Quantum Chemistry of Atoms and Molecules
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Lecture – 33
Multi Electron Atoms

We are learning about many electron atoms. Today, we are going to learn how to write their wavefunctions using a particular form.

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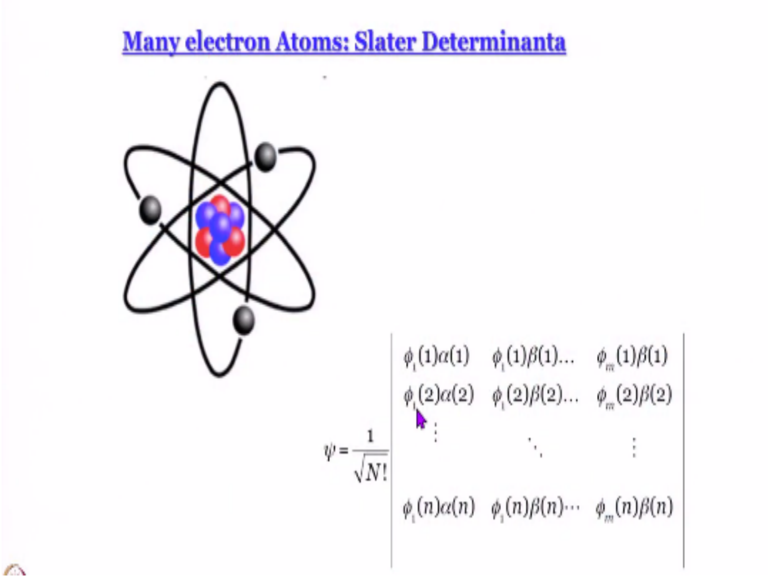

Many electron Atoms: Slater Determinanta

$$\psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1)\alpha(1) & \phi_1(1)\beta(1)\ldots & \phi_m(1)\beta(1) \\ \phi_1(2)\alpha(2) & \phi_1(2)\beta(2)\ldots & \phi_m(2)\beta(2) \\ \vdots & \ddots & \vdots \\ \phi_1(n)\alpha(n) & \phi_1(n)\beta(n)\cdots & \phi_m(n)\beta(n) \end{vmatrix}$$

We learn how to write the wavefunctions as what are called Slater determinants which look sort of like this.

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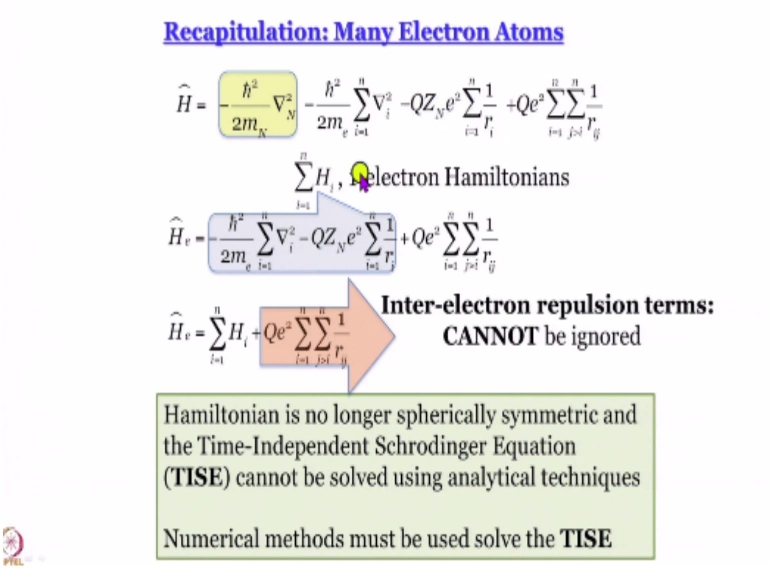

Recapitulation: Many Electron Atoms

$$\hat{H} = \boxed{-\frac{\hbar^2}{2m_N}\nabla_N^2} - \frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla_i^2 - QZ_Ne^2\sum_{i=1}^{n}\frac{1}{r_i} + Qe^2\sum_{i=1}^{n}\sum_{j>i}^{n}\frac{1}{r_{ij}}$$

$\sum_{i=1}^{n} H_i$, 1-electron Hamiltonians

$$\hat{H}_e = \boxed{-\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla_i^2 - QZ_Ne^2\sum_{i=1}^{n}\frac{1}{r_i}} + Qe^2\sum_{i=1}^{n}\sum_{j>i}^{n}\frac{1}{r_{ij}}$$

$$\hat{H}_e = \sum_{i=1}^{n} H_i + \boxed{Qe^2\sum_{i=1}^{n}\sum_{j>i}^{n}\frac{1}{r_{ij}}}$$

Inter-electron repulsion terms:
CANNOT be ignored

Hamiltonian is no longer spherically symmetric and the Time-Independent Schrodinger Equation (**TISE**) cannot be solved using analytical techniques

Numerical methods must be used solve the **TISE**

But before that let us recapitulate very quickly what we have studied in the earlier modules. We have learned that the way you write the Hamiltonian for many electron atom is that first of all you separate out the term for the kinetic energy of the nucleus or the center of mass. What you are left with is sum of n number of kinetic energy terms one for each electron, sum of n number of nucleus electron.

