Particle spin as quantum statistics identifier

~~However,~~ In addition to the magnetic momentum contribution, spin has a profound effect on the particle statistics!

In quantum physics identical particles must be indistinguishable => if two particles are exchanged, the physical reality must not change

$$\overset{1}{\bullet} \quad \overset{2}{\bullet} \iff \overset{2}{\bullet} \quad \overset{1}{\bullet}$$

$$|\psi(\vec r_1, \vec r_2)|^2 = |\psi(\vec r_2, \vec r_1)|^2$$

two possibilities

wave function is symmetric

$$\psi(\vec r_1, \vec r_2) = \psi(\vec r_2, \vec r_1)$$

Integer spin

photons $S = 1$

wave function is anti-symmetric

$$\psi(\vec r_1, \vec r_2) = -\psi(\vec r_2, \vec r_1)$$

Half-integer spin

e, p, n $S = 1/2$

The symmetry of a wave function has a dramatic consequences!

Two independent distinguishable particles

$$\psi(\vec r_1, \vec r_2) = \psi_1(\vec r_1)\,\psi_2(\vec r_2)$$

For indistinguishable particles:

symmetric wave function

$$\psi(\vec r_1, \vec r_2) = \frac{1}{2}\left(\psi_1(\vec r_1)\psi_2(\vec r_2) + \psi_1(\vec r_2)\psi_2(\vec r_1)\right)$$

Two particles can be in the same state!

$$\psi_1 = \psi_2 = \psi_0$$

$$\psi(\vec r_1, \vec r_2) = \psi_0(\vec r_1)\,\psi_0(\vec r_2)$$

Bosons

Integer spin particles
(photons)

Fermions

Half-integer spin particles
(electrons, protons, neutrons)

That means that for very low temperature all particles will ~~collect~~ accoumulate in the same ground state : Bose-Einstein condensate

Thus, integer-spin particles are called **bosons**

Anti-symmetric wave function

$$\psi(\bar{r}_1, \bar{r}_2) = \frac{1}{\sqrt{2}}\left(\psi_1(\bar{r}_1)\psi_2(\bar{r}_2) - \psi_1(\bar{r}_2)\psi_2(\bar{r}_1)\right)$$

If $\psi_1 = \psi_2 = \psi_0 \Rightarrow \psi(\bar{r}_1, \bar{r}_2) = 0$

two particles cannot be in the same quantum state

Spin $1/2$ particles are called fermions

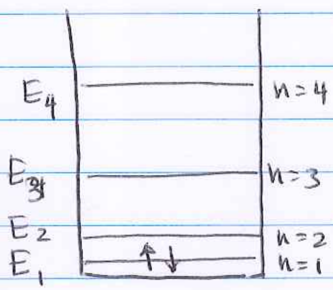
Pauli exclusion principle: No two electrons (or any other fermions) can occupy the same quantum state.

Electrons ~~are~~ are spin-$1/2$ particles (fermions), and Pauly exclusion principle shapes the ~~str~~ atomic structure for all elements in the universe!

Examples of Pauli principle applications

a) 1 D infinite square well

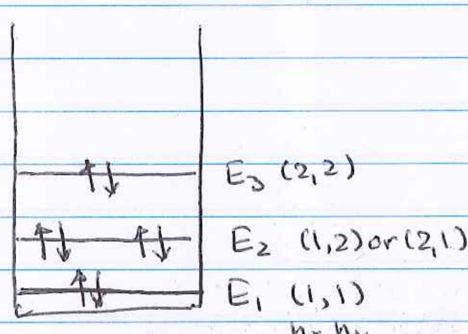
Energy levels : no degeneracy



Let's put the first $\bar{e}$ in the ground state E_1
Thus, if we want to place the second electron in the lowest energy state, the only option for it to go to E_1 is if its spin state is different from the first one
(Electrons can be only in two orthogonal spin states $m_s = \pm 1/2$, "up" or "down")

The third electron will have to go to E_2, and so on.
So max # of electrons on a non-degenerate energy level is 2.

b) 2 D Square well



E_1: non-degenerate, 2 electrons
E_2: doubly-degenerate: 4 electrons
(one pair at $n_x=1, n_y=2$ state
one pair at $n_x=2, n_y=1$ state)

Multi-electron atoms

Half-integer spin particles (fermions)

$$\psi(\bar r_1, \bar r_2) = \frac{1}{2}\left(\psi_1(\bar r_1)\psi_2(\bar r_2) - \psi_2(\bar r_1)\psi_1(\bar r_2)\right)$$

two particles <u>cannot</u> be in the same state

Pauli exclusion principle
No two electrons (or any fermions) can occupy the same quantum state.

