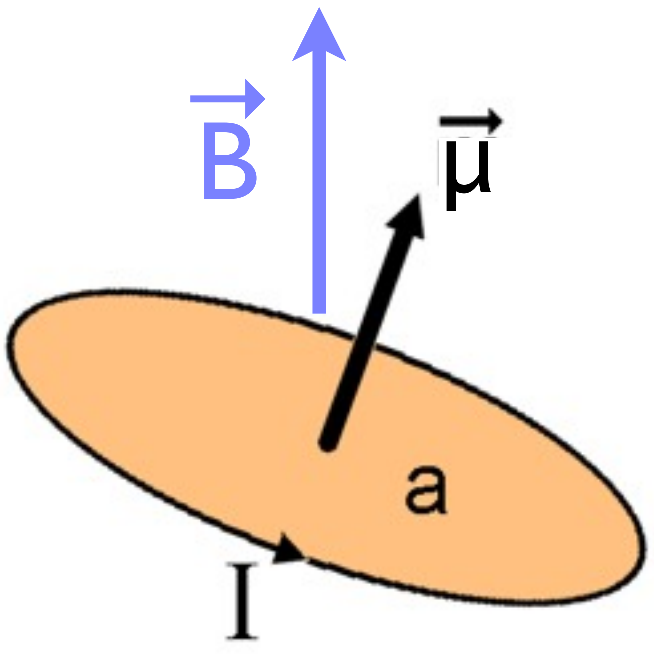
Classical Electron Spin

$\vec{s}$ =spin =intrinsic angular momentum

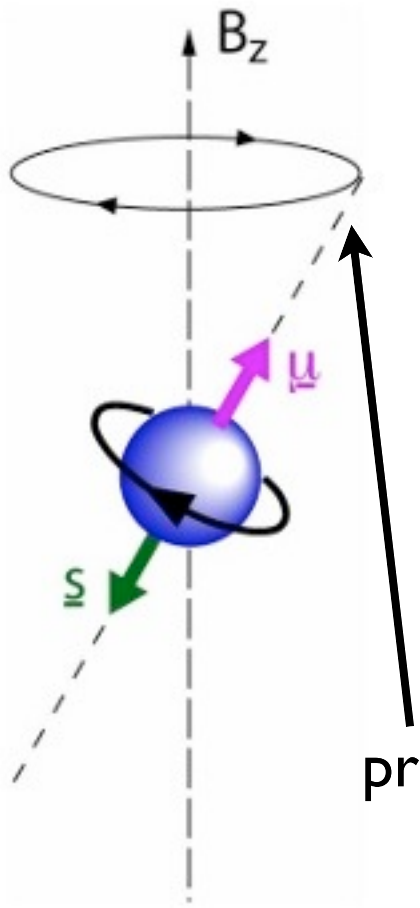
Moving charges create magnetic fields.

