Nuclear Physics Fundamentals and Applications Prof. H. C. Verma Department of Physics Indian Institute of Technology, Kanpur

Lecture - 17 Shell Model

In atoms you know you have shells, major shells, then sub shells and all that chemistry is based on that you have inert gases or noble gases. So, there the shells are major shells are closed and then when one more electron you put, a new shell starts in periodic table and new period is starts right. So, you have that hydrogen then you have lithium below that right, below that you have sodium, potassium. So, these are the elements at which a new shell starts and there are many things common, they are all called alkali metals.

So, there are many of the properties are common, because they all have close shell and one more electron a new shell has just started. So, there are many of the properties, which are common in this, similarly if you go for a 2 electrons beyond a close shells you get that a period to a magnesium, beryllium though. So, there also the properties many of the properties are common all kinds of chemical bonds and theses things valence these things are common.

So, the properties are largely decided by those extra valence electrons. Once the shell is closed then those extra valence electrons they decide the properties. Those inner electrons are not that much participating in all kinds of interactions. Then these reactivity also you know that if you have those helium and argon and neon close shell elements. There the chemical reactivity is very small they are that is why they are called inert and once you have theses alkali metals or alkaline earth metals the reactivity is very high.

So, all these things depend on the shell structure the energies are, so arranged that when you start filling up then somewhere you have major gap in the energy. And you say that here the shell closes and here a new shell starts. Now, this reflects in many things, yes last lecture we talked about ionization energy, if you want to pull 1 electron out, so when you have this close shell then pulling 1 electron out is difficult. They are extra stable, but if you have just a new shell has just started the, it is easy, so you can pull it very easily.

So, ionization energy will go down there and then gradually it will increase and when the shell closes the energy is highest. Similarly, many properties radius, atomic radius many properties you see that the shell reflects the shell shows up. The similar thing also happens in a nucleus, in a nucleus also the number of neutrons and number of protons. How many neutrons are there and how many protons are there.

So, the a similar shell structure it is seen, if you look at the properties then there are certain numbers says when this proton number or neutron number just crosses that. You look for 1 nucleus then next nucleus and then next nucleus by putting 1 more proton or 1 more neutron and so on. The front nuclei when you compare although the life is slightly more complicated because here they are 2 kinds, protons and neutrons. There you had only 1 kind it was only electron.

So, you talk in terms of 20 electrons or 21 electrons, but here there are 2 of them protons and neutrons, but still you have certain numbers. If z is equal to that number or n is equal to that number, then it is extra stable it is radius suddenly show the discontinuity. It is protons separation energy which is something like that ionization energy, there you remove 1 electron and ask how much energy is needed. Here, you remove 1 proton and ask how much energy is needed. So, proton separation energy neutron separation energy all the many things are there which show some structures.

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I will just show some of them to you from a book, which is this is by Richard A Dunlap by this Thomson Brooks Kole. I will just draw there things for you some of the things, now this is figure 5.3 at page 16 page 46. This talks of binding energy which binding energy per nucleon, you remember this curve binding energy per nucleon as a function of A.

So, measured value and minus binding energy per nucleon as calculated from that semi empirical mass formula right. One can calculate that and 1 can measure that, so this some difference in that and that difference is plotted this quantity is plotted on the y axis side. And x axis side it is A, I will just draw the diagram may be some time I will show you on the screen and it is something of this sort. So, there are periodic humps and these humps where they occur the numbers are n is 28, z is 28 for this hump.

Then n is equal to 50 this hump, n is equal to 82, z is equal to 50, then here it is n is equal to 126, z is equal to 82. Remember, the semi empirical mass formula we derived was semi empirical, we did talk of some asymmetry energy. And said that it is coming because of those energy levels and fermions and therefore, if you have more neutrons than protons, neutrons are forced to go into the higher energy levels and so on.. So, that shell structure is actually included there little bit, but only little bit largely it was based on like we drop model.

So, you do expect that if shell effects are large you will have deviation from this semi empirical mass formula. And you can see here that at certain numbers this 28 or 50 or 82 1 as certain numbers when z acquires that number or n acquires that number the deviations are large. So, near shell closer the shell effects are largest as a closed shell and a new nucleon comes and a new shell starts. So, there is there where you will see that shell effect most permanently correct.

