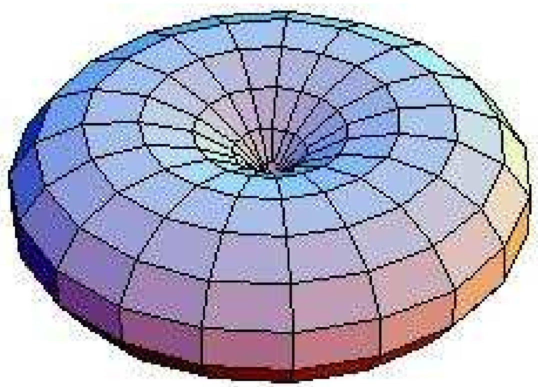
Wave functions with properties that resemble Bohr orbits

$$\Phi(r,\vartheta,\varphi) = R_{n\,n-1}(r)Y_{n-1,\pm(n-1)}(\vartheta,\varphi) \propto e^{-\frac{1}{n a_0}r}\left(r\sin\vartheta\right)^{n-1} e^{\pm i(n-1)\varphi}$$

$$\rho(r) = 4\pi r^2 \,|\,\Phi\,|^2 \propto r^{2n} e^{-\frac{2}{n a_0}r} \quad \rightarrow \quad 2n\, r_{\max}^{2n-1} - \frac{2}{n a_0} r_{\max}^{2n} = 0$$

$$l = n-1, \quad m = \pm l \quad \rightarrow \quad r_{\max} = \frac{1}{n^2} a_0$$



$$|\,\Phi\,|^2 = const.$$

$$E_n = -\frac{1}{n^2}\frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2} = \underbrace{\frac{1}{2}mv^2}_{-E_n} - \underbrace{\frac{e^2}{4\pi\varepsilon_0 r}}_{-2E_n}$$

$$v = \sqrt{\frac{-2E_n}{m}}\,, \quad r = \frac{1}{-E_n}\frac{e^2}{8\pi\varepsilon_0} = \frac{1}{-2E_n}\sqrt{\frac{-E_n n^2\, 2\hbar^2}{m}}$$

$$\omega_{rot} = \frac{v}{r} = \sqrt{\frac{-2E_n}{m}}\sqrt{\frac{-2E_n m}{n^2\hbar^2}} = \frac{2E_1}{n^3\hbar}$$

$$\Psi(\vec{x},t) = \Phi(\vec{x})e^{-i\frac{E_n}{\hbar}t} \propto e^{-\frac{1}{n a_0}r}\left(r\sin\vartheta\right)^{n-1} e^{i[(n-1)\varphi - \frac{E_1}{n^2\hbar}t]}$$

$$\dot{\varphi}_{group} = \frac{\partial}{\partial n}\left(\frac{E_1}{n^2\hbar}\right) = -\frac{2E_1}{n^3\hbar} = \omega_{rot}$$

Georg.Hoffstaetter@Cornell.edu

Spin-Orbit coupling energy

$S_z = \pm\hbar/2$ but the magnetic moment is $\mu_z = \pm\frac{q}{2m}\hbar = \mu_B = g\, m_s \mu_B$ with $g \approx 2$

Classical picture: The magnetic moment of the electron experiences in its rest frame a magnetic field due to the circling proton.

Assuming the circular motion of a Bohr atom:

$$B_z = \mu_0 \frac{1}{2r} I = \mu_0 \frac{1}{2r}\frac{qv}{2\pi r} = \mu_0 \frac{q}{4\pi m r^3} L_z = \frac{\mu_0}{2\pi r^3}\mu_B m \approx \frac{2\cdot 10^{-7} 9.27\cdot 10^{-24}}{10^{-30}} m \approx m \cdot 2T$$

Order of magnitude estimate of spin-orbit coupling (fine structure of the spectrum):

$$\Delta E = -\vec{\mu}\cdot\vec{B} = \pm\mu_B B \approx \pm 9\cdot 10^{-24}\,\frac{J}{T}\,2T = \pm\frac{1.8\cdot 10^{-23}}{1.6\cdot 10^{-19}} eV \approx \pm 0.1 meV$$

Reality:

Fine structure splitting of Hydrogen l=1 line: 0.09meV

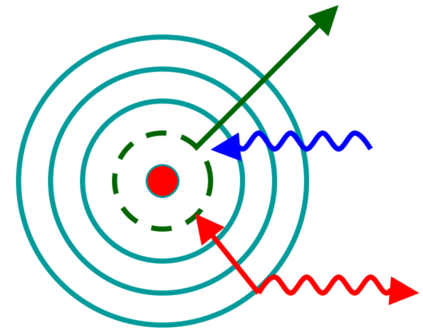
Fine structure splitting of Sodium l=1 line: 2.1meV

The energy of states with l=0 do not change due to spin orbit coupling, since no magnetic field is produced for l=0.

