

PART XII

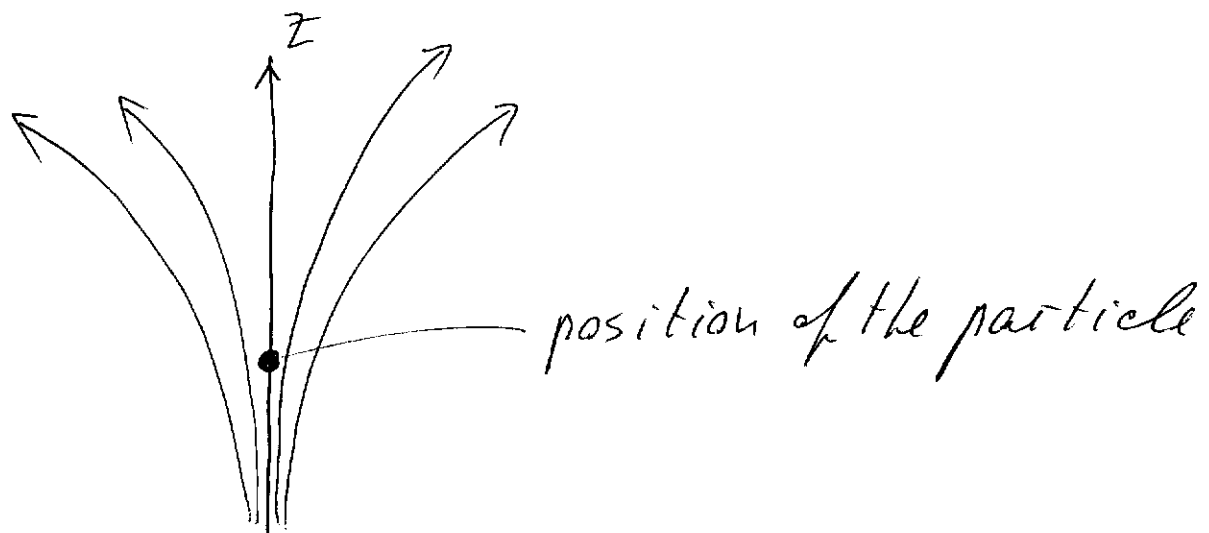
Force acting on a magnetic moment in a nonuniform magnetic field.
Stein-Gerlach experiment (Ag).

$$\hat{H} = -g \frac{e\hbar}{2m} \vec{s} \cdot \vec{B}$$

state "up" $|\uparrow\rangle$: $E_{\uparrow} = -\frac{g e \hbar}{2} \frac{1}{2m} B$

state "down" $|\downarrow\rangle$: $E_{\downarrow} = \frac{g e \hbar}{2} \frac{1}{2m} B$

Consider a nonuniform magnetic field.



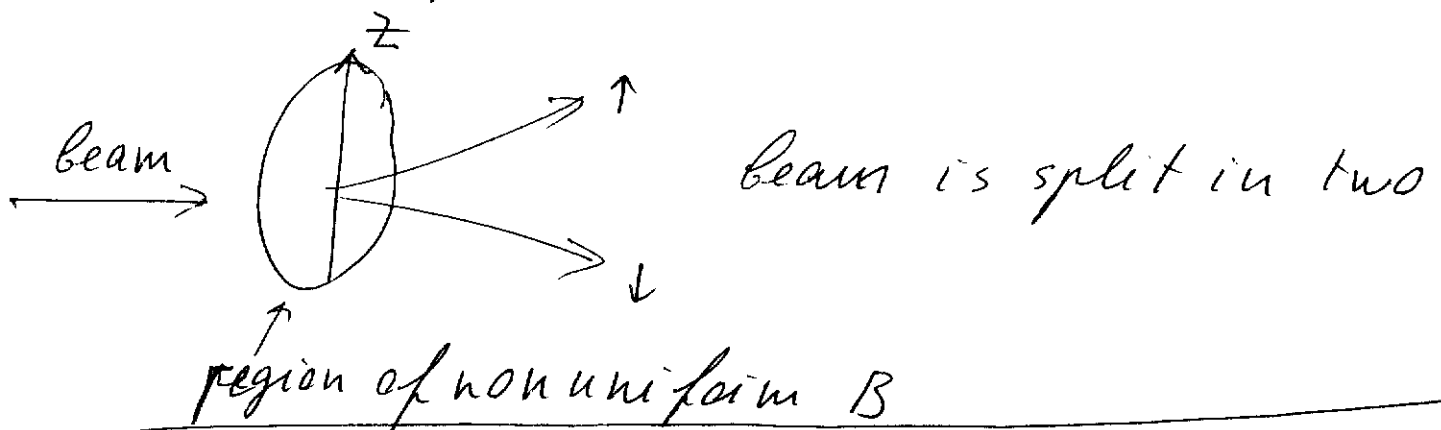
Then there is a force acting on the particle and direction of the force depends on polarization of the particle.

$$F_{\uparrow} = - \frac{\partial E_{\uparrow}}{\partial z} = g \frac{e\hbar}{4m} \frac{\partial B}{\partial z}$$

$$F_{\downarrow} = - \frac{\partial E_{\downarrow}}{\partial z} = -g \frac{e\hbar}{4m} \frac{\partial B}{\partial z}$$