$\vec{\mu}$ =magnetic moment

$$\boxed{\vec{\mu} \propto \vec{S}}$$



current loop



spinning electron

spin selection

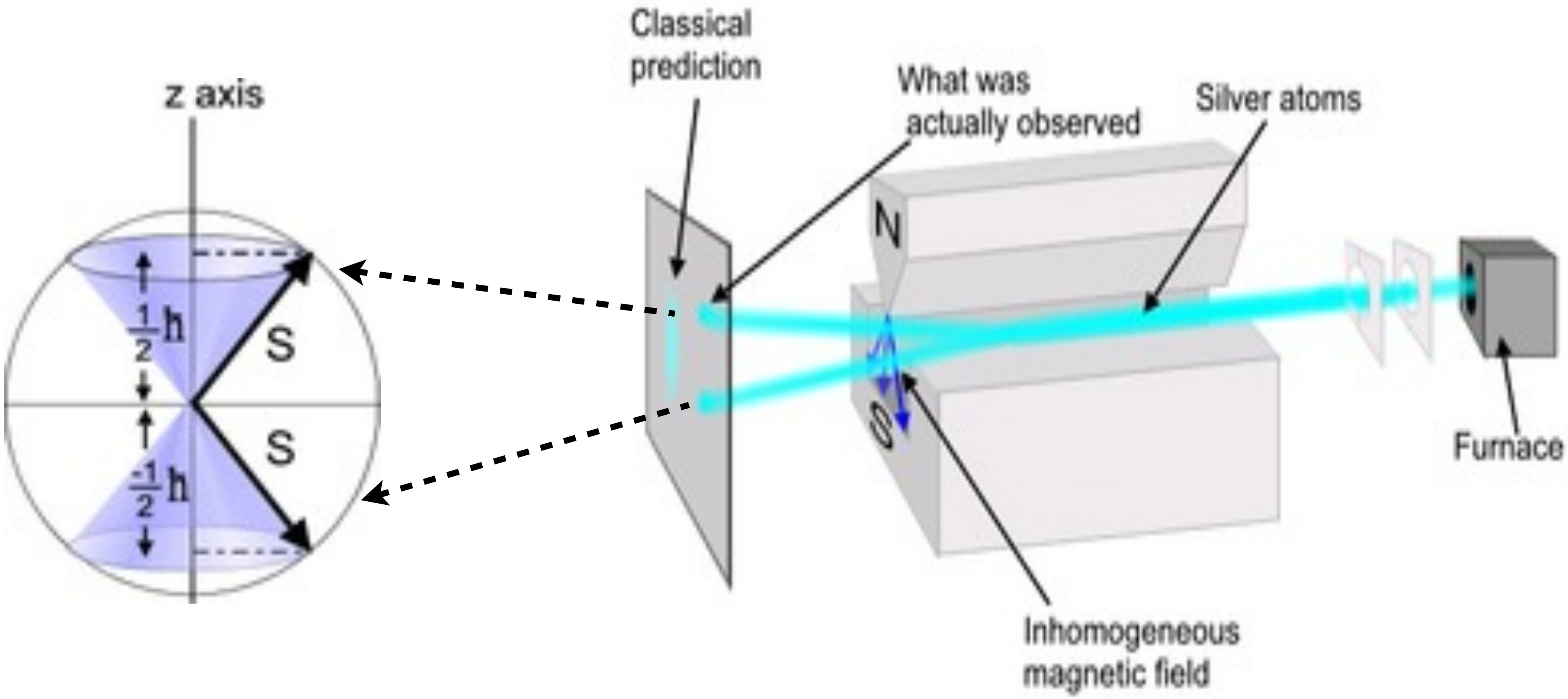
$\vec{F} = -\vec{\nabla} U$

$$\boxed{\begin{array}{l} U = -\vec{\mu} \cdot \vec{B} \\ \vec{\tau} = \mu \times \vec{B} \end{array}}$$