Photon electron you can say attraction terms - QN e square sum over i to n 1 / ri and you have this problematic + Qe square it is a double summation 1 / rij terms. So these turn out to be the one electron Hamiltonians these ones that is not a problem, but what you are left with is this electron-electron repulsion terms which we have established that we cannot ignore.

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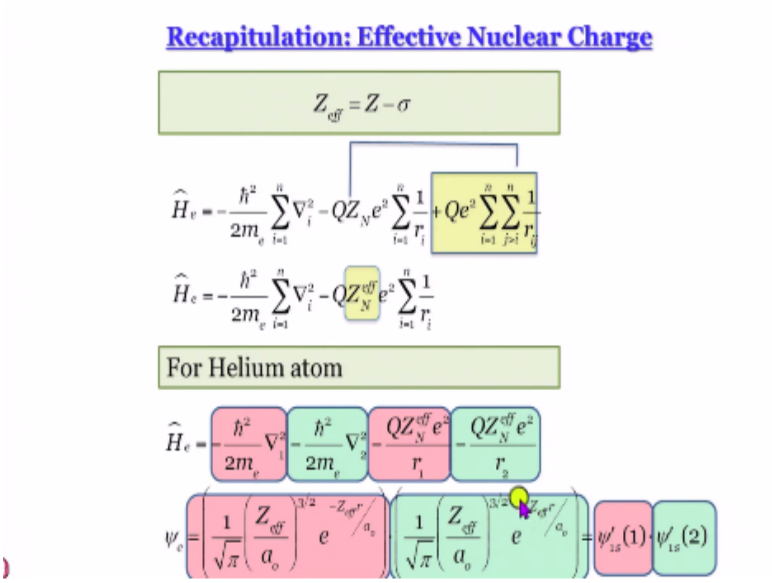

Recapitulation: Effective Nuclear Charge

$$Z_{eff} = Z - \sigma$$

$$\hat{H}_e = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla_i^2 - QZ_N e^2\sum_{i=1}^{n}\frac{1}{r_i} + Qe^2\sum_{i=1}^{n}\sum_{j>i}^{n}\frac{1}{r_{ij}}$$

$$\hat{H}_e = -\frac{\hbar^2}{2m_e}\sum_{i=1}^{n}\nabla_i^2 - QZ_N^{eff} e^2\sum_{i=1}^{n}\frac{1}{r_i}$$

For Helium atom

$$\hat{H}_e = -\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{QZ_N^{eff}e^2}{r_1} - \frac{QZ_N^{eff}e^2}{r_2}$$

$$\psi_e = \left[\frac{1}{\sqrt{\pi}}\left(\frac{Z_{eff}}{a_o}\right)^{3/2} e^{-Z_{eff}r/a_o}\right]\left[\frac{1}{\sqrt{\pi}}\left(\frac{Z_{eff}}{a_o}\right)^{3/2} e^{-Z_{eff}r/a_o}\right] = \psi'_{1s}(1)\,\psi'_{1s}(2)$$

So, what we do is that we incorporate this electron-electron repulsion term into the shielding constant and we work with not the actual nuclear charge, but the effective nuclear charge and that is how we write these one electron wavefunctions by replacing the actual nuclear charge by effective nuclear charge and for helium atom for example the Hamiltonian is going to be a sum of for 4 terms and I have shown the terms due to each electron in a different color.

And the wavefunction could also be a product of 2 wavefunctions. One in electron 1, one is electron 2 and to start with we work within the ambit of orbital approximation which says that the orbital shear are essentially the wavefunctions here are essentially atomic orbital. In case of helium these are 1s orbitals. We are now familiar with the form of 1s orbitals only radius dependent part no theta phi dependence.

And here once again the only change from the hydrogen atom system, hydrogen atom scenario is that you write Z effective instead of actual Z. So, this is how we have formulated the Hamiltonian, this is how we have written the wavefunction.

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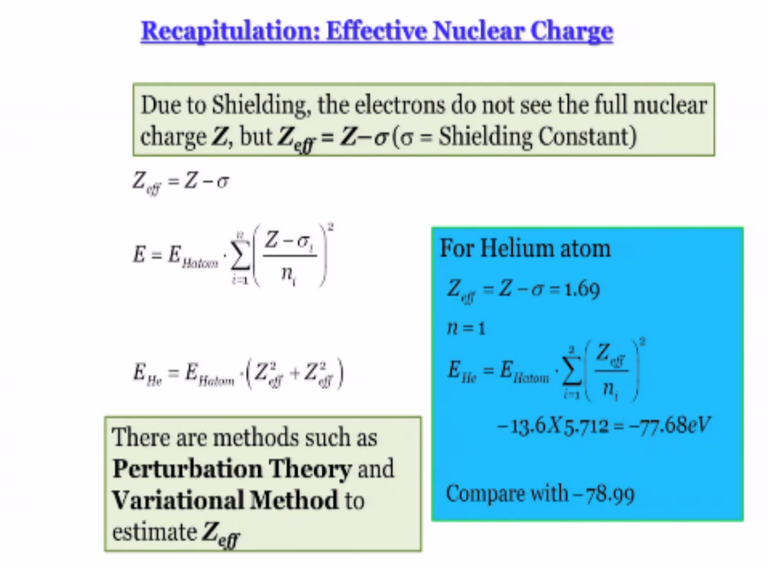