Thus particles with polarization up are deflected in positive z direction and particles with polarization down are deflected in negative z direction

This is Stern-Gerlach experiment originally performed with Ag atoms

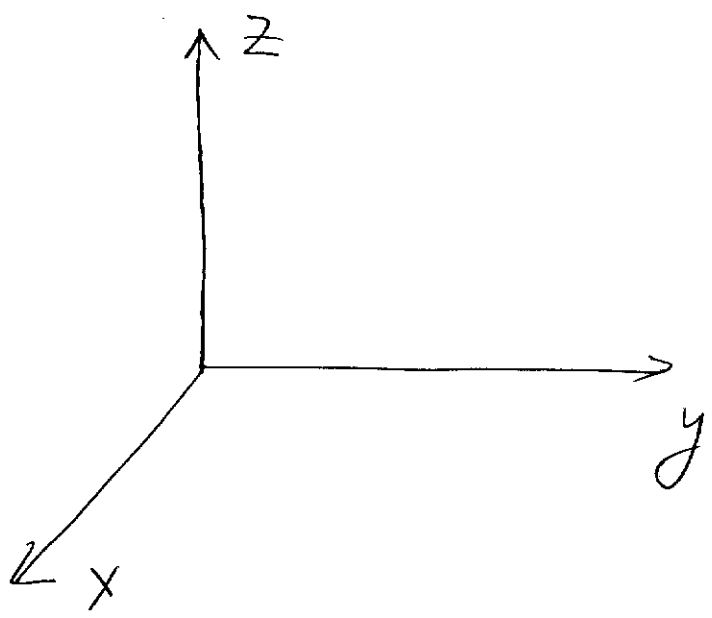


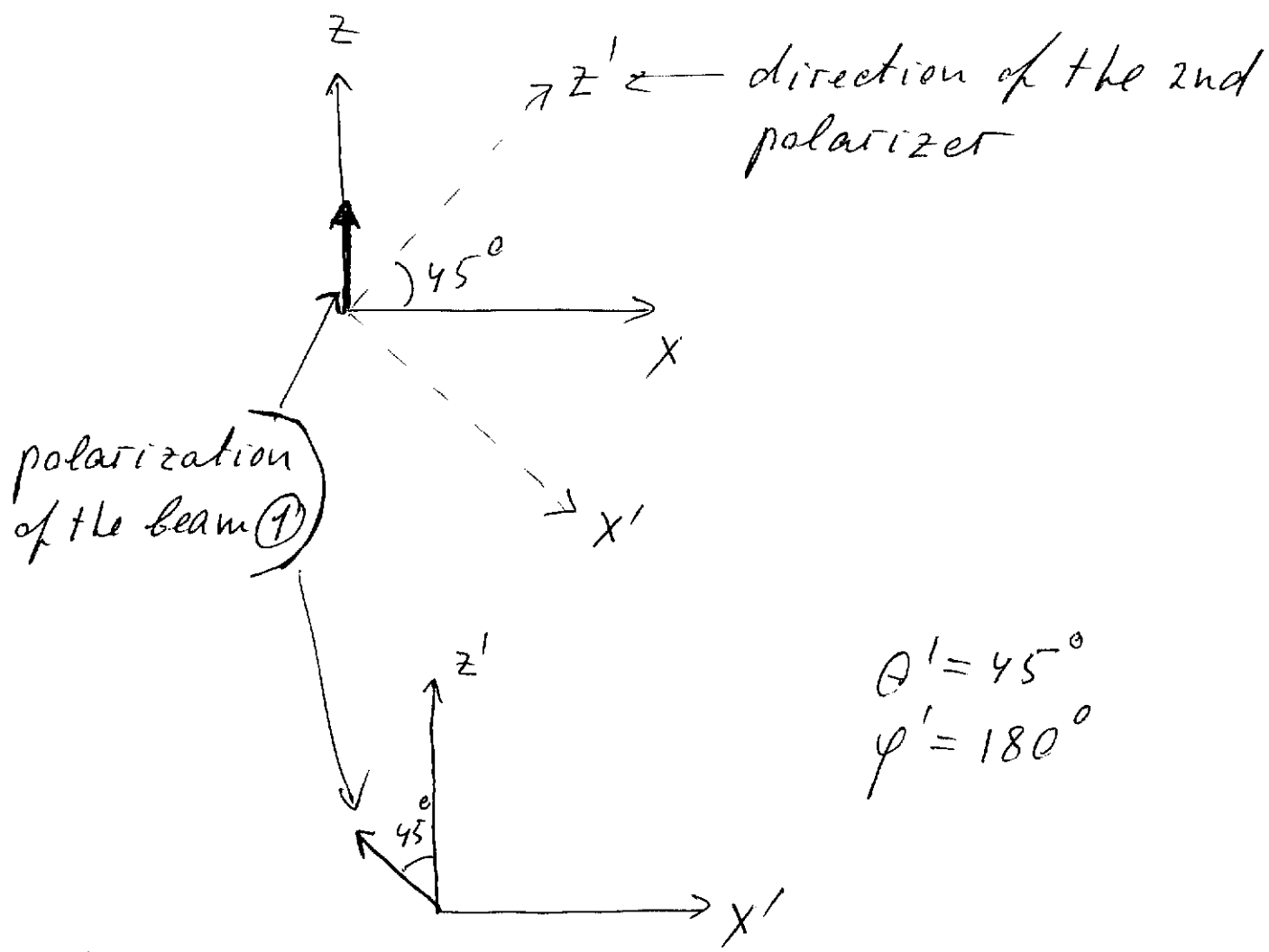
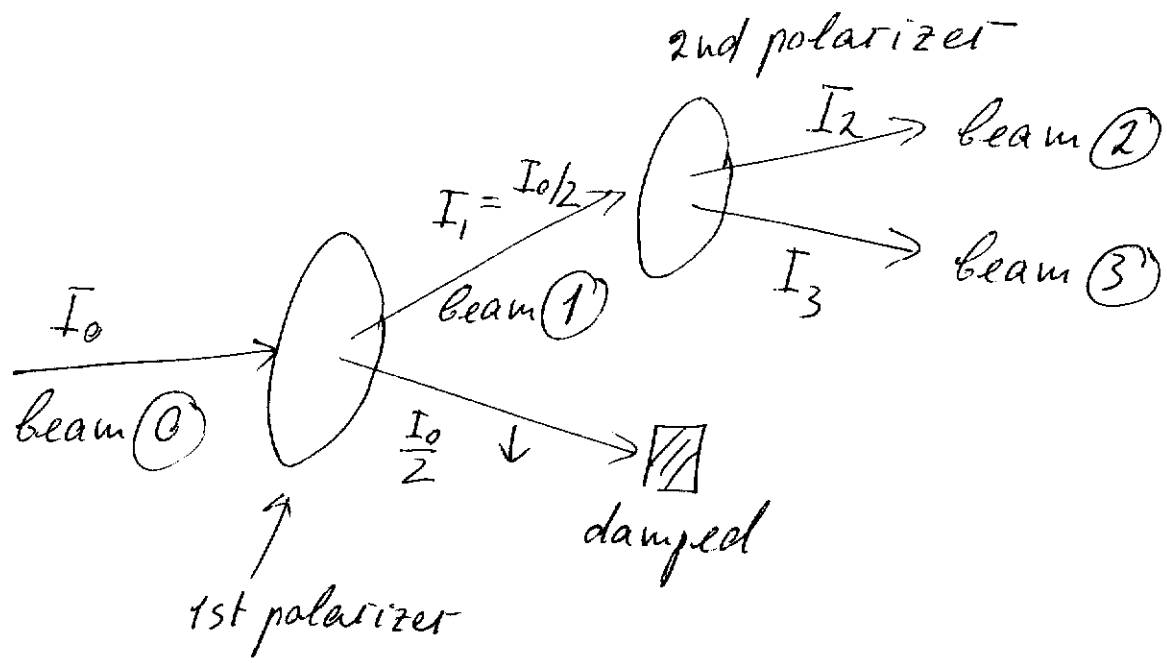
Comment: Here we use quantum description of spin and semiclassical description of translational motion. It is semiclassical because we use "force" which generally cannot be defined in quantum mechanics (see pages 105-107). Semiclassical description is justified because we consider heavy particles: atoms, neutrons.