precession

Images: http://www.st-andrews.ac.uk
http://www.phys.au.dk

Quantum Electron Spin

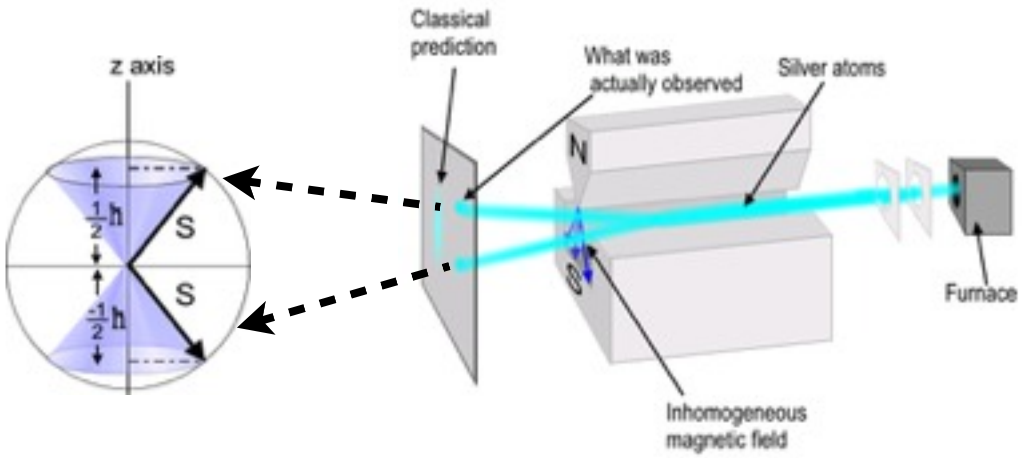


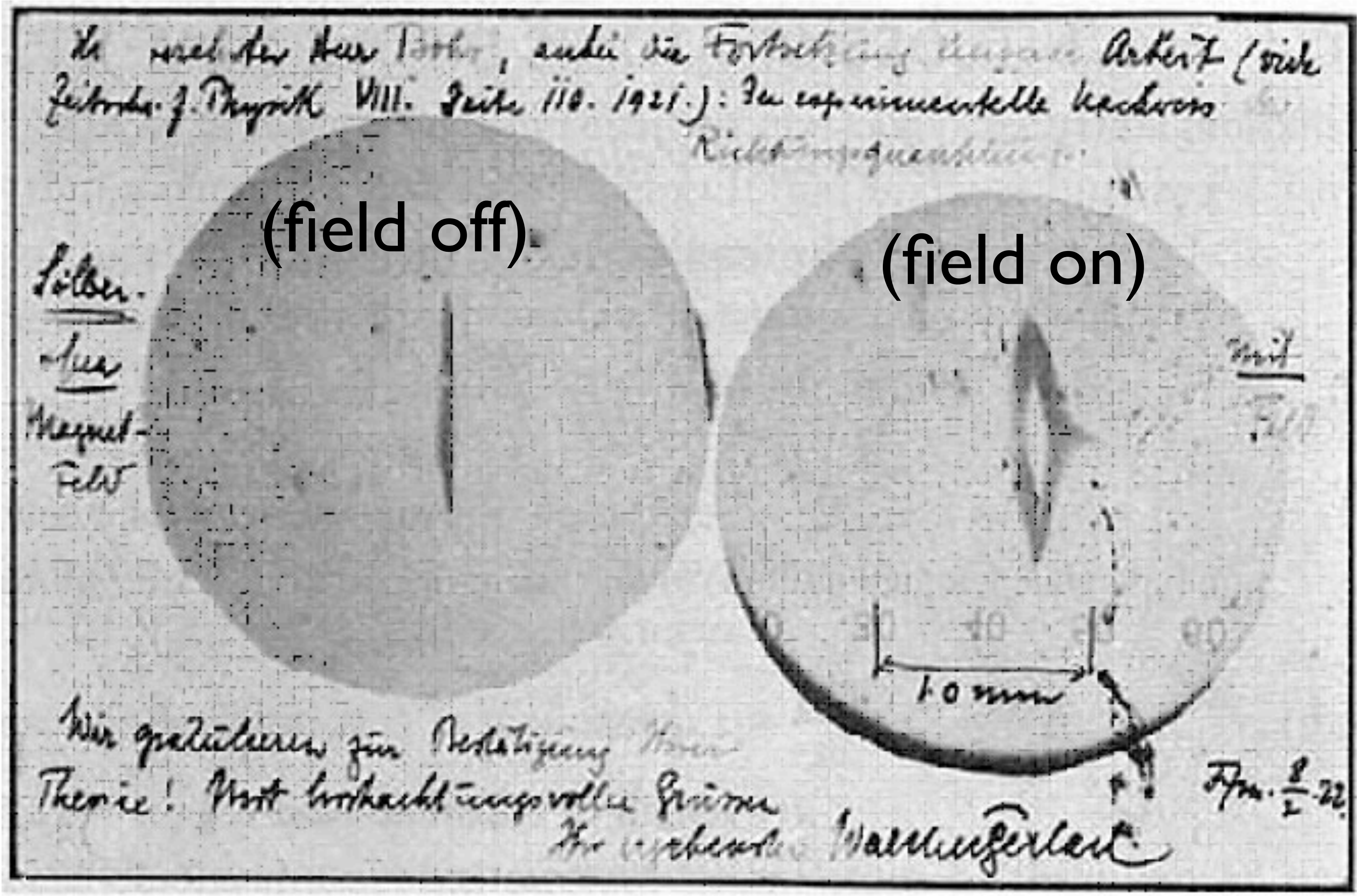
Stern-Gerlach Experiment (1922)