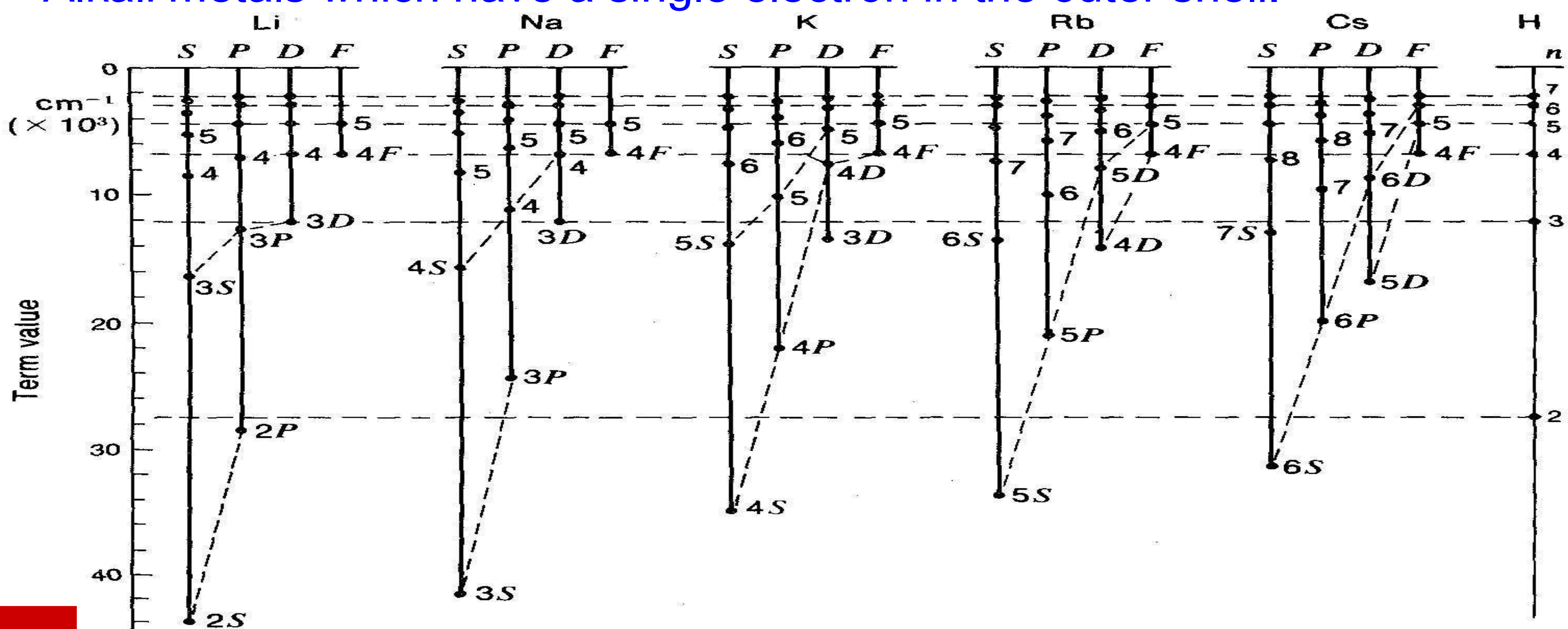
Georg.Hoffstaetter@Cornell.edu

Hydrogen-like systems

- Highly ionized atoms, with only one electron left: $E_n \propto Z^2$
- Energy levels of innermost electrons, which experience a nearly unshielded potential. These lines become visible when a innermost electron (K-electron) has been expelled.



- Alkali metals which have a single electron in the outer shell.



Energy levels of Alkali atoms versus Hydrogen

Georg.Hoffstaetter@Cornell.edu