This principle guides the composition of all atoms

In an atom electron's state is now defined by <u>5</u> quantum numbers

$n, \ell, m_\ell, \quad s = 1/2, \quad m_s = \pm\frac{1}{2}$

Total degeneracy of an n-state is $2n^2$

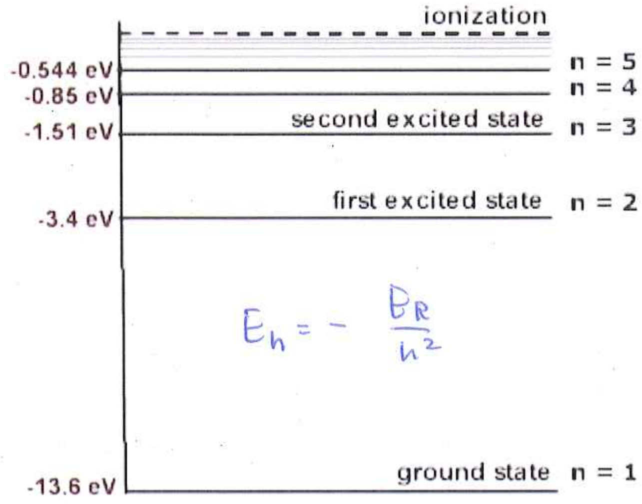
Thus only $\underline{2n^2}$ electrons can ~~occupy~~ have the same energy!

$3s \ \overline{\ 2\bar e\ }$ $\quad 3p \ \overline{\ 6\bar e\ }$ $\quad 3d \ \overline{\ 10\bar e\ }$

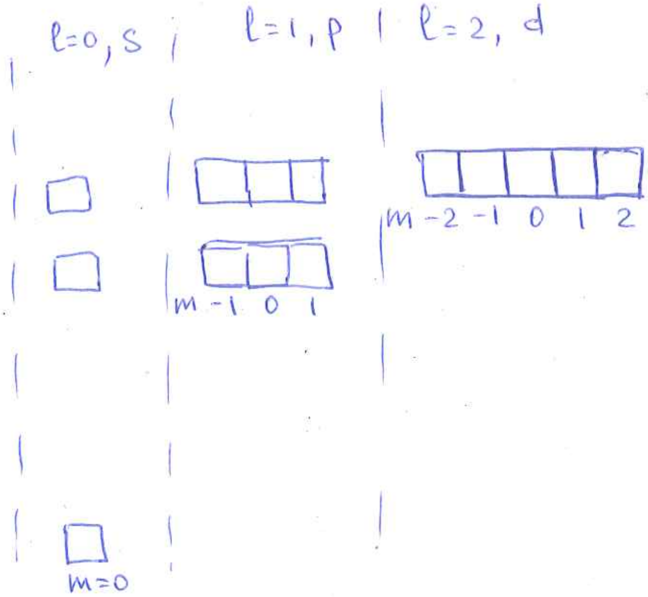
$2s \ \overline{\ 2\bar e\ }\ \uparrow\downarrow \quad 2p \ \overline{\ 6\bar e\ }\ \boxed{\uparrow\downarrow|\uparrow\downarrow|\uparrow\downarrow}$ $\quad n=2 \quad \ell=0 \quad m_\ell=0 \quad m_s=\pm 1/2$

$m_\ell = -1 \ 0 \ 1$ $\qquad \ell=1 \quad m_\ell = 0, \pm 1, \quad m_s = \pm\frac{1}{2}$

$1s \ \overline{\ 2\bar e\ }\ \uparrow\downarrow \qquad n=1, \ \ell=0, \ m_\ell=0, \ m_s = \pm 1/2$



$$E_n = -\frac{E_R}{n^2}$$



$l=0 \rightarrow s$ (for sharp)
$l=1 \rightarrow p$ (principle)
$l=2 \rightarrow d$ (diffuse)
$l=3 \rightarrow f$ (fundamental)
g
h
...

Pauli exclusion principle

no two electrons are in the same state

Multy - electron atom $+Ze$ - nuclei charge
Z electrons

In a stationary case these electrons will fill in Z low energy states available

$Z = 2$ He $-$ 2e $1s$ $\boxed{\uparrow\downarrow}$ closed shell
very stable configuration

$Z = 3$ $Li \rightarrow 3e$ $1s$ $\boxed{\uparrow\downarrow}$ $2s$ $\boxed{\uparrow}$ $1s^2 2s^1$
one unpaired electron
expect H-like behaviour
(same is true for all alkali metals)

$Z = 4$ $Be \rightarrow 4e$ $1s^2 2s^2$ $1s$ $\boxed{\uparrow\downarrow}$ $2s$ $\boxed{\uparrow\downarrow}$

$Z = 5$ $B \rightarrow 5e$ $1s^2 2s^2 2p^1$ $1s$ $\boxed{\uparrow\downarrow}$ $2s$ $\boxed{\uparrow\downarrow}$ $2p$ $\boxed{\uparrow \,|\, \;\, |\, \;\,}$

$Z = 6$ $C \rightarrow 6e$ $1s^2 2s^2 2p^2$ $\underbrace{\boxed{\uparrow\downarrow}}_{1s}\underbrace{\boxed{\uparrow\downarrow}}_{2s}\underbrace{\boxed{\uparrow}\boxed{\uparrow}\boxed{\;\;}}_{2p}$

$Z = 7$ $N \rightarrow 7e$ $1s^2 2s^2 2p^3$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$

$Z = 8$ $O \rightarrow 8e$ $1s^2 2s^2 2p^4$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow}\boxed{\uparrow}$

$Z = 9$ $F \rightarrow 9e$ $1s^2 2s^2 2p^5$ $\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow}$

$Z = 10$ $Ne \rightarrow 10e$ $1s^2 2s^2 2p^6$ $\underbrace{\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}\boxed{\uparrow\downarrow}}$
closed shell

$Z = 11$ $Na \rightarrow 11e$ $[Ne]\,3s_1$ $[Ne]\underset{3s}{\boxed{\uparrow}}$