- Spin angular momentum quantized: ħ/2!

Images: http://en.wikipedia.org

Stern-Gerlach Experiment





Hochverehrter Herr Bohr, anbei die Fortsetzung unserer Arbeit (vergl. Zeitschr. f. Physik VIII. Seite 110. 1921.): den experimentellen Nachweis der Richtungsquantelung.

Silber. Ohne Magnet-Feld

Mit Feld

Wir gratulieren zur Bestätigung Ihrer Theorie! Mit hochachtungsvollen Grüssen

Ihr ergebenster Walther Gerlach

Ffm. 8/2.22

Gerlach's postcard, dated 8 February 1922, to Niels Bohr. It shows a photograph of the beam splitting, with the message, in translation: "Attached [is] the experimental proof of directional quantization. We congratulate [you] on the confirmation of your theory." (Physics Today December 2003)

Otto Stern
1888-1969
Nobel Prize 1943

Walter Gerlach
1889-1979

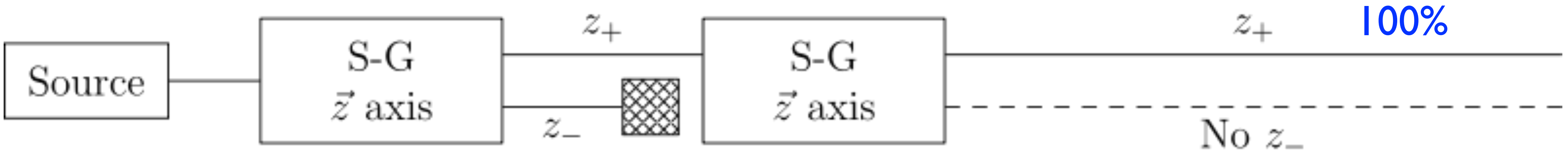
Images: http://en.wikipedia.org

Concept Test

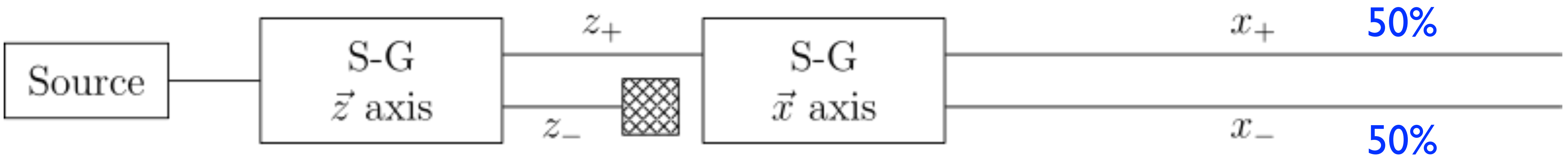
- A beam of unpolarized silver atoms is passed through a x-axis Stern-Gerlach device. On the screen one finds
  - One spot
  - [✓ Two spots]
  - Three spots
  - No spots