So, at those places where neutron number or proton number is like this 50, 82, 126 you see that your prediction of semi empirical mass formula and the measured binding energy per nucleon they differ. So, that is 1 then another thing is this is change in the measured nuclei radius this is phi of 5.5. Change in a measured nuclear radius for a change in neutron number delta n equal to normalized to change predicted by that radius equation delta r measured by delta r calculated.

What is delta r? Delta r is that this n is increased to n plus 2 and how much is the radius change all right n is increased by because there is some even odd effect also. So, to remove that it is changed in steps of 2, if it is even all even and so on, so the 1 which you calculate using they R naught A power 1 by 3 and 1 which you measure right. So, that ratio again shows similar kind of fluctuations from sketching it. So, these type of ups and downs are observed and once again the numbers which are here are n is equal to 20, 28, 50, 82 and so on right. Then you have number of stable isotones as a function of n, this I believe I have on slide look at your screens.

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This is number of stable isotones as a function of neutron number n. So, on the horizontal axis you have neutron number, on this axis you have neutron number. So, here you have neutron number n, n is plotted here. This is n equal to 10 this is 20, 30, 40, 50, 60, 70, 90, 100 here, and this side number of stable isotones. You know what is number of stable? What is isotone? Isotope you know, what is isotope?

Student: Number of equal number of.

Same number of protons you can put more neutrons. So, all those nuclei are called isotope of a particular element right, similarly if you fix neutron number n and then ask you put more z. So, you can ask what are those nuclei with this particular capital N they are called isotones, if n is fixed you have several nuclei in which neutron number is

same. Then these nuclei are called isotones, if you have several nuclei in which proton number it is same then these nuclei are called

Student: isotopes

Isotopes.

And if you have several nuclei in which capital A is fixed, z is also varying n is also different, but z plus n is same. So, those nuclei are called

Students: isobars.

Isobars right. So, for a particular n you can ask how many isotones are there stable isotones are there. So, how many different nuclei which different proton numbers can exist to that capital N that is number of isotones.

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Now, look at the screen again. So, on this vertical axis side you have number of stable isotones right, here it is say this is 20 and the corresponding point is here, this is 5. So, with n equal to 20, you have 5 stable isotones with neutron number 20 by putting different number of protons you have 5 stable nuclei.

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But, if you look at the 19 or 18 or 17 this number is 3, 10 this number is 2 or this side 21 this number is 3 and so on. And here 28, 28 again it becomes 5 this is 28 this is 20. Then it is here, here, here, here, here, here and all of sudden here. this is 50, this n is equal to 50. So, with n is equal to 50 you have 6 stable isotones, then these are numbers fluctuations and n is equal to 82.

Again you have 7 stable isotones with n equal to 82. So, these numbers that you are seeing here 50 82 28 20 these show that n is equal to 1 of these. You have even if you put 1 more proton or you remove 1 proton still it remains a stable. So, this n equal to 50 or n equal to 82 or 28 or 20, it is providing extra stability. Even if there are some more protons are number of protons is somewhat less, it does not be dedicate.

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So, this is about this stability, now from the same book you have figure 5.7 which talks of absorption cross section for 1 m v neutrons. So, if you have a nucleus and you send a neutron with certain energy here, it is 1 mega electron energy. What is the probability that this neutron will be absorbed in the nucleus n will become n plus 1. So, if you have closed shell right extra stable shell, then getting a 1 neutron absorb there will be difficult.

Neutrons are being bombarded on the nuclei and the probability of their getting absorbed. And nucleus becoming 1 more neutron in the nucleus that situation is looked for probability. For that absorption cross section for that, that is plotted on this side. This is absorption cross section in on the vertical side and horizontal side, it is n. And can you see the drops? You have numbers here, in some unit is numbers here, this increasing neutrons can get absorbed, but all of sudden here you can see a fall.

The absorption cross section as you have as you are increasing the n, the absorption cross section on the average increases, but here there is sudden fall. And that is at n equal to 50, this point is n is equal to 50. Then again once you cross that 1 then again you have larger cross sections larger cross section, but all of sudden it falls here. And this number here 82, these are all experimental results and these results are taken from physical review volumes are 78 19 50, can you see this page number 632.