Example: Unpolarized beam of neutrons (unpolarized = equal numbers of "up" and "down" neutrons) is moving in y direction and has intensity I_0 .

The beam is transmitted through a region of nonuniform magnetic field directed along z, $\vec{B} = (0, 0, \vec{B})$ and then the upper beam is transmitted through a region of nonuniform \vec{B} directed at 45° in zx-plane, $\vec{B} \sim (0, 1, 1)$.

Find intensities of beams after the second polarizer





According to results on page 201 the spin state of neutrons in the beam (1) is (I use the coordinate system of the 2nd polarizer)

$$\Psi_{11} = \begin{pmatrix} e^{-i\frac{\phi'}{2}} \cos \frac{\theta'}{2} \\ e^{i\frac{\phi'}{2}} \sin \frac{\theta'}{2} \end{pmatrix} = \begin{pmatrix} e^{-i\frac{\pi}{2}} \cos \frac{\pi}{8} \\ e^{i\frac{\pi}{2}} \sin \frac{\pi}{8} \end{pmatrix} = \begin{pmatrix} -i \cos \frac{\pi}{8} \\ i \sin \frac{\pi}{8} \end{pmatrix}$$

Hence

$$I_1 = \frac{I_0}{2} \left| \cos \frac{\pi}{8} \right|^2 = I_0 \frac{\sqrt{2}+1}{4\sqrt{2}} = 0.4268 I_0$$

$$I_2 = \frac{I_0}{2} \left| \sin \frac{\pi}{8} \right|^2 = I_0 \frac{\sqrt{2}-1}{4\sqrt{2}} = 0.0732 I_0$$

Comment: It is somewhat similar to optics, but answers are different because in optics we deal with vector polarization and in this case (neutrons) we deal with spinor polarization.