Recapitulation: Effective Nuclear Charge

Due to Shielding, the electrons do not see the full nuclear charge **Z**, but $\boldsymbol{Z_{eff} = Z-\sigma}$ (σ = Shielding Constant)

$$Z_{eff} = Z - \sigma$$

$$E = E_{Hatom}\cdot\sum_{i=1}^{n}\left(\frac{Z-\sigma_i}{n_i}\right)^2$$

$$E_{He} = E_{Hatom}\cdot\left(Z_{eff}^2 + Z_{eff}^2\right)$$

There are methods such as **Perturbation Theory** and **Variational Method** to estimate Z_{eff}

For Helium atom

$Z_{eff} = Z - \sigma = 1.69$

$n = 1$

$E_{He} = E_{Hatom}\cdot\sum_{i=1}^{2}\left(\frac{Z_{eff}}{n_i}\right)^2$

$-13.6X5.712 = -77.68eV$

Compare with -78.99

And then we did a quick fact check and we saw that for helium atom when we work with Z effective actually we have not told you how we get the sigma, but there are ways I think most of you would know of the empirical rules by which one can determine the value of sigma for different kinds of electrons and an atom and using this, we showed you that you get a theoretical value of energy which is close to the actual experimental value that is there and the point to note is that in theoretical value is more positive than the experimental value which is the real value. We are going to have more to say about this in the future modules.

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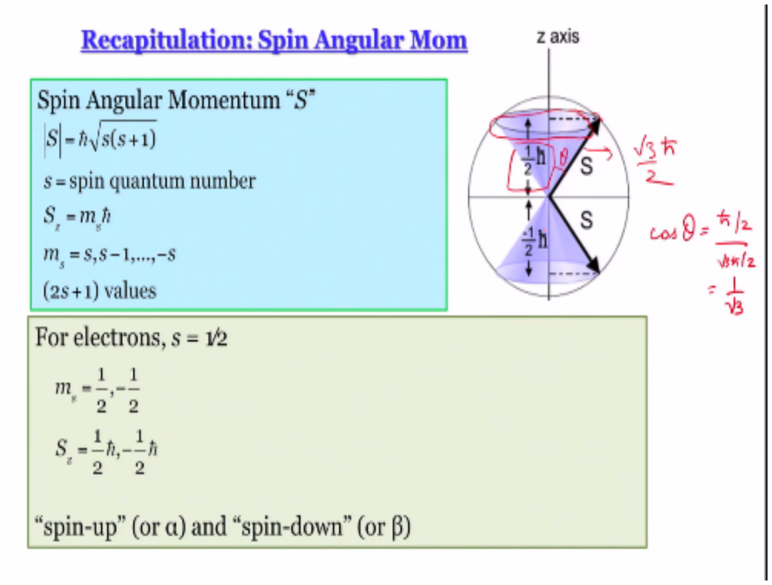

Recapitulation: Spin Angular Mom

Spin Angular Momentum "*S*"

$|S| = \hbar\sqrt{s(s+1)}$

s = spin quantum number

$S_z = m_s\hbar$

$m_s = s, s-1, \ldots, -s$

$(2s+1)$ values

For electrons, $s = 1/2$

$m_s = \frac{1}{2}, -\frac{1}{2}$

$S_z = \frac{1}{2}\hbar, -\frac{1}{2}\hbar$

"spin-up" (or α) and "spin-down" (or β)

Next, we came to this very, very important concept of spin. I sort of rush through this part and once again I want to rush through this part today, but I hope this is something familiar to us we know very well that there is something called a spin quantum number. The only confusion that is usually there is that in many books it is written for electrons s = + - 1 / 2. No, please remember for electrons the spin quantum number s is 1 / 2 and ms, ms is the spin magnetic quantum number that can take up values of + 1 / 2 and – 1 / 2.

So Z component of angular momentum can be plus minus h cross / 2 and the length of this arrow or the magnitude of the spin angular momentum as such is equal to h cross multiply it by square root of s into s + 1. So, we have actually learnt about angular momentum and we know very well why is it that magnetic quantum number cannot take up sorry about this is not Mom recapitulation spin angular momentum.

