. So, we have the 42 neutrons all paired up. So, this 33rd proton, what is the spin state of the proton, you can see here last proton state f 5/2. f 5/2 is the occupied state. And according to this one, it should be 5/2-. But actually, the observed value is 3/2. So, here I try to explain the f 7/2 will be 28 protons, then we have after that 2p3/2. So, according to shell model, the proton should occupy f 5/2 and hence its spin should be 5/2-. But you see here, just before that there is a p3/2 level. And that p3/2 level is, so instead of the 33rd proton occupying f 5/2, the pair goes to f 5/2 and the odd proton occupies the p3/2. So, this is what happens that the paired configuration is having lower energy if it is in a high spin state. And so, the f 5/2 gets stabilized by a paired nucleon configuration and the odd nucleon goes into p 3/2.

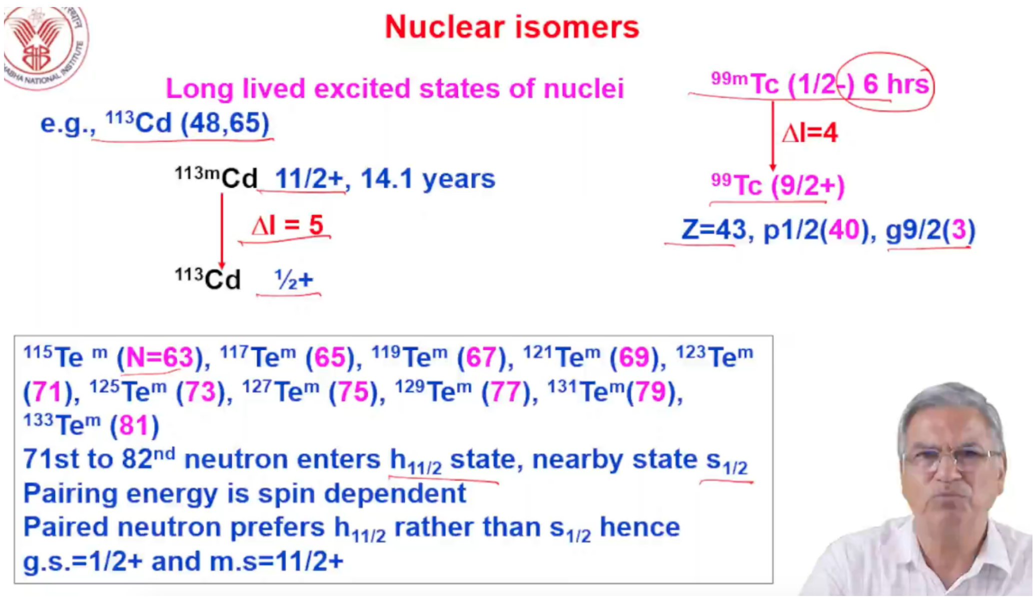
Similarly, iodine 127, Z equal to 53. So, 53rd proton, you can see the last proton state is g7/2. So, it should be 7/2+. And so, you can see here the shell model states the 50 neutron, 50 proton configuration, 50 numbers here and then we have the g7/2 and the d 5/2. So, the 53rd proton could have occupied 1g7/2 and spin state would have been 7/2+. But experimental value of this nucleus is 5/2 +. And again, you can see here that the next state, so this is d 5/2 which is vacant. So, the odd proton in the g 7/2 is not preferred over that in the d 5/2. So, that is the explanation that the odd proton will prefer to remain in a lower j value compared to that in the higher j. Paired configuration will remain in the higher j value. So, this is one of the explanations for discrepancies in the shell model predictions over the experimentally observed values.

So, many cases you will find that this kind of changes will take place. And then another explanation, another, there are some cases where, you know, even this pairing energy effect cannot explain the ground state spin and parity, particularly in the case of mid shell nuclei. So, this mid shell nuclei, what I mean by mid shell nuclei, so when we have 50, 82, 126, these are shell somewhere here. So, if around 100, if the proton number is 100 or neutron number is 100, then for those nuclei, the nucleus is deformed in their ground state. And for such nuclei again, you will find, you can just to give an example to illustrate this point, Erbium-169 has got N equal to 101. And so the 101st neutron, if you see the shell model state, it should occupy the f5/2 state and accordingly its spin should be 5/2-. But actually the observed spin is ½-. And there is no ½- state, there is no s orbital, p orbital, actually you can see it should be corresponding to p1/2. But there is no p orbital p1/2 in the vicinity of this f5/2. And therefore, it was becoming difficult to explain how you can get this kind of ground state spins. So, one of the explanations is the collective motion. Collective model means in the nucleus, other than the shell model, there is one more model called collective model, which I am not able to discuss because of the paucity of time.