So, these are all experimental results, measured results here are the cross sections, absorption cross sections and all of it sudden it drops here and this number is 126. To

many of these properties each 1 showing discontinuity at the same values 50 82 126. For all these experiments suggest that there are some kind of shell structure and there are some kind of shell closer.

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>(1, 0, 4) -_

And those numbers where were shell close from the experiment, those numbers are 2 8 20 28 50 82 126. Now beyond that we do not have stable nuclei, but then things are being studied in laboratory where, nuclei with much higher nucleon number A mass number A are created. For some time of course, they are not stable at such and then studied. So, you have magic numbers beyond this also you will talk about later, but with the commonly available nuclei these are the number, these are called magic numbers.

Essentially, these are the numbers where the measure shell closes and there is in energy gap. If you wants to put 1 more electron, 1 more neutron or 1 more proton if the number is this then there is a bigger energy gap, so there is a kind of shell closer there. This is a suggestions from experiments, this is results coming from experiment various different kinds of properties, not just 1 different kinds of property.

All showing discontinuity are these same numbers, so these same numbers are built in the structure or the theory. So, how do we understand why n equal to 50 nucleus is extra stable or z is equal to 50 nucleus is extra stable. So, how that results from where these numbers come. So, just like in atomic physics here also the scheme is the same you

assume what we call a single particle potential or 1 particle potential. In the nucleus you have, so many protons and so many neutrons.

And if you pick up 1 and ask what is the field that this proton is seeing because of the rest of the nucleus. So, that we approximate by in the first attempt by a central potential some kind of central potential. So, if a particular proton is experiencing that central potential, because of all other then each of the other protons and each of the other neutrons, they also experience the same potential. So, that is single particle or mean potential theorem, mean potential theory that you assume that this whole nucleus is giving and average kind of potential to each of it is constituents.

That is how in atomic physics also it is done, where multi electron system, but then you say that the whole atom is giving particular potential to each of the electrons right. And then with that potential you solve for a possible energy levels and these energy levels are open to all those electrons. But, then electrons are fermions and in 1 state not more than 2 can go in 1 state, in fact, not more than 1 can go and so on. So, there is a huge bough principle of filling it up and all that.

So, similar structure we barrow in nuclear physics also, we assume that for each of the constituents protons and neutrons. This nucleolus is providing some kind of potential and we will solve the energy levels for that particular potential. So, you will get some energy levels, then you will say that protons and neutrons will fill these levels from below and taking a count of that they are fermions. So, this is how the things will go and if you find that there are gaps in the energy levels are grow up then the shell structure will come out.

So, with that expectation the first the question the major question is what kind of potential that average potential 1 starts with, 2 nucleon potential is even you know how complicated it was. So, at the whole idea of this single particle potential is forget that come out with something simple. One of the very simple potentials is infinity square well potential that give me that try. So, infinity square well potential of some width r naught. So, it is V r is equal to 0 for r less than r naught and is equal to infinity for r greater than r naught, this will called infinity square well potential. And if you it is a central potential why is it a central potential, because it does not depend on theta and phi.

Any potential that depends only on r naught on theta phi is a central potential, so that means, there is no direction dependence. If r is less than r naught that is a spherical

volume, in any direction you go in this volume you have the same potential. It does not depend on theta phi, so that is why it is a central potential? And if it is a central potential, then you can write the wave function or the Eigen functions of energy r theta phi. The potential does not depend on theta phi, but the wave function does depend on theta phi.

So, this is a that radial part you write u r by r, and then it will be Y l m theta phi where, Y l m theta phi are spherical harmonics good. So, this theta phi function, we already know what are those functions sin theta, cos theta, e to the power I phi and all those things. And this u r by r as we have done earlier, this satisfies the equation minus h cross square by 2 m, then d 2 u d r square and plus v, so for I am writing r less than r naught, so v 0.

So, it is or let me first write it and then we will put 0 V r plus 1 l plus 1 h cross square by 2 m r square u r and is equal to e times u r these are the energies. So, this equation to be solved to get u and once you get u you put it here and we get the energy Eigen functions. And you have those boundary conditions, the wave function should be continues everywhere and slope should be same and all those things are there. Now, when you apply a it is to the infinity square well potential it is this V r is 0.