Unfortunately, some kind of reformatting has taken place please do not worry about it. So, we have studied angular momentum and we know that the magnetic angular momentum has an upper cap. Let us do a small calculation now which sort of started, but we did not complete in one of the earlier modules. What I want to say is this that this length here as we said is root over 3 / 2 is not it? Why? Because s is equal to 1/ 2, 1/ 2 into 3 / 2 that is 3 / 4 under root sign root 3 divided by well 4 comes out as a root sign and you get 2 in the denominator.

Of course, if you want I can write root 3 h cross / 2 reason why I did not write it is that in quantum mechanics often you write quantities in terms of h cross h cross is like the unit and here it is shown here that the Z component is equal to h cross / 2. So, if we take say this angle theta. What is cos theta? Cos theta is equal to h cross / 2 divided by root 3 h cross / 2 you are left with 1 / root 3.

Is that right 1 / root 3 do you remember where we encounter this 1 / root 3 earlier. What this essentially means is if you take square on the both sides you get 3 cross square theta – 1 = 0. So you see this cos theta well theta is again the same magic angle that we get. So this is a value of theta. What is the value of phi? We do not know, cannot say. That is why usually it is written like this, this tip of the arrow is usually shown to define the edge of a cone.

And in the classical picture interestingly for spin one can actually get away using a nice classical vector picture and it works. So sometimes people get confuse that is a problem. The name spin itself is very confusing because you might get the idea that the electron is spinning about its own axis pretty much like the spinning motion of the earth which is there in addition to its revolution round the sun.

Now the thing is this spin quantum number or spin angular momentum they do not arise from actual spinning motion of electron. If you work out the energy associated to find out that the electron has to actually spin at velocity is greater than light if this angular momentum has to arise from a really circular motion of some sort. So that is not realistic. So, let me just tell you that spin arises out of relativistic treatment of electron.

Spin is a product of relativistic quantum mechanics which we are not going to study in this course. Interestingly, this spinning is in terms of some kind of an imaginary coordinate omega, but you can have its component in real space. So, it is a rather intriguing quantity. It is highly possible that we do not exactly understand what is going on here, but the mathematics is not impossible to understand and also it is manifested in experiments.

As I told you earlier experimental results are the only truth as Max Plank has said. So, this spin what we will do is we are going to just deal with this spin angular quantum number in the way that we are talking about right now. So what we have said is spin is associated with some kind of an angular momentum, we know the magnitude, we know the direction also and we have also understood that phi is undefined.

Phi is completely undefined so this tip of the arrow could be actually anywhere if you are talking about one spin. So, since for electron ms can take a values of plus 1/ 2 and minus 1 / 2. Your z component can be h cross / 2 or – h cross / 2 that determines whether the angular momentum, spin angular momentum is pointing up or pointing down these are called spin up or spin down states.

Spin up state is assigned a wavefunction alpha. Spin down is assigned of wavefunction beta. Right now let us not worry about what is the actual functional form of alpha and beta is. It suffices our purpose if we just think that the wavefunction for up spin is alpha, wavefunction for down spin is beta, but remember these are wavefunctions spin wavefunction that is all.

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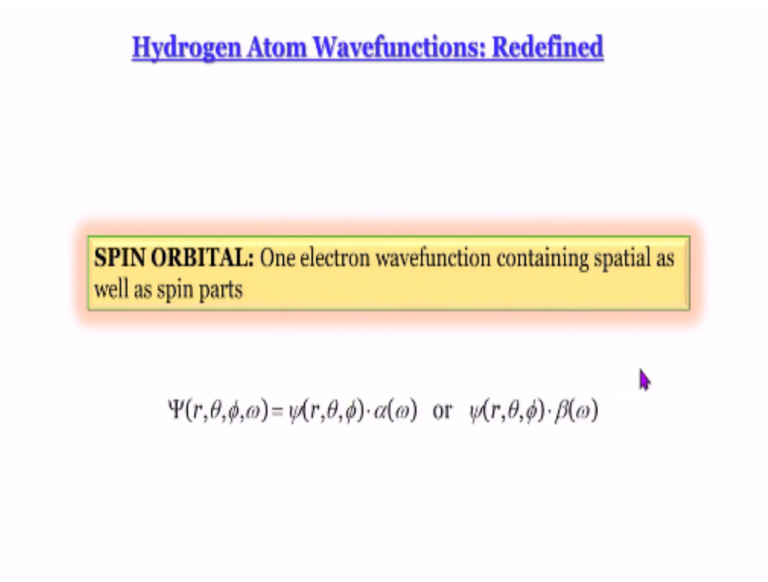

Hydrogen Atom Wavefunctions: Redefined

SPIN ORBITAL: One electron wavefunction containing spatial as well as spin parts

$$\Psi(r,\theta,\phi,\omega)=\psi(r,\theta,\phi)\cdot\alpha(\omega) \text{ or } \psi(r,\theta,\phi)\cdot\beta(\omega)$$

Now let us go ahead. So what we said is now if you want to talk about multi electron atoms it is not sufficient to talk about n, l and m we also have to talk about ms not s remember ms for all electrons s is 1 / 2 anyway. So, this total wavefunction psi which is a function of r theta phi and omega the spin coordinate is given by psi r theta phi the wavefunction is spatial coordinates multiplied by the wavefunction in spin coordinates alpha or beta.