Addition of angular momenta

Consider two electrons, $s_1 = \frac{1}{2}$, $s_2 = \frac{1}{2}$

Question: How to construct states with given total spin of the pair, $\hat{S} = \hat{S}_1 + \hat{S}_2$!

Two starting points:

- 1) Wave function of two particles is product of single particle wave functions.
- 2) One can construct four products

$$|A\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$$

$$|B\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2$$

$$|C\rangle = |\downarrow\rangle_1 |\uparrow\rangle_2$$

$$|D\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2$$

$$\hat{S}_z = \hat{S}_{1z} + \hat{S}_{2z} \Rightarrow$$

$$\hat{S}_z |A\rangle = \left(S_{1z} |\uparrow\rangle_1 \right) |\uparrow\rangle_2 + \left(S_{2z} |\uparrow\rangle_1 \right) |\uparrow\rangle_2 =$$

$$= \frac{1}{2} |\uparrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 \frac{1}{2} |\uparrow\rangle_2 = \left(\frac{1}{2} + \frac{1}{2} \right) |\uparrow\rangle_1 |\uparrow\rangle_2$$

Obviously, in general case, if the state is $|m_1\rangle_1 |m_2\rangle_2$ then $M = m_1 + m_2$.

So, z-projections are added as usual numbers.

Thus, the state $|A\rangle$ has $S_z = 1$

$|B\rangle$ has $S_z = 0$

$|C\rangle$ has $S_z = 0$

$|D\rangle$ has $S_z = -1$.

There is only one state with $S_z = 1$ (state $|A\rangle$).

Therefore

1) maximum value of total spin is $S = 1$

This is because S_z always takes values $S_z = -S, -S+1, \dots, +S$

2) The state $|A\rangle$ must have definite value of total spin, $\hat{S}^2 |A\rangle = S(S+1) |A\rangle = 2 |A\rangle$

Thus $|S=1, S_z=1\rangle = |A\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$

Similarly $|S=1, S_z=-1\rangle = |D\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2$

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Situation with $|B\rangle$ and $|C\rangle$ is more complicated because both have $s_z = 0$. and hence generally one can write

$$|S=1, s_z=0\rangle = b|B\rangle + c|C\rangle,$$

where b and c are some coefficients.

An orthogonal combination must describe state with total spin zero

$$|S=0, s_z=0\rangle = -c|B\rangle + b|C\rangle$$

The coefficients b and c are called Clebsch-Gordan coefficients.

How to find them?

$$\left. \begin{aligned} \hat{S}_x &= \hat{S}_{1x} + \hat{S}_{2x} \\ \hat{S}_y &= \hat{S}_{1y} + \hat{S}_{2y} \end{aligned} \right\} \Rightarrow \begin{aligned} \hat{S}_+ &= \hat{S}_x + i\hat{S}_y = \hat{S}_{1+} + \hat{S}_{2+} \\ \hat{S}_- &= \hat{S}_x - i\hat{S}_y = \hat{S}_{1-} + \hat{S}_{2-} \end{aligned}$$

Let us take the state

$|S=1, S_z=1\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2$ and act on this state by the operator \hat{S}_- .

$$\hat{L}_- |L, m\rangle = \sqrt{(L+m)(L-m+1)} |L, m-1\rangle, \text{ see page 117}$$

Therefore

$$\hat{S}_- |1, 1\rangle = \sqrt{(1+1)(1-1+1)} |1, 0\rangle = \sqrt{2} |1, 0\rangle$$

on the other hand

$$\begin{aligned} \hat{S}_- |1, 1\rangle &= (\hat{S}_{1-} + \hat{S}_{2-}) |\uparrow\rangle_1 |\uparrow\rangle_2 = \\ &= (\hat{S}_{1-} |\uparrow\rangle_1) |\uparrow\rangle_2 + |\uparrow\rangle_1 (\hat{S}_{2-} |\uparrow\rangle_2) = \\ &= \sqrt{\left(\frac{1}{2} + \frac{1}{2}\right)\left(\frac{1}{2} - \frac{1}{2} + 1\right)} |\downarrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 \sqrt{\left(\frac{1}{2} + \frac{1}{2}\right)\left(\frac{1}{2} - \frac{1}{2} + 1\right)} |\downarrow\rangle_2 = \\ &= |\downarrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 |\downarrow\rangle_2 \end{aligned}$$

Hence

$$\left[|1, 0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2) \right]$$

The state $|0,0\rangle$ follows from the orthogonality condition

$$\langle 1,0|0,0\rangle = 0$$

hence

$$|0,0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$$

Thus

$$\begin{cases} |1,1\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2 \\ |1,0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2) \\ |1,-1\rangle = |\downarrow\rangle_1 |\downarrow\rangle_2 \end{cases}$$

$$|0,0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$$

Generally adding $\vec{j}_1 + \vec{j}_2$ one gets

$$\vec{J} = \vec{j}_1 + \vec{j}_2$$

triangle rule $\left\{ \begin{array}{l} J_{\max} = j_1 + j_2 \\ J_{\min} = |j_1 - j_2| \end{array} \right.$
 allowed values of J are: $J = J_{\min}, J_{\min} + 1, \dots, J_{\max}$

assignment PHYS 3010

add $\vec{1} + \vec{1/2}$

Identical particles and quantum statistics (222)

Consider two identical particles

2 electrons

2 neutrons

2 photons

2 π^+ mesons

...

$$\Psi = \Psi(\Gamma_1, S_1; \Gamma_2, S_2)$$

Γ_1, S_1 - variables of the 1st particle

Γ_2, S_2 - variables of the 2nd particle

The particles are identical \Rightarrow the state is not changed under permutation

$$\Psi(\Gamma_2, S_2; \Gamma_1, S_1) = R \Psi(\Gamma_1, S_1; \Gamma_2, S_2)$$

R is a coefficient.