So, for r less than r naught just put V r is equal to 0 and you get this equation u this is to be solved with the condition that r equal to r naught. This u should become 0 because the outside the potential is infinity, u is 0 and the value is must be continues. So, this the solution of this turns out to be some Bessel functions, these are the solutions r times j l k r.

So, at r equal to 0 it is any way 0, it should be and r equal to r naught, this should be 0. So, when you apply that condition, it is j l k what is k by the way all of sudden I brought k here. This k is related to this E and this k is square root of 2 m E over h crosses square. This 2 m by h crosses square you take to other side, so it will become 2 m E by h crosses square that is written as k square. So, once you know k you know energy E and which mass is this mass of

Student: proton.

Proton. Yes it is mass of proton we are writing single particle potential, so each proton and each neutron is expected to experience this potential. So, this are single particle energy levels, if you have 1 proton in 1 particular level, you say that this proton has this much of energy. So, these energies that we are writing here they are single particle energies and therefore, this m that appears that is also for that single particle which can proton which can be neutron, so that m is there.

Now, this is Bessel function, so the with the you can 1 can write the expression for Bessel function or solve this is equal to 0. So, what is the value of k r naught, r naught is already fixed from the potential that you have chosen 2 femto meter or whatever you choose and correspondingly you can get those k. Now, it depends on 1 because the Bessel function that is written here has different functional form for different 1. If 1 is equal to 0, it is simple sin function.

If it is 1 is equal to 1, it will be more complicated 1 equal to 2 more. So, you start with 1 particular 1, say 1 is equal to 0 and then you have a wave function and then ask, when this function becomes 0. So, what are those values? And take those values and from there you find different values of k and therefore, different values of E. So, there will be a list of values, then you take 1 equal to 1 and which 1 equal to 1 it is a different function now.

And that function equal to 0 will give another set of values of this k r naught. And from there you get another set of values of this k and therefore, another set of values of this E. So, all those energies, so you have to list all those energies which comes after what, so that you get that energy level diagram. Now, the order relative order I will show you.



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So, l is equal to 0 which l is equal to 0, you get the smallest value of this k r naught, then next larger, then next larger, then like next larger. Those are termed as n equal to equal 1, n equal to 2, n equal to 3, n equal to 4, n equal to 5 and so on. So, which l is equal to 0 you will have n is equal to 1, n is equal 2, n is equal to 3 and so on. This will be 1 set then you will start with l is equal to 1 will be at different functional form and when you solve that equal to 0. You again get values certain values of k r naught and the first value will be called n equal to 1, next value will be called n equal to 2 and so on.

So, with 1 is equal to 1 you will have n equal to 1, n equal 2, n equal to 3 and so on. Similarly, for 1 equal to 2 and so on. So, this n and 1 does not bear the same relation as in atomic physics the 1 is orbital angular momentum that is fine 1, 1, 1, 1 plus 1 h crosses square by, but the n and 1 relation of that. Here, 1 equal to 0 you have a full series, 1 equal to 1 you have a full series, 1 equal to 2 you have a full series and so on fine independently. So, I will show the order of energies each of this corresponds to 1 particular energy.

And the symbols are same I equal to 0 are called s states, I equal to 1 are called p states, then I equal to 2 are called d states, then f, then g, then h, then I and so on. So, these symbols we will be using, so in what sequence these energies appear n n l. So, I will shown on the on the screen.

	3s	
1h	2d	
1g		Infinite square well
	2p	Potential
1f		
1d	2s	
1p		
1s		

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This is infinity square well potential and the first lowest energy comes 1 s when 1 is equal to 0, and n equal to 1 the lowest 1. Next, energy appear somewhere here 1 p, so this is n is equal to 1 and 1 is equal to 1. In atomic physics you do not have 1 p state, atomic physics you have 1 s and 2 s 2 p. Here, we you will have 1 p 1 d everything, next higher energy comes here 1 d, then comes 2 s. And after that it is 1 f, 2 p, 1 g, 2 d, 1 s, 3 s, there will be more we do not have to work with 1000 nuclei, so we do not have to go much beyond this.

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So, this is the sequence, now let me draw this sequence on the board also, let me draw this on the board and help me what is the lowest 1 s. Next is 1 p, then 1 d, and 2 s, is close to it right 1 d, and then here 2 s, and 1 f, 2 p and 1 g is closed 2 d, 1 h and 3 s all quite close right. Now, let us look at the ((refer time: 35:06)) and see if it is fermion, then 1 quantum state will accommodate 1, but we have not taken spin of that particle into account.