So, if you just take one electron then it can reside in the same orbital in two ways. One, in which it has up spin, one in which it has down spins. So two wavefunctions are now possible very incorporate spin. Now this state is called a doublet state. Why doublet? Because they are actually 2 wavefunctions when you consider the spin part as well.

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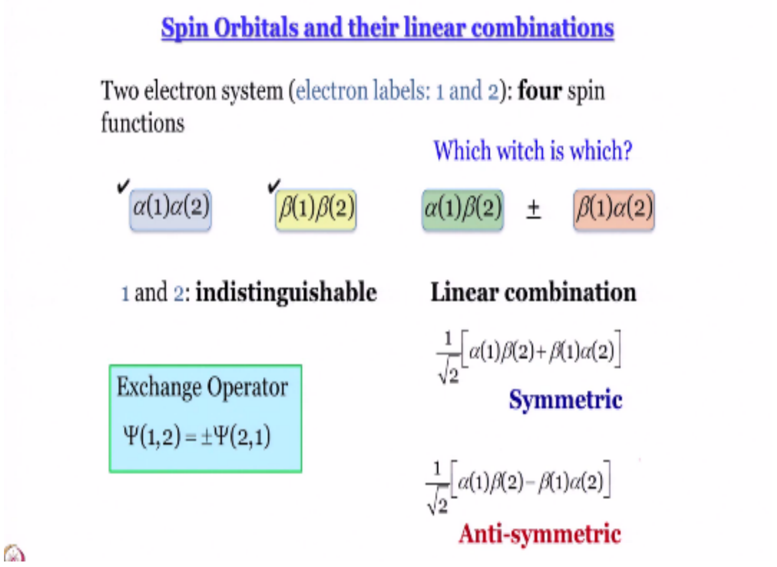

Spin Orbitals and their linear combinations

Two electron system (electron labels: 1 and 2): **four** spin functions

Which witch is which?

✓ $\alpha(1)\alpha(2)$ ✓ $\beta(1)\beta(2)$ $\alpha(1)\beta(2)$ ± $\beta(1)\alpha(2)$

1 and 2: **indistinguishable**

Linear combination

$$\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)+\beta(1)\alpha(2)\right]$$

Symmetric

$$\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)-\beta(1)\alpha(2)\right]$$

Anti-symmetric

Exchange Operator

$$\Psi(1,2)=\pm\Psi(2,1)$$

Now, let us make things a little interesting. Let us talk about 2 electron system remember that is what we want to do anyway not only 2 we want to talk about maybe 5 electron, 6 electron, 10, 12 electron systems. To start with, let us understand how to go about it by considering a 2 electron system. So, here we are using electron labels of 1 and 2. So 1 and 2 are like the names of the electron, electron number 1, electron number 2.

So, as you understand we can construct 4 different spin wavefunctions using electron number 1 and 2 and at this stage in case you do not have a pen and notebook please pause the video, go and fetch them and start writing. As I said earlier we have to keep writing so that we understand. So what are the 4 spin functions that we can think of? First of all, both electron number 1 and 2 can have up spin.

So that is written as alpha 1, alpha 2 alpha the one in bracket then alpha 2 in bracket. This means electron number 1 has alpha spin electron number 2 also has alpha spin alpha 1, alpha 2. Similarly, both can have beta spins that wavefunction will be beta 1, beta 2 no problem so far. Things get interesting when we think of mix spin systems. What happens when one spin is alpha, one spin is beta.

Do I think of writing like this alpha 1, beta 2 or we might think of writing like this beta 1, alpha 2. Now, if you look at this terms what does this first wavefunction say? The first wavefunction says electron number 1 has up spin, electron number 2 has down spin. This one says electron number 1 has down spin, electron number 2 has up spin. Do you get the point if not let us just say it once again.

What it says here this alpha 1, beta 2 is that it is electron number 1 and not electron number 2 that has alpha spin. It also says it is electron number 2 and not electron number 1 that has beta spin. Similarly, in this function we say that it is electron number 1 and not electron number 2 that has beta spin and electron number 2 and not electron number 1 that has alpha spin. Now we encounter a problem.

What is the problem? If we say alpha 1, beta 2 and in fact it is 1 and not 2 electron I mean electron number 1 and not electron number 2 that has alpha spin then, what we are saying essentially is that we can differentiate between electron number 1 and 2. Can we really do that? Yeah, actually we cannot. So, if you are going there alpha, alpha 2 is fine, beta 1, beta 2 is fine. Problem is 1 and 2 are indistinguishable.