Double permutation = 1 \Rightarrow

$$\Rightarrow R^2 = 1 \Rightarrow R = \pm 1.$$

Spin-statistics theorem can be proven in relativistic quantum mechanics:

Particles with integer spin have $R = 1$, they are called bosons (Bose-Einstein statistics).

Particles with half-integer spin have $R = -1$, they are called fermions (Fermi-Dirac statistics).

Comment: Do not mix permutation with parity, these are different operations

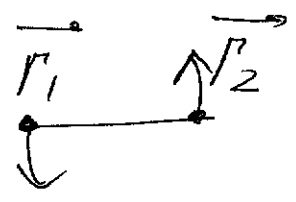
$$\Psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2) \xrightarrow{\text{permutation}} \Psi(\vec{r}_2, \vec{s}_2; \vec{r}_1, \vec{s}_1)$$

$$\Psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2) \xrightarrow{\text{space reflection}} \Psi(-\vec{r}_1, \vec{s}_1; -\vec{r}_2, \vec{s}_2)$$

Example: Statistics influence rotational spectra of diatomic molecules.

Consider rotational spectrum of the O_2 molecule consisting of two ^{16}O isotopes of carbon.

A ^{12}C nucleus has spin = 0 \Rightarrow it is a boson.



spin wave functions.

$$\psi(1,2) = \chi(|\vec{r}_1 - \vec{r}_2|) Y_{em}(\vec{r}_1 - \vec{r}_2) \psi_1 \psi_2$$

$$\text{spin} = 0 \Rightarrow \psi_1 = \psi_2 = 1.$$

permutation

$$\begin{aligned} \psi(2,1) &= \chi(|\vec{r}_2 - \vec{r}_1|) Y_{em}(\vec{r}_2 - \vec{r}_1) \psi_2 \psi_1 = \\ &= (-1)^l \chi(|\vec{r}_1 - \vec{r}_2|) Y_{em}(\vec{r}_1 - \vec{r}_2) \psi_1 \psi_2 = \\ &= (-1)^l \psi(1,2) \end{aligned}$$

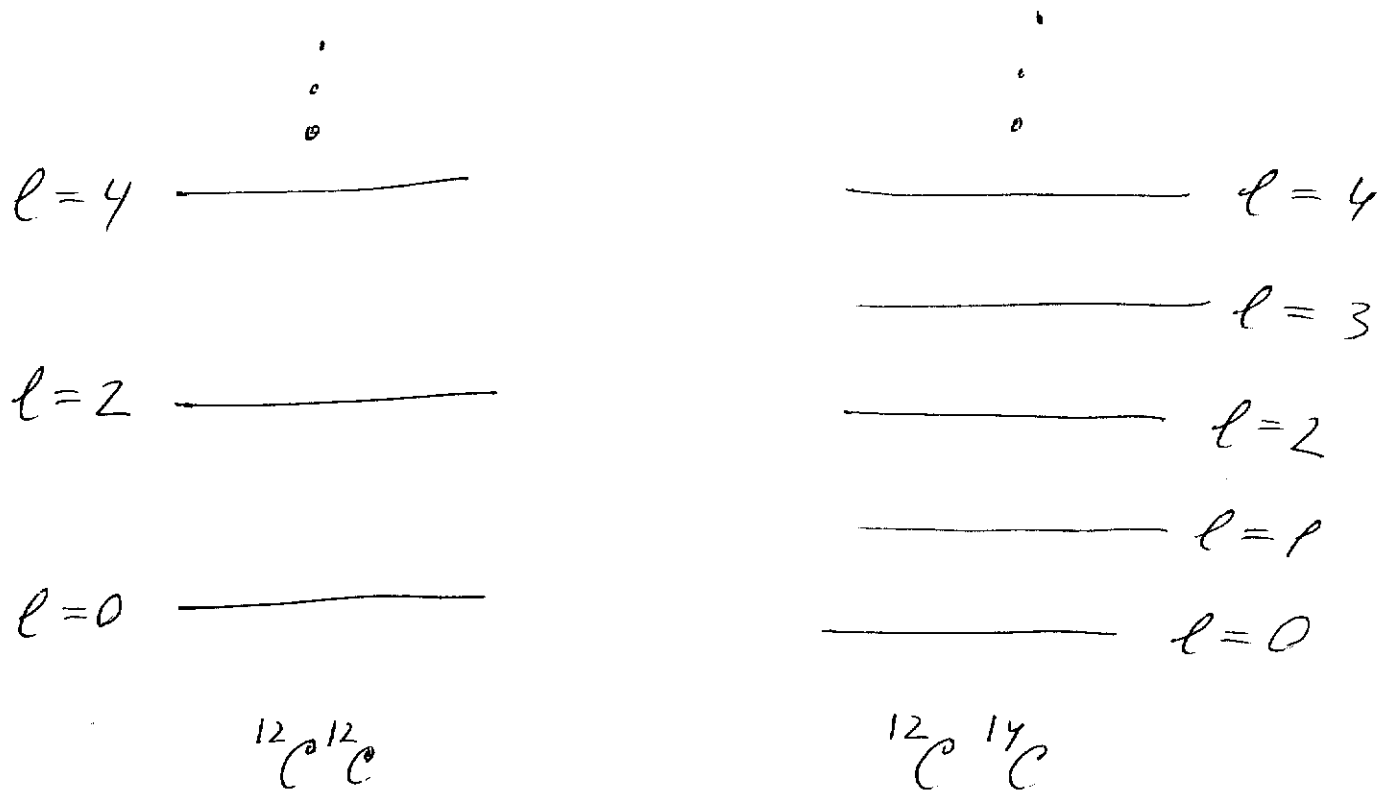
I've used the relation $Y_{em}(-\vec{r}) = (-1)^l Y_{em}$,