Multiple Analyzers

consistency



s_x and s_z different



definite s_x: indefinite s_z

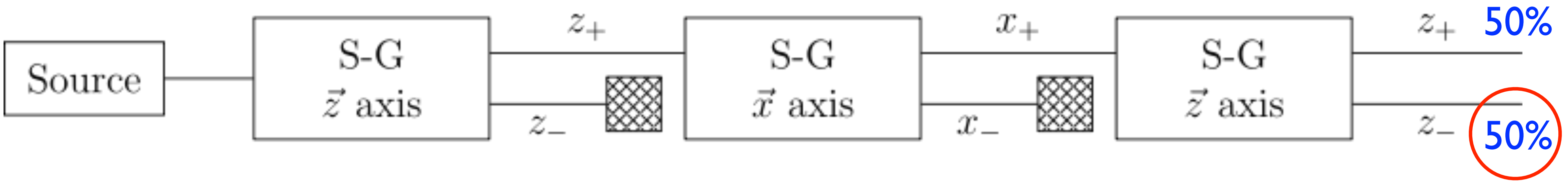
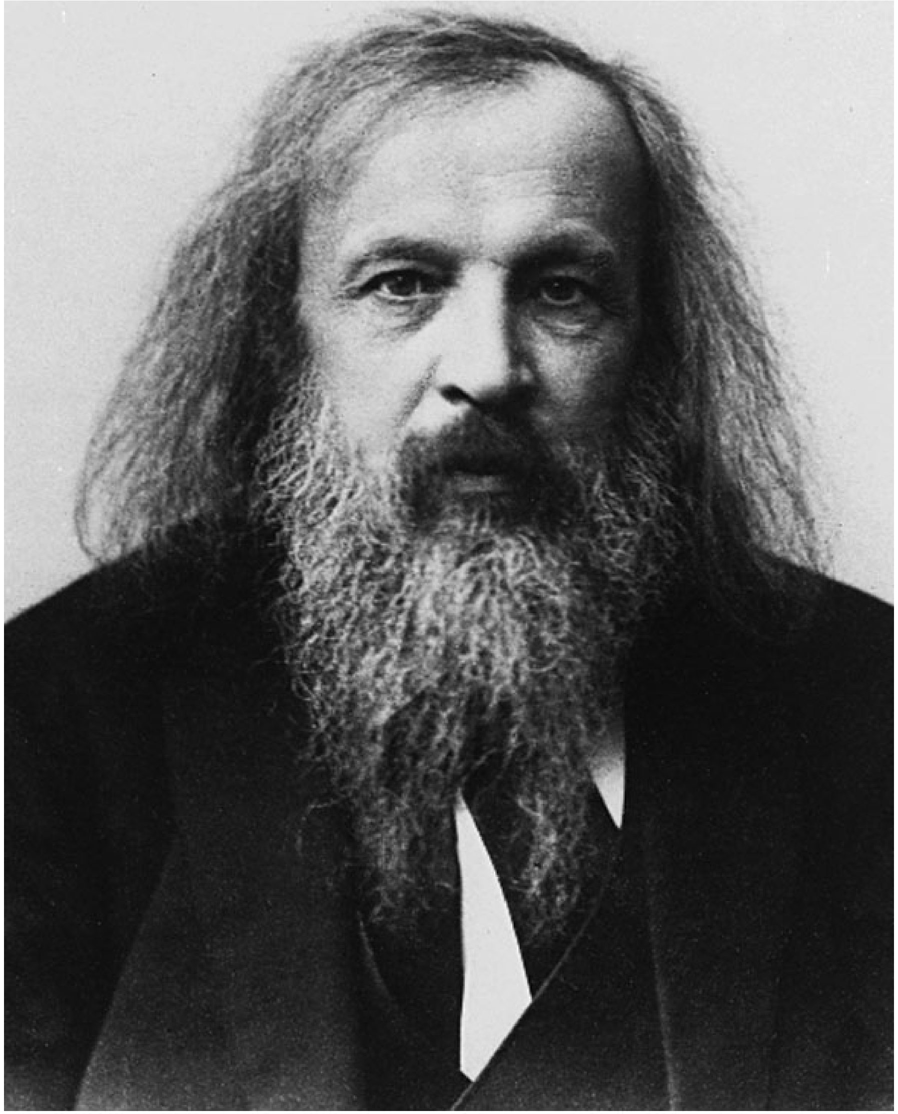


Image: http://en.wikipedia.org

Atomic Structure



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The first systematic organization of the chemical elements was made by Dimitri Mendeleev (1834-1907). He organized the elements using atomic weight and was able to predict undiscovered elements.

