Ionization Energy

- amount of energy needed to remove one electron

\[ E(\text{eV}) \]

filled shells, subshells shield nuclear potential

Spin- Spin Coupling

\[ s = \frac{1}{2} \]

for two electrons \( s' = s_1 + s_2 \)

\[ s = \sqrt{s(s+1)} \frac{1}{\hbar} \]

\( s = 0, 1 \)

electrons with some spin are "pushed" apart by Pauli exclusion principle, lowering energy.
Orbital - orbital coupling

\[ L = L_1 + L_2 \]
\[ l = |l_1 - l_2| \ldots l_1 + l_2 \]
\[ L = \sqrt{l(l+1)} \hbar \]

Larger \( l \) values correspond to states where electrons are further apart. This gives lower energy for larger \( l \).

Spin - orbit coupling

\[ J = L + S \]
\[ j = |l-s| \ldots l+s \]

Small compared to spin - spin, orbital - orbital

Consider 2 electrons in 2p state

Wave function must be anti-symmetric from Pauli exclusion principle

Write \( \Psi_{\text{total}} = \Psi_{\text{space}} \Psi_{\text{spin}} \)

\[ \Psi_A = (\Psi_{\text{space}})_A (\Psi_{\text{spin}})_S \]

or \[ \Psi_A = (\Psi_{\text{space}})_S (\Psi_{\text{spin}})_A \]

\( S = 1 \) - symmetric

\( S = 0 \) - anti-symmetric
States with $\ell$ odd - anti-symmetric
$\ell$ even - symmetric

$\Psi_{\ell m, s} = (-1)^{\ell+s+1} \Psi_{\text{total}}$

only $\ell+s+1$ - odd are allowed

$S = 1, \quad \ell = 1$

$J = 0, 1, 2$

$S = 0$

$\ell = 0, 2$

$J = 0, 2$

no further splitting of levels beyond orbital-orbital.
$J_J$ Coupling

When $z$ is large, spin-orbit dominates over spin-spin, orbital-orbital coupling.

Treat each electron independently.

\[
\begin{align*}
\tilde{J}_1 &= \tilde{L}_1 + \tilde{S}_1 \\
\tilde{J}_2 &= \tilde{L}_1 + \tilde{S}_2 \\
\tilde{J} &= \tilde{J}_1 + \tilde{J}_2
\end{align*}
\]
Singlet, triplet states

Consider the helium atom

total spin quantum number, $S = 0, \frac{1}{2}$

$S = 0 \quad m_s = 0 \quad $ singlet - para helium

$S = 1 \quad m_s = \begin{cases} 0 \\ \frac{1}{2} \end{cases} \quad $ triplet - ortho helium

ground state - $1s^2$, $S = 0$

$1s\,2p$ and $1s\,2s$ can both have singlet, triplet states

triplet states, $S = 1$, cannot decay to ground state because $S$ would be $1$

Selection rules

$\Delta S = 0$

$\Delta \ell = \pm 1$
Atoms in external magnetic fields

**Weak field**
\[
\Delta E = \frac{e}{2m} \left( \vec{L} + \vec{S} \right) \cdot \vec{B}
\]

Cannot just use \( \vec{L} \) and \( \vec{S} \) since they are coupled through spin-orbit.

Must use \( \vec{J} = \vec{L} + \vec{S} \)

\[
\Delta E = \frac{e}{2m} \left[ \frac{(\vec{L} + \vec{S}) \cdot (\vec{J})}{J^2} \right] \left( \frac{\vec{J} \cdot \vec{B}}{J} \right)
\]

Assume \( \vec{B} \) is in \( z \) direction

\[
\Delta E = \frac{e}{2m} \left[ \frac{(\vec{L} + \vec{S}) \cdot (\vec{L} + \vec{S})}{J^2} \right] J \cdot \vec{B}
\]

\( J_z = n \hbar \)

\[
\Delta E = g_L m_J J \hbar B
\]

\[
g_L = \frac{3 J^2 - L^2 + S^2}{2 J^2}
\]

**Strong field**

Breaks spin-orbit coupling

\[
\Delta E = (m_e + 2m_s) \beta \nu_B
\]