see page 129

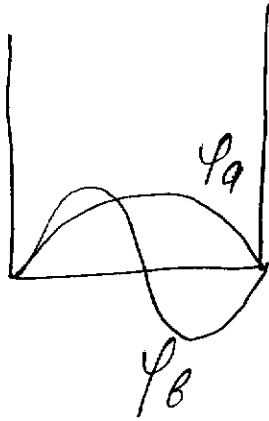
Requirement of Bose statistics:
 $\psi(2, 1) = \psi(1, 2)$

Hence only even values of l are allowed in the rotational spectrum of C_2 consisting of two ^{12}C isotopes.

If we take two different isotops, say $^{12}C^{13}C$ or $^{12}C^{14}C$ the all values of l are allowed.



Two fermions in a box



ψ_a and ψ_b are single particle states.

non-interacting

Let us put two electrons with parallel spins in the box.

requirement of Fermi statistics:

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

Therefore

$$\psi(1,2) = A[\psi_a(r_1)\psi_b(r_2) - \psi_a(r_2)\psi_b(r_1)] \uparrow_1 \uparrow_2$$

$$\text{if } \psi_a = \psi_b \Rightarrow \psi = 0$$

Thus, one cannot put two fermions in the same single-particle quantum state

This is Pauli exclusion principle

If spins of the electrons are opposite then the single particle states are different, ψ_a and ψ_b . Such two-electron state is possible.

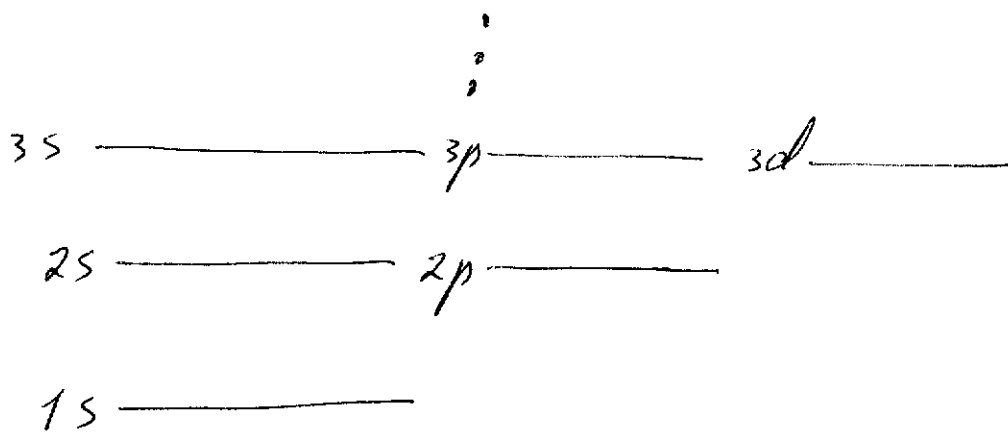
$$\Psi(1,2) = \psi_a(r_1)\psi_b(r_2) \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle_1 |\downarrow\uparrow\rangle_2 - |\downarrow\uparrow\rangle_1 |\uparrow\downarrow\rangle_2 \right)$$

Multi-electron atoms and periodic table

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{ Periodic table is a consequence of the
{ Pauli exclusion principle.

Single electron levels in Coulomb field



Filling of the single-electron states.

1s - Hydrogen, H

1s² - Helium, He closed shell.

1s²2s - Lithium, Li

1s²2s² - Beryllium, Be closed shell

1s²2s²2p - Boron, B

1s²2s²2p² - Carbon, C

1s²2s²2p³ - Nitrogen, N

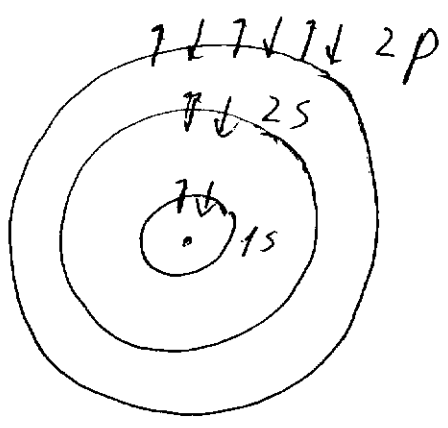
1s²2s²2p⁴ - Oxygen, O

1s²2s²2p⁵ - Fluorine, F

1s²2s²2p⁶ - Neon, Ne closed shell.