A qualitative understanding of Mendeleev's empirical periodic table was possible when the Schroedinger treatment of hydrogen, including electron spin, became available. The explanation uses Wolfgang Paul's exclusion principle

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Pauli exculsion principle:
No two electrons in an atom may have the same set of quantum numbers (n, ℓ, m_ℓ, m_s).

The ordering in the periodic table can be understood using these two rules:

1. The electrons in an atom tend to occupy the lowest energy levels available to them.
2. Only one electron can be in a state with a given (complete) set of quantum numbers (Pauli principle).

For hydrogen, the complete set of quantum numbers is (1,0,0, ±1/2). Since these states have equal energy, either will do for the ground state.

For helium, the two electrons must have (1,0,0,1/2) and (1,0,0,-1/2) by the Pauli principle. The actual spin state in He is

$$\Xi(1,2) = \frac{1}{\sqrt{2}}\left(\chi_1^+\chi_2^- - \chi_1^-\chi_2^+\right) = -\Xi(2,1).$$

The complete wave function for He is

$$\psi(\vec{r}_1, \vec{r}_2) = \frac{1}{4\pi} R_{10}(r_1) R_{10}(r_2) \Xi(1,2).$$

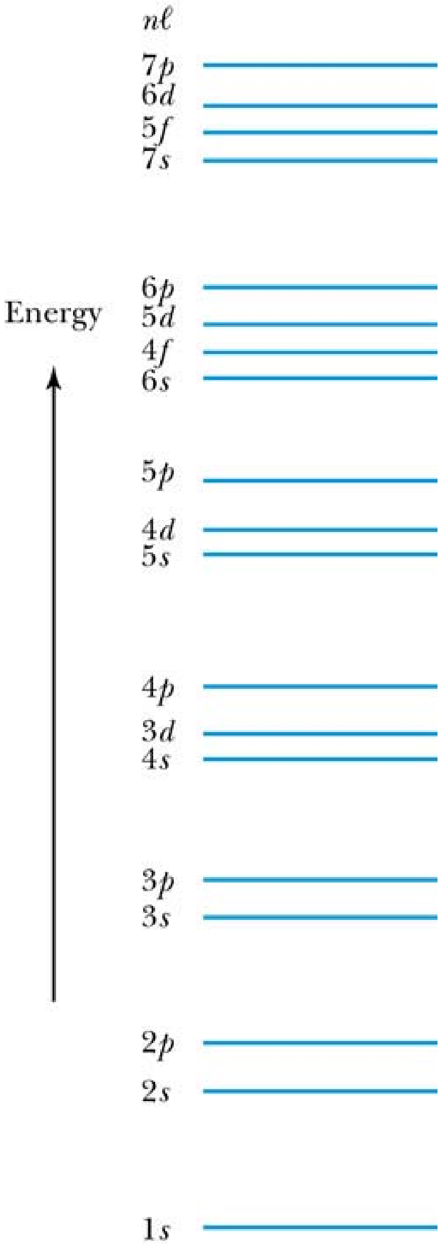
Notice that the wave function changes sign if 1 and 2 are interchanged.

Because the energies of hydrogen are so degenerate, it is convenient to define <u>shells</u>.

$$\begin{array}{lccccc} n & = & 1 & 2 & 3 & 4 & \ldots \\ \text{Letter} & = & K & L & M & N & \ldots \end{array}$$

The K shell consists of the two 1s levels denoted $1s^1$ and $1s^2$. The L shell has $2s^1$, $2s^2$ as well as $2p^1$, $2p^2$, ..., $2p^6$. The 2s and 2p level sets are <u>subshells</u> of the L shell.