This is the only l part orbital part, so with this 1 s, I will have 2 protons or 2 neutrons can go there 1 with spin up 1 with spin down. The quantum state will be defined by this is special part plus this spin part. So, there are in fact 2 quantum states at this level 1 with spin up 1 with spin down each other. So, the it can accommodate 2 p 6 d s f p g 18 d h 22 18 then 22 s 2. So, this is 1 gap, so your shell is here and after the gap another big gap here.

So, next will be next shell closer will be here, so it total of 8 particles and the shell will close here. So, 8 then 10 into there close enough, so this is 1 group, so 8 and plus 12 20 and then there is a gap. So, the next shell closer will be 20 nice magic numbers are coming, then this is what 14 and then there is a gap, of course, so this comes at 34. That is not a magic number suggested by the experiments. There is no such discontinuities at this, then you will have what do I do 40 and then no this you this is 1 group.

They are close enough, so 10 then how much is this total 34 and add to it 92. So, worked up to here and yeah these are right numbers, we were expecting and beyond this everything goes that. So, may be that infinity square well potential I had taken is not the right potential to take change to something else and perhaps things will improve. So, second potential that I know, how to solve is linear harmonic not linear 3 dimensional harmonic potential. A 3 dimensional harmonic potential I do not have to do much energy levels are very nicely given by a simple formula.

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So, if you have single particle potential as V r is equal to half m omega square r square, this is the potential and similar rite Schrödinger equation and in terms of u and this also central potential. So, Y 1 m theta phi will be there and solve for u with this V. Let me write, so phi r is u r by r same thing. In fact, repeat repeated y 1 m theta phi, this portion will not change.

This theta phi part will not change, as long as it is central potential that theta phi part will be same. And this u will be now minus h cross square by 2 m d 2 d r square plus V r, V r is this, V r is half m omega square r square plus 1 l plus 1 h crosses square by 2 m r square u is equal to E u. So, this is to be solved and from here using the boundary conditions those should not become infinity another things and get the values of E. And this E turns out to be 2 n plus 1 plus 3 by 2 times h cross omega, energy depends on n n l and this is how it depends.

And you can put n going from 0 onwards and 1 is again 0 1 2 3 4 So, although this n is 0 1 2 3 4, but the label that we will put will be 1 more than this. So, n equal to 0 we will write that as 1 say n equal to 0, 1 equal to 0 we will write at 1 s, so the label will be 1 more this an if you wish you can call it n prime. And then n will be n prime plus 1 or you can call it 2 n plus 1 minus 1 by 2, then it will match over.

So, let us look at the energies, so you can write this as capital N plus 3 by 2 h cross omega and this capital N can take values starting from 0 when n 1 l both are 0. This will be 0, so 0 1 2 3 and so on. Let me do it here, so what is the lowest energy? how many h cross omega, 3 by 2 h cross omega when this capital N is 0 then the energies 3 by 2 h cross omega, it has the minimum energy. So, you have a line here, put a line here this is a lowest energy and this capital N is equal to 0.

This is 0 that will happen only when N is equal to 0 and 1 is equal to 0. And so capital N is equal to 0 these are lowest energy, this will happen when N is equal to 0 and 1 is equal to 0 and we will write it as 1 s. So, you have 1 s here, next energy, next higher energy phi by 2 h cross omega. When this capital N is equal to 1, what are the values of small n and 1 to make capital N equal to 1. So, this is 1, so n is equal to

Student: 1

l is equal to...

Student: 1

1.

So, n is equal to 0 and 1 is equal to 1, what is this is state called 1 p. So, we will put 1 p here, that gap is h cross omega. Next, 1 will be N is equal to 2, this capital N should be 2 what are values of small n and what are values corresponding value of small 1.

Student: ((Refer Time: 43:36))

1 is equal to 0.

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Students: ((Refer Time: 43:43))
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1 is equal to 0, n equal to 1 anything else, capital N is 2 n plus l, I need capital N equal to2. 1 solution you gave put what n equal to 1 and l is equal to 0 any other combination.