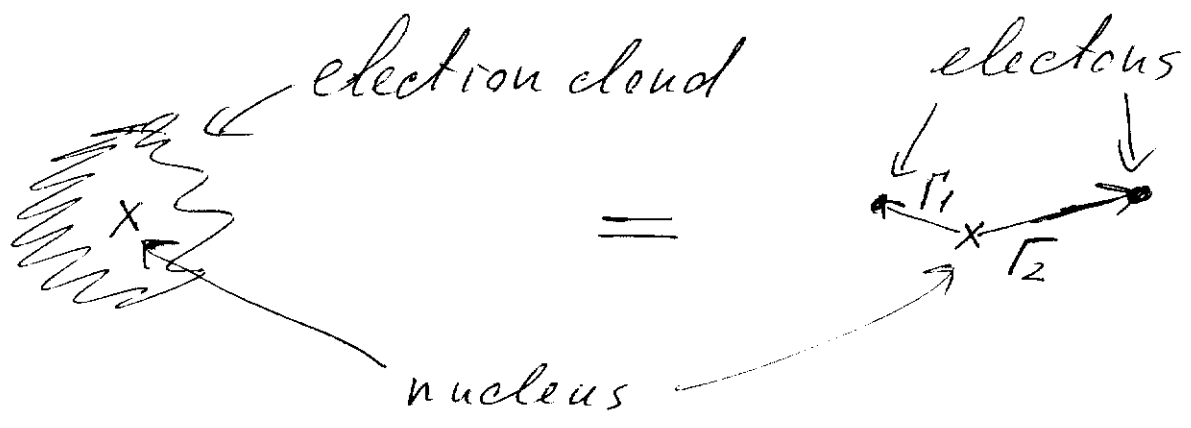
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Effective self consistent potential.



Why 2s state is filled before 2p?
Naively one shall expect simultaneous filling.

Consider He atom as an example.



$$\hat{H} = \frac{\hat{p}_1^2}{2m} + \frac{\hat{p}_2^2}{2m} - \frac{2e^2}{4\pi\epsilon_0 r_1} - \frac{2e^2}{4\pi\epsilon_0 r_2} + \frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}$$

$$\hat{U}\Psi(\vec{r}_1, \vec{r}_2) = E\Psi(\vec{r}_1, \vec{r}_2)$$

$$\langle r_1 \rangle = \int r_1 |\Psi|^2 d^3r_1 d^3r_2$$

$$\langle r_2 \rangle = \int r_2 |\Psi|^2 d^3r_1 d^3r_2$$

$$\langle r_1 \rangle = \langle r_2 \rangle \sim a_B$$

Let us assume that wave functions of electrons are uncorrelated

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

This is called mean field or selfconsistent field approximation.

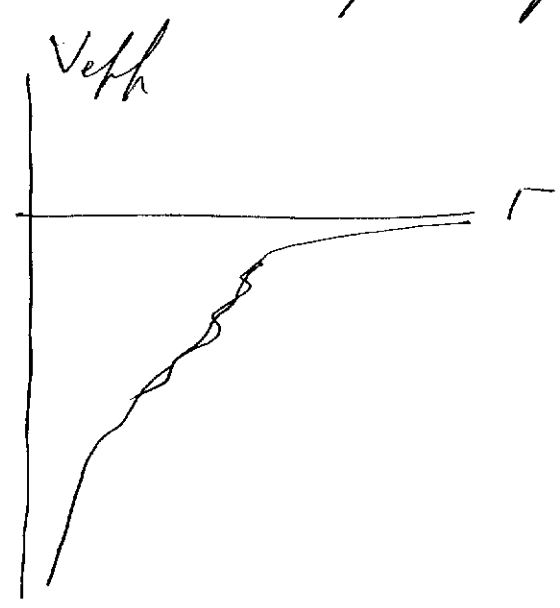
In this approximation the effective potential acting of the 1st electron is

$$V_{eff}(r_1) = \int \left[-\frac{2e^2}{4\pi\epsilon_0 r_1} + \frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|} \right] |\psi(r_2)|^2 d^3r_2$$