In describing the filling of the shells, we can ignore m_l and m_s because their values don't affect the atom's energy.



The shells fill as indicated in the Figure. Note that the 4s subshell fills before the 3d subshell. This is because all s states are finite at r = 0 and their Coulomb energy is lower due to the attractive interaction with the nucleus.

According to this scheme, the electronic structure of K (Z = 19) is

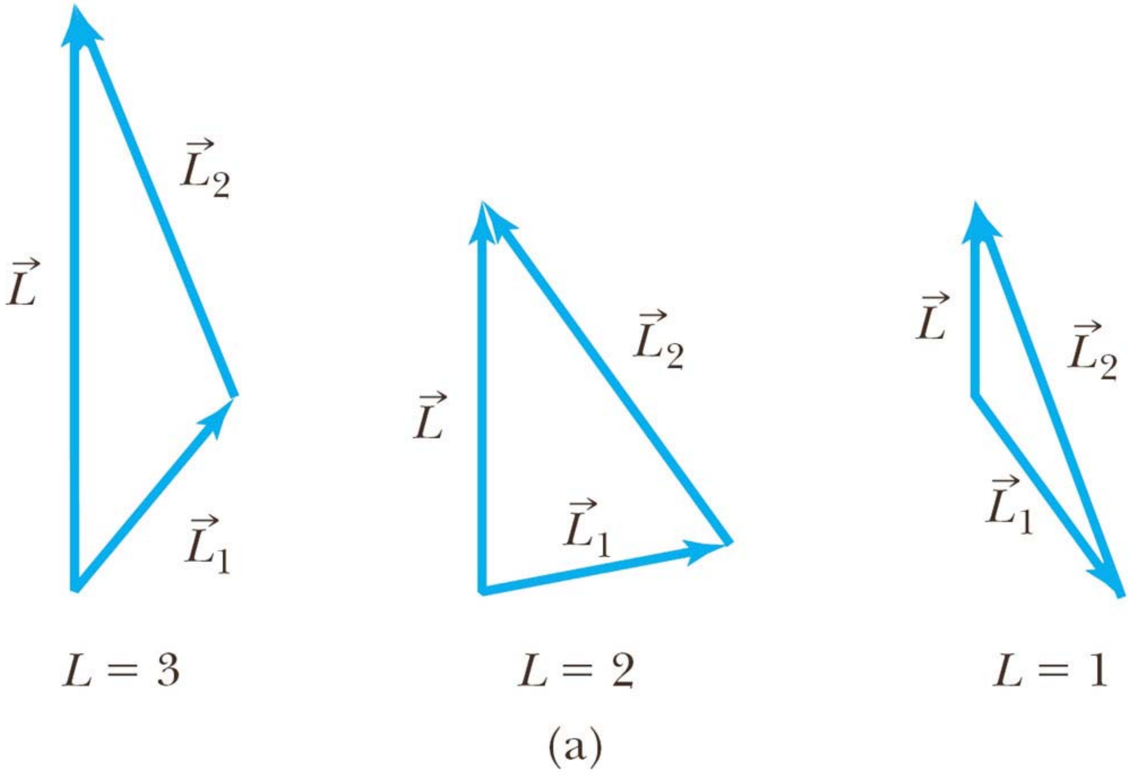
$$1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^1.$$

For atomic ground state electron configurations, we can get away with considering only the electrons outside the last closed shell. For the case of two active electrons, we have two angular momenta and two spins. The most common way to treat this system is by using spin-orbit (L-S) coupling.

