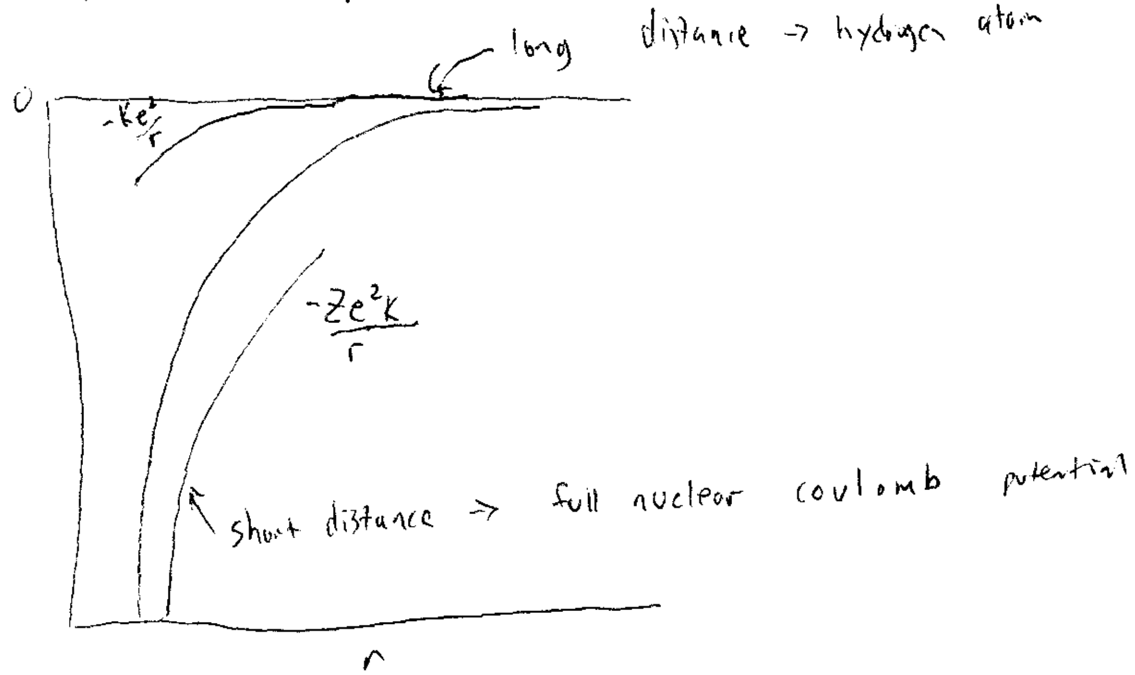
Multi-electron Atoms

Independent particle Approximation

electrons don't feel each other, just a modified central potential $\sim \frac{1}{r}$



potential is similar to hydrogen so we can still use quantum numbers

n, l, m_l, m_s

Pauli Exclusion principle

only one electron can have a set of quantum numbers

n, l, m_l, m_s

Wave function symmetry

Schrödinger equation for two electron atom

$$-\frac{\hbar^2}{2m}\left[\nabla_1^2\psi(\vec{r}_1,\vec{r}_2)+\nabla_2^2\psi(\vec{r}_1,\vec{r}_2)\right]+V(\vec{r}_1,\vec{r}_2)\psi(\vec{r}_1,\vec{r}_2)=E\psi(\vec{r}_1,\vec{r}_2)$$

$$|\psi(\vec{r}_1,\vec{r}_2)|^2=|\psi(\vec{r}_2,\vec{r}_1)|^2$$

$$\psi_S(\vec{r}_1,\vec{r}_2)=\psi_S(\vec{r}_2,\vec{r}_1) \quad \text{- symmetric}$$

$$\psi_A(\vec{r}_1,\vec{r}_2)=\psi_A(\vec{r}_2,\vec{r}_1) \quad \text{- anti-symmetric}$$

$$\vec{a}=(n,\ell,m_\ell,m_s) \quad \text{- electron 1}$$

$$\vec{b}=(n,\ell,m_\ell,m_s) \quad \text{- electron 2}$$

$$\psi_S(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left[\psi_{\vec{a}}(\vec{r}_1)\psi_{\vec{b}}(\vec{r}_2)+\psi_{\vec{b}}(\vec{r}_1)\psi_{\vec{a}}(\vec{r}_2)\right]$$

$$\psi_A(\vec{r}_1,\vec{r}_2)=\frac{1}{\sqrt{2}}\left[\psi_{\vec{a}}(\vec{r}_1)\psi_{\vec{b}}(\vec{r}_2)-\psi_{\vec{b}}(\vec{r}_1)\psi_{\vec{a}}(\vec{r}_2)\right]$$

if $\vec{a}=\vec{b}$ $\quad \psi_A=0$

half integer spin particles must be written with anti-symmetric wave functions - fermions

Particle conservation doesn't allow $\vec{a}=\vec{b}$ for fermions

electron - $s=\frac{1}{2}$

shell structure

N_n - number of possible electrons with principle quantum number 'n'

$$N_n = 2 \sum_{l=0}^{n-1} (2l+1)$$

↑ number of possible m_l values

$$= 2n^2$$

electrons with same 'n' form a shell

electrons with same l form a subshell

n	shell	# possible e^-	configuration
1	K	2	$1s^2$
2	L	8	$2s^2 2p^6$
3	M	18	$3s^2 3p^6 3d^{10}$
4	N	32	$4s^2 4p^6 4d^{10} 4f^{14}$

Energy Dependence on ℓ

$$E_{1s} \approx (Z-1)^2 (-13.6\ eV)$$

↑ shielded by other electron

$$E_{2s} \approx (Z-2)^2 (-3.4\ eV)$$

↑ shielded by two 1s electrons

2s electrons are closer to the nucleus than 2p electrons. They feel less shielding

$$E_{2s} < E_{2p}$$

and

$$E_{3s} < E_{3p} < E_{3d}$$