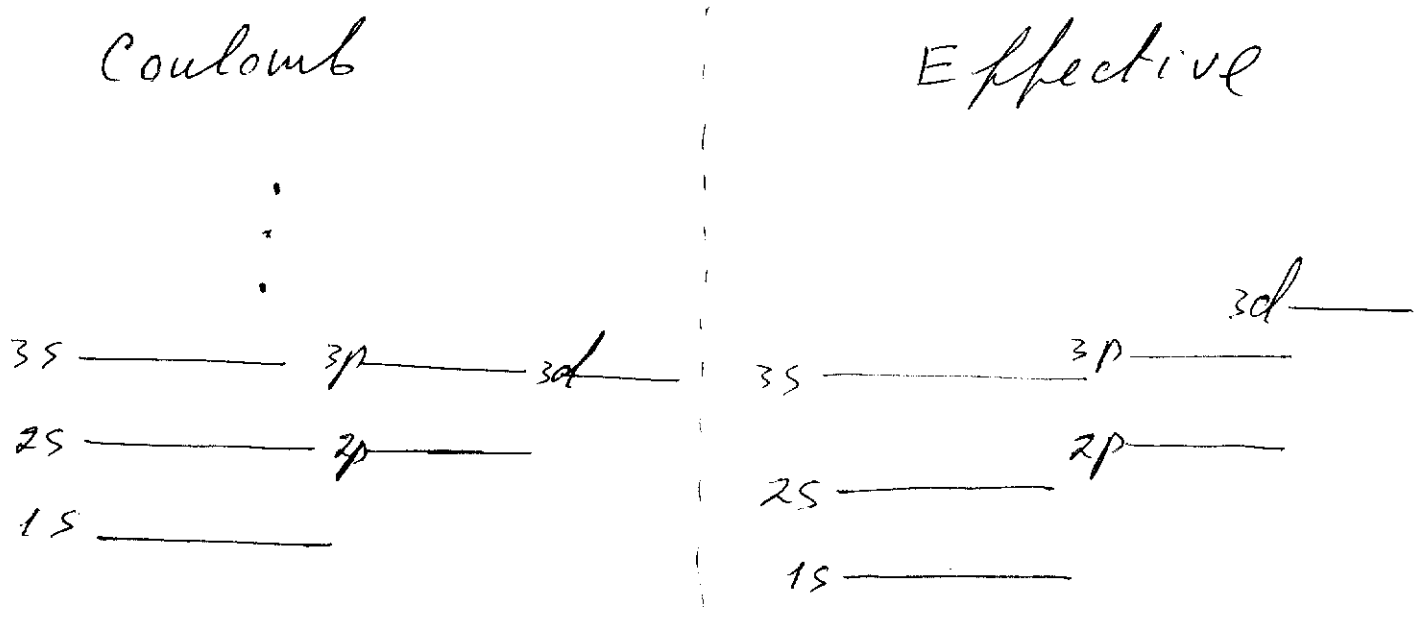
$$r_1 \ll a_B : V_{eff}(r_1) = - \frac{2e^2}{4\pi\epsilon_0 r_1}$$

$$r_1 \gg a_B : V_{eff}(r_1) = - \frac{e^2}{4\pi\epsilon_0 r_1}$$

Thus the effective potential is different from that of the pointlike nucleus.



Therefore degeneracy of states with the same principal quantum numbers is lifted



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This is why 2s is filled before 2p,
3s before 3p, etc.

Spin-orbit interaction.

The interaction is due to relativistic effects

$$\hat{H}_{es} = a(r) \vec{l} \cdot \vec{s}, \text{ where } a(r) \text{ is some function}$$

Hydrogen atom

$$\hat{H} = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} + \hat{H}_{es} \quad \downarrow \text{very small relativistic correction}$$

Because of \hat{H}_{es} the angular momenta \vec{l} and \vec{s} are not conserved. Only total angular momentum $\vec{j} = \vec{l} + \vec{s}$ is conserved

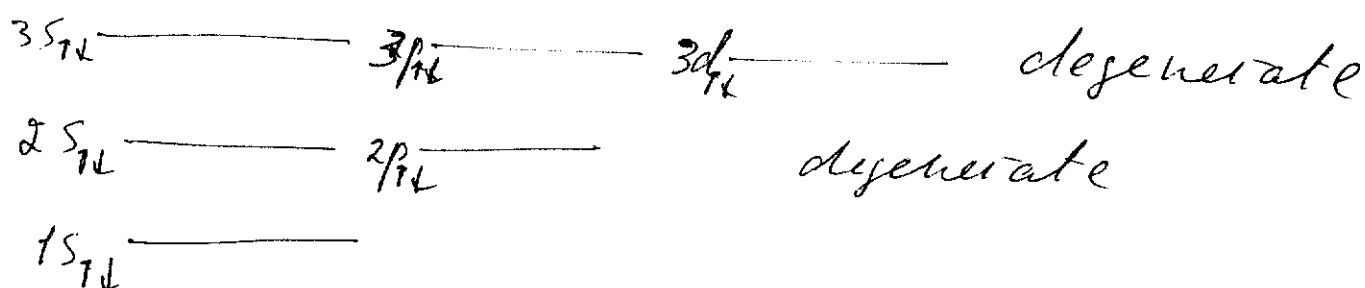
For $l=0$, $j = \frac{1}{2}$

For $l=1$ j takes values

$$j = \begin{cases} 1 + \frac{1}{2} = \frac{3}{2} \\ 1 - \frac{1}{2} = \frac{1}{2} \end{cases}$$

follows from addition of angular momenta (assignment)

Structure of Hydrogen levels without account of \hat{H}_{es}



Structure of Hydrogen levels with account of \hat{H}_{es} (real Hydrogen atom)