The collective model considers that all the nucleons inside the nucleus undergo a collective motion, like the molecules have vibrations and rotations. The nucleus also has its vibrational states and the rotational states. They are called the collective states of the nuclei. And so apart from liquid drop and shell model, there is one more model called collective model. And the collective model has been validated by observation of the spectra, the rotational spectra.

Rotational spectra, the low lying states of even-even nuclei have spins as 0, 2+, 4+. And the energy gaps from the moment of inertia, rotational energy of the nucleus, you can predict B J(J+1), where B is h cross square by 2I, where I is the moment of inertia. And so people have even found out the moment of inertia. There is a fixed ratio of the energy states for the nearby low lying states of a collective nucleus. For the collective motion, people have seen that if the nuclei follow that kind of relationship, you can associate this with the rotational states of the nuclei.

And so there is a mixing of collective states and the single particle states or shell model states. And that is one of the explanations for this observed spin values being quite different from shell model predictions. So this is another area where the discrepancies can be explained.



Nuclear isomers

Long lived excited states of nuclei

e.g., ^{113}Cd (48,65)

^{113m}Cd 11/2+, 14.1 years

ΔI = 5

^{113}Cd ½+

^{99m}Tc (1/2-) 6 hrs

ΔI=4

^{99}Tc (9/2+)

Z=43, p1/2(40), g9/2(3)

^{115}Te^{m} (N=63), ^{117}Te^{m} (65), ^{119}Te^{m} (67), ^{121}Te^{m} (69), ^{123}Te^{m} (71), ^{125}Te^{m} (73), ^{127}Te^{m} (75), ^{129}Te^{m} (77), ^{131}Te^{m}(79), ^{133}Te^{m} (81)

71st to 82nd neutron enters $h_{11/2}$ state, nearby state $s_{1/2}$

Pairing energy is spin dependent

Paired neutron prefers $h_{11/2}$ rather than $s_{1/2}$ hence g.s.=1/2+ and m.s=11/2+

And lastly, I will discuss the nuclear isomers. The nuclear isomers are the long-lived excited states of nuclei. And it happens whenever there is a large difference between the excited state and the ground state of the nucleus. So the gamma decay is not easy to happen. And so the gamma decay is hindered. So when the gamma decay is hindered, the nucleus, the excited state has got a long lifetime. So you can see here, cadmium-113, 48 protons and 65 neutrons, the excited state of this nucleus is 11/2+ and ground state is ½+.

So the shell model can predict the ground state of nuclei and excited states. So there is a large spin change ΔI, in the gamma decay. And therefore, this isomeric state has a half-life of 14.1 years. Similarly, the technetium-99m, excited state ½-, ground state 9/2+, because of the large change in the spin during the gamma decay, this decay is hindered and therefore isomeric state has got a half-life of 6 hours. So again, you can see here, the state, Z is equal to 43 for technetium, the 9/2 in the ground state, so it is the 43rd proton will go to 9/2 state. And then there is a excited state. So if you populate the excited state ½- its decay to ground state is hindered. And so we can see, this ^{99m}Tc is the workhorse of nuclear medicine used in single photon emission computer tomography.

And it so happens, the isomeric states are found just below the magic number. So you can see here, the magic number is 82 and right from 70 to 82, or even right from 63, so these are the other tellurium isotopes having these odd number of neutrons have got isomeric states. So the 71st to 82nd neutron enter h11/2 state and nearby s1/2 is there. So again, the nucleon decides where to occupy, the pair will go to h11/2 and the odd nucleon will go to s1/2. So whenever there is a magic shell configuration just below that, there is a large difference in the spin states of the levels and the excited state and ground state have this difference and therefore the gamma decay is hindered. So this is what explains the nuclear isomers. There are several nuclei having isomeric states, many of them are having half lives in seconds to hours to even years. So shell model can therefore explain the properties of nuclei which are based on the, wherever there is a fluctuation in the property of the nucleus in terms of the mass or in the ground state spin and parities, binding energies and so on. This can be explained by shell model very well. Thank you very much.