First, we add the four spin states to get

$$\begin{aligned}
\Xi_1 &= \frac{1}{\sqrt{2}}\left(\chi_1^+\chi_2^- - \chi_1^-\chi_2^+\right) \ \text{(singlet)} \\
\Xi_3^{m_s} &= \begin{cases} \chi_1^+\chi_2^+ \\ \frac{1}{\sqrt{2}}\left(\chi_1^+\chi_2^- + \chi_1^-\chi_2^+\right) \ \text{(triplet)} \\ \chi_1^-\chi_2^- \end{cases}
\end{aligned}$$

The singlet combination has spin 0 and the triplet combination has spin 1. Next, the two orbital angular momenta are added.



$$\vec{L} = \vec{L}_1 + \vec{L}_2,\ \ell_1 = 1,\ \ell_2 = 2,\ \ell = 1, 2, 3.$$

Once the possible L's and S's are determined, the two sets are combined into J values using

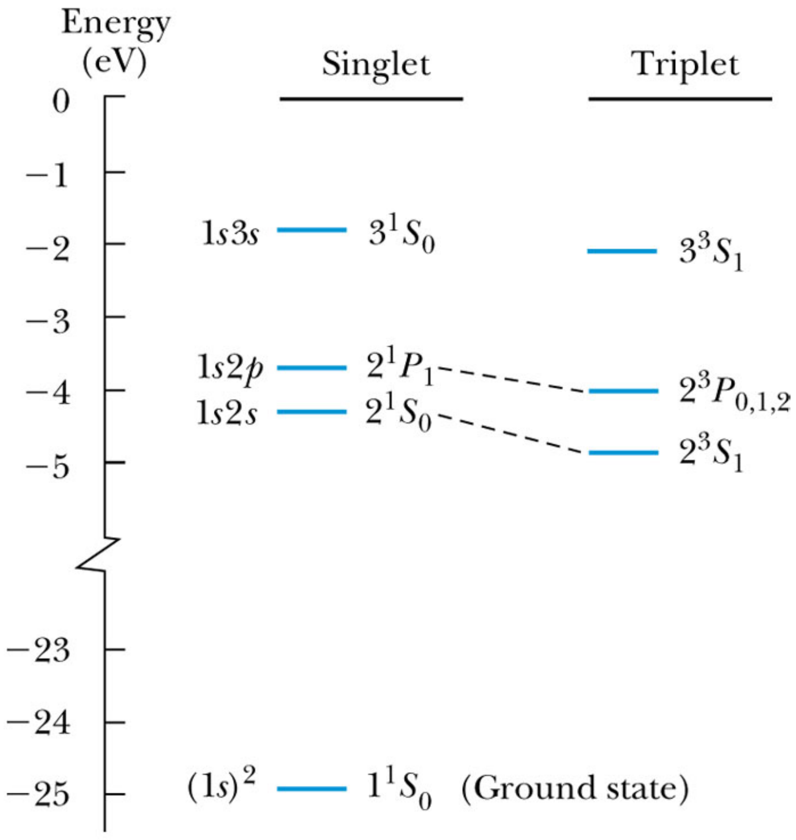
$$\vec{J} = \vec{L} + \vec{S},\ j = |\ell - s|, \ldots, \ell + s.$$

The ground state is determined using the rules (Hund)

Rule 1. The total spin angular momentum S should be maximized to the extent possible without violating the Pauli principle.
Rule 2. Insofar as rule 1 is not violated, L should be maximized.
Rule 3. For atoms having subshells less than half full, J should be minimized.

For He in the first excited state

$$\begin{aligned} \ell_1 &= 0, \quad \ell_2 = 0, \quad \ell = 0 \\ s_1 &= 1/2, \; s_2 = 1/2, \; s = 0, 1 \\ j &= 0, 1 \end{aligned}$$



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There are two combinations of L and S

$$^1S_0 \text{ and } {}^3S_1.$$

Notice that the triplet state has the lowest energy.

For the $2s^1 2p^1$ level in He, $\ell = 1$ and $s = 0,1$. Adding the singlet state ($S = 0$) to $\ell = 1$ gives $j = 1$ and adding the triplet state ($s = 1$) to $\ell = 1$ gives $j = 0,1,2$. The resulting states are

$$^1P_1,\ ^3P_2,\ ^3P_1,\ ^3P_0.$$

In this case, the state with lowest energy is the $j = 0$ triplet state.