Electrons do not wear jerseys with their names or numbers written on them. Electrons do not have the numbers in printed on them. We are designating them 1 and 2 to formulate the problem, but actually the 2 electrons are absolutely indistinguishable. You cannot say that it is electron number 1 and electron number 2 or electron number 2 and electron number 1 that has a particular spin state.

What you can say is like one of the electrons has alpha spins and one of the electrons has beta spin that much is okay, but you cannot say at least this and that or this and not that or that and not this that has alpha spin or beta spin. I hope I am able to make the point. Yeah, so I have say 2 boys in a room and there is an apple and then after a while I come back and I see that the apple is not there somebody has eaten it.

Without asking them shall I able to say that well this is a bad example because they could have shared the apple. Let us say they cannot, let us say that it is an apple that cannot be shared then I cannot say that it is boy A and not boy B who has eaten the apple I cannot say the other way round. What I can say is that one of them has eaten it provided the apple has not been shared that is another problematic situation fortunately which is not relevant to our discussion.

So, what we do is we write the way function like this since we cannot figure out which, which is which we take a linear combination. When we take a linear combination we end up getting 2 functions one with a plus sign between these two and one with minus sign and we have to normalize. So we multiply by 1 / root 2. Now if I look at this what does it say? The first term says that it is electron number 1 and not number 2 that has alpha spin and electron number 2 and not number 1 that has beta spin.

The second one says exactly the opposite it says electron number 1 has beta spin, electron number 2 has alpha spin. So, if I combine the two remember probability. What is the probability of simultaneous occurrence or product? What is the probability of either this or that happening some. The probability of raining is 1 / 2 the probably of not raining is 1 / 2. So it cannot rain and not rain if it could than the probability of that would have been 1 / 4.

But the total probability that it might rain or might not rain that is 1 / 2 + 1 / 2 = 1 once again I think we have very bad examples today. Anyway, so what is the significance of this plus and minus at this point nothing, significance is there profound significance is there we will come to that, but at this point we are just combining the two terms using plus or minus. The two terms which say that one of the electrons has alpha spin and the other one has beta spin.

I can say that using plus or minus there is no reason at least now to discard one in favor of the other so we write both. So what have we learned? We have learned that if both the spins are up or both the spins are down you can happily write alpha 1, alpha 2 or beta 1 or beta 2 if one is up spin, one is down spin then we must necessarily write two terms. In the first one electron number one should have alpha spin, electron number two should have beta spin.

And the second one it should be other way round and then we connect them using either plus or minus sign. So, we take these two linear combinations. Now, to develop the discussion of why this linear combinations are important at all. We will bring in the concept of symmetry. What is the meaning of symmetry? Let us say I have an exchange operator, exchange operator means an operator by which the labels are interchanged.

When you apply exchange operator to psi 1, 2 then it can become either plus psi 2, 1 or minus psi 2, 1 something like that not all wavefunctions will be like that, but we are going to work only with wavefunctions that are either symmetric. Symmetric means eigen function of 1 the sign is plus and it is or anti-symmetric, anti-symmetric means eigen function of minus 1 now we have minus sign here.

So, we are going to work only with wavefunctions that are either symmetric or anti-symmetric with respect to exchange. Exchange means exchange in the labels. Now whatever is in 1 becomes in terms of 2, whatever is in terms of 2 becomes in terms of 1 that is all. What about the first one is it symmetric or is it anti-symmetric with respect to exchange and here how I wish there was a chat window where you people could respond.

Unfortunately, we do not at least think first. The first one, the first linear combination that we have shown upon applying exchange operator does it change sign, does it not change sign? Obviously it does not change sign. So, it is symmetric with respect to exchange. What about the second one? If we exchange the labels 1 and 2 then what do you get? Simply exchange the labels you get of course you get 1 / root 2 let us not worry about that.

Then you get alpha 2, beta 1 – beta 2, alpha 1 wait - this is beta 2, alpha 1. What have I done? I have just interchanged 1 and 2. So what do I get here I get 1 / root 2 let us take this second term first and write in the same sequence as far as possible beta 2, alpha 1 is the same as alpha 1, beta 2 minus, but wait there is a minus sign in front of this so I would better take this minus sign out – 1 / root 2 alpha 1, beta 2.

Now I can write another minus because this is plus sign minus and minus is plus minus I will write it as beta 1, alpha 2. What is that you recognize it? If this is psi then this is minus sign. So after erasing so what we see is that upon applying the exchange operator the second wavefunction changes sign. So the second wavefunction must be anti-symmetric with respect to exchange. So what we see here is that the wavefunctions that we generate by taking linear combinations are either symmetric or anti-symmetric with respect to exchange.