Student: ((refer time: 44:03))

That 2 possibilities, 1 is you put 1 here and 0 here or you put 0 here and 2 here then also you will get this. So, 1 possibility is you put 1 here and 0 here, so n is equal to 1 and 1 is equal to 0, and together with this you can also have n equal to 0, 1 is equal to 2. Both of these combinations will give you capital N equal to 2. So, this energy can be obtained this will be 2 s, this 2 s n equal to 1 and 1 equal to 0, it is 2 s and what is this 1 d 2 s and 1 d energies will concede. So, next energy which is h cross omega above this you have 2 s and 1 d, so 1 d and 2 s.

All this will have the same energy, next capital 1 is equal to 3. How can you get this capital N equal to 3 n equal to 1 l equal to 1 anything else.

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Student: ((Refer Time: 45:35))
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n is equal to 0 l is equal to 3 that is all for capital N equal to 3 you cant do anything else. So, this is l equal to 3 n equal to 0 l equal to 3 what it will be called...

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Students: ((Refer Time: 45:56))
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1 d is already there...

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Students: 1 f.
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1 f l equal to 0 is s l equal to 1 is p l equal to 2 is d and l equal to 3 is f. So, this is 1 f same difference this is 1 f and the other 1 is what is this 2 p this is 2 and this is p. So, at

the same level at the same energy you have 1 f and 2 p. Next n equal to 4 small n equal to here it is I need capital N equal to 4

Students: ((Refer Time: 46:44))

n equal to 1 l is equal to 2 next 2 anything else.

Student: ((Refer Time: 46:56))

n equal to 0 and 1 equal to 4. So, this was 1 f and now it is 1 g n equal to 0 n equal to 3 was 1 f, n equal to 0, 1 equal to 4 1 g, and so this is then this 1 2 d. So, 2 d and this one 3 s and similarly you can construct others. Let us look at the occupancies at this energy level how many protons can we put

Students: 2.

2 protons can be put 2 neutron can also be put, here.

Students: 6.

6 here.

Students: 12

Very good 10 here and 2 here, so 12 so you can put 12 here

Students: ((Refer Time: 48:20))

f is...

Students: 14

14 and p is.

Students: 20

20 right 20. Now here, so 4 up g let us do it that way g is 18. Let me write s p d f h 2 6 10 14 18 22. So, 1 g is 18 then 2 d is 18 plus 10 28 and plus s 30. So, here it is 30. Now, without going trough this can you see this sequence and tell me what it what it will be here, pattern reorganization see 1 s 1 p 1 d 1 f 1 g 1 h should be here right. Then 2 s 2 p 2

d 2 f should be here, 3 s is already here, so 3 p do I have 4 s here. See 1 s is here then 2 s starts here 1 jump 3 s starts here, so 4 s will go here no 4 s just pattern reorganization. And how much will be the occupancy h 22 plus f 14 36 and plus p 42, so this will be 42 this level will accommodate 42.

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Now, accumulative from the bottom 2 shell closes with a gap, then 2 plus 6 8 shell closes this is a gap 8 plus 12 20 and then 40 out. Does not help weather this is infinity square well potential or it is harmonic potential it is all the same first 3 are reproduced and the rest or not. So, now, both these potentials have some problems, both are infinite I infinite means if a part p is bound you just can not take it out by giving any amount of energy. Infinity square potential is infinite and this harmonic potential also goes to infinity so it is un realistic.

In a nucleus we know that if I give certain energy the proton can be taken out, that is proton separation energy or if in give a certain amount of energy a neutron can be taken out that is neutron separation energy. But, the potentials that we have chosen are infinite potentials that is you can never take a nucleon out of that, so this is indeed an unrealistic potential both of them are unrealistic potential. So, next level would be that 1 should try more realistic potential of finite potential. So, that at least I should be able to take that nucleon out.

So, for finite potentials also we have certain choices finite square well potential could be 1 that 1 can see. Then finite square well potential with exponential edges because you know the nucleus is not something where you have sharp edges it is diffused. The charge distribution you solve boot section potential, boot section distribution it is all diffused.

And any realistic system does not suddenly jump up to here it is this and then suddenly it becomes 0. So, if the above edges are rounded, so a square well potential type, but the edges are rounded that is another possibility. So, many other things can be tried with finite potentials and may be next lecture I will show the results for such calculations. In fact, in those day it was very, very fascinating.