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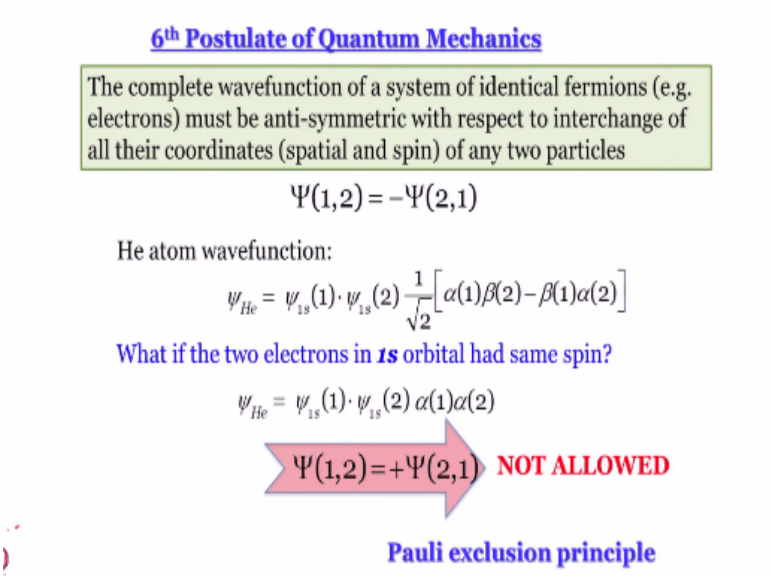

6th Postulate of Quantum Mechanics

The complete wavefunction of a system of identical fermions (e.g. electrons) must be anti-symmetric with respect to interchange of all their coordinates (spatial and spin) of any two particles

$$\Psi(1,2) = -\Psi(2,1)$$

He atom wavefunction:

$$\psi_{He} = \psi_{1s}(1)\cdot\psi_{1s}(2)\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)-\beta(1)\alpha(2)\right]$$

What if the two electrons in *1s* orbital had same spin?

$$\psi_{He} = \psi_{1s}(1)\cdot\psi_{1s}(2)\,\alpha(1)\alpha(2)$$

$$\Psi(1,2)=+\Psi(2,1)$$ NOT ALLOWED

Pauli exclusion principle

Why would we bother about that? We bother about that because there is something called 6th postulate of quantum mechanics and I will just read it for you. So it is important to understand this. It says the complete wavefunction of a system of identical fermions. What is fermion? Spin 1 / 2 integral multiple of 1 / 2 that is what this spin number is. So fermions like electrons must be anti-symmetric with respect to interchange of all their coordinates spatial and spin of any two particles. I will read that again.

For identical fermions the complete wavefunction must be anti-symmetric with respect to interchange of all their coordinate of any 2 particles which means that if I just interchange 1 and 2 then psi should become minus sign that is all it means. This is true for fermions. For bosons it is not the case for bosons they are actually symmetric the wavefunctions are symmetric with respect to interchange.

So, now let us try to write the helium atom wavefunction knowing very well that the complete wavefunction has to be anti-symmetric with respect to exchange of any coordinates. First of all let us start with this. Psi 1 is 1, psi 1 is 2. We encountered this in the previous slide I hope you remember. This means both the electrons are in the 1s orbital then what will the corresponding spin part be. Say that first tell me or tell yourself is this psi s1, psi s2 symmetric or anti-symmetric with respect to exchange.

This is a very easy question because just take 1 here, take 2 here psi 1 s1, psi 1 s2 becomes psi 1s 2 psi 1 s1 and these are functions these are not operators. So the sequence of multiplication does not matter. So what we get then is helium atom wavefunction given by psi s1 multiplied by psi s2 is symmetric with respect to exchange. Now, let us go back to the 6th postulate. This is also called by the way Pauli principle.

Ring a bell you remember something. Well, it does not say Pauli exclusion principle I did not say Pauli exclusion principle I said Pauli principle. Pauli principle is that for fermions the total wavefunction including the spin part has to be anti-symmetric with respect to exchange. As we will see our familiar Pauli exclusion principle is going to follow from here, but until now what we have stated the 6th postulate it is really Pauli principle.

So now this is symmetric so if the total wavefunction has to be anti-symmetric then I must multiply this by an anti-symmetric spin part. Remember there are 2 spin parts that were there well 2 kinds of spin parts alpha 1, alpha 2 symmetric or anti-symmetric. So if I just write this if I write say alpha 1, alpha 2 then what is the problem. The problem is this is symmetric with respect to exchange this here is symmetric with respect to exchange.

So the product is also symmetric, but then we have just learned that for identical fermions the complete wavefunction must be anti-symmetric with respect to exchange. So this is not an acceptable wavefunction. The moment you bring in these spin part some of the spatial wavefunctions are not going to be allowed anymore okay sorry about that let us just go ahead.

So, now what we have then is we multiply it by the anti-symmetric combination remember there are 4 spin wavefunction alpha, alpha which is symmetric, beta, beta which is symmetric alpha, beta plus beta, alpha which is symmetric. The only anti-symmetric spin wavefunctions in our hand is 1 / root 2 multiply it by alpha 1 beta 2 – beta 1 alpha 2. So what we are saying is that only this anti-symmetric spin part can be multiplied with this symmetric spatial part to give us an acceptable total wavefunction.

So this is this is only spin part that is going to work all other spin wavefunctions are not compatible you can say with psi 1 s1 multiplied by psi 1 s2 because we need an anti-symmetric total wavefunction. Shall we go ahead? Let us. Now see what happens if the 2 electrons in 1s orbital has same spin. So what we imply by saying this is that at the moment we say that alpha 1, alpha 2, beta 1, beta 2 these are not going to exist.

It automatically says that 2 electrons in 1s orbital must not have the same ms numbers, not the same spin if I say loosely and that essentially is your Pauli exclusion principle that in an atom for an electron all 4 quantum numbers cannot be the same. If N, L, M are the same at least MS should be different. So now we are asking the question what happens if two electrons in 1s orbital has the same spin.

So, it is like this alpha 1, alpha 2 multiply it by psi He = psi 1 S1 multiplied by psi 1 S2. So see this is symmetric with respect to exchange. So, since it is symmetric it does not stand the test of your 6th postulate of quantum mechanics. So it cannot be taken, it turns out that upon applying the exchange operator you get back the same psi 1, 2, psi 2, 1 wavefunction no change in sign. So this is not allowed by the 6th postulate of quantum mechanics.

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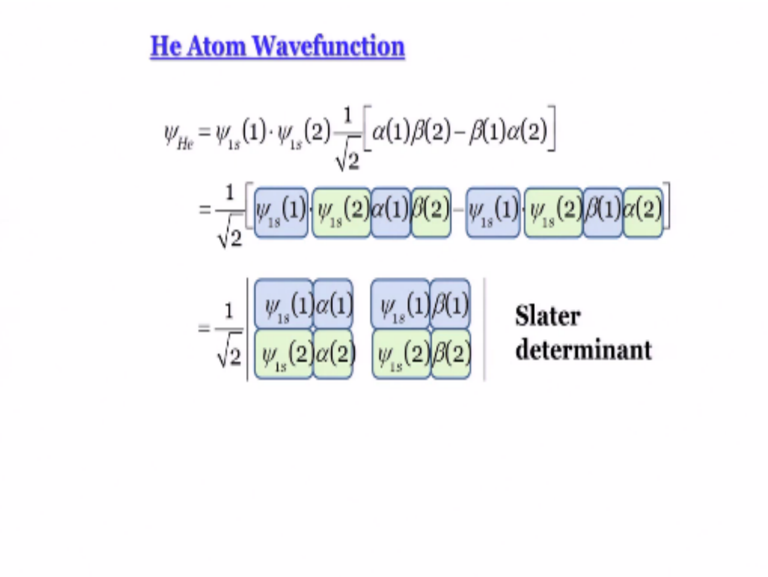

He Atom Wavefunction

$$\psi_{He} = \psi_{1s}(1)\cdot\psi_{1s}(2)\frac{1}{\sqrt{2}}\left[\alpha(1)\beta(2)-\beta(1)\alpha(2)\right]$$

$$= \frac{1}{\sqrt{2}}\left[\boxed{\psi_{1s}(1)}\cdot\boxed{\psi_{1s}(2)}\boxed{\alpha(1)}\boxed{\beta(2)}-\boxed{\psi_{1s}(1)}\cdot\boxed{\psi_{1s}(2)}\boxed{\beta(1)}\boxed{\alpha(2)}\right]$$

$$= \frac{1}{\sqrt{2}}\begin{vmatrix} \boxed{\psi_{1s}(1)}\boxed{\alpha(1)} & \boxed{\psi_{1s}(1)}\boxed{\beta(1)} \\ \boxed{\psi_{1s}(2)}\boxed{\alpha(2)} & \boxed{\psi_{1s}(2)}\boxed{\beta(2)} \end{vmatrix}$$

Slater determinant

The only thing that is allowed I hope it is not very difficult for you to see is 1 / root 2 alpha 1, beta 2 – beta 1, alpha 2. So, we expand this is what you get. What I have done here is I have labeled all the functions in a particular coordinate using the same color and all functions in another particular coordinate in a different color. Now, we are already familiar with matrices because we talked about them while discussing your angular momentum.

Now see this not matrices determinants. Now when you look at this do you see that it is very simple to collect the terms in the same atom sorry same electron and write this whole thing in the form of a determinant. Let me do it for you. First of all, in this 1, 1 location we are going to write psi s1, alpha 1. What is that psi s1, alpha 1? That is a spin orbital then psi s1, alpha 1 is multiplied by psi 1 s2 multiplied by beta / 2.

So, the only way you can get it is by incorporating psi 1s 1 sorry psi 1 s2 beta 2 in the diagonal block of the determinant we are getting and the other 2 terms come here simple. Let us get ahead. So this is what we have. We have this determinant and now this is called a Slater determinant. Let us have a closer look at the determinant what has happened? Look at row number 1 when you go from left to right what has remained the same, what has changed. But let us do something let us wait here we will come back and continue from here in the next module.