### Possible Values of $l$ and $m_l$ for $n = 1, 2, 3$

<table>
<thead>
<tr>
<th>$n$</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l$</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>$m_l$</td>
<td>0</td>
<td>0</td>
<td>$-1, 0, +1$</td>
</tr>
</tbody>
</table>

| Number of degenerate eigenfunctions for each $l$ | 1 | 1 | 3 | 1 | 3 | 5 |
| Number of degenerate eigenfunctions for each $n$ | 1 | | 4 | | | 9 |
### Some Eigenfunctions for the One-Electron Atom

<table>
<thead>
<tr>
<th>Quantum Numbers</th>
<th>Eigenfunctions</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n ) ( l ) ( m_l )</td>
<td>( \psi_{00} = \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} )</td>
</tr>
<tr>
<td>1 0 0</td>
<td>( = \left( \frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} )</td>
</tr>
<tr>
<td>2 0 0</td>
<td>( \psi_{200} = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \left( 2 - \frac{Zr}{a_0} \right) e^{-Zr/2a_0} )</td>
</tr>
<tr>
<td>2 1 0</td>
<td>( \psi_{210} = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos \theta )</td>
</tr>
<tr>
<td>2 1 ( \pm 1 )</td>
<td>( \psi_{21 \pm 1} = \frac{1}{8\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \sin \theta ) e( \pm i\phi )</td>
</tr>
<tr>
<td>3 0 0</td>
<td>( \psi_{300} = \frac{1}{81\sqrt{3\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \left( 27 - 18 \frac{Zr}{a_0} + 2 \frac{Z^2r^2}{a_0^2} \right) e^{-Zr/3a_0} )</td>
</tr>
<tr>
<td>3 1 0</td>
<td>( \psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \left( 6 - \frac{Zr}{a_0} \right) \frac{Zr}{a_0} e^{-Zr/3a_0} \cos \theta )</td>
</tr>
<tr>
<td>3 1 ( \pm 1 )</td>
<td>( \psi_{31 \pm 1} = \frac{1}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \left( 6 - \frac{Zr}{a_0} \right) \frac{Zr}{a_0} e^{-Zr/3a_0} \sin \theta ) e( \pm i\phi )</td>
</tr>
<tr>
<td>3 2 0</td>
<td>( \psi_{320} = \frac{1}{81\sqrt{6\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \frac{Z^2r^2}{a_0^2} e^{-Zr/3a_0} (3 \cos^2 \theta - 1) )</td>
</tr>
<tr>
<td>3 2 ( \pm 1 )</td>
<td>( \psi_{32 \pm 1} = \frac{1}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \frac{Z^2r^2}{a_0^2} e^{-Zr/3a_0} \sin \theta \cos \theta ) e( \pm i\phi )</td>
</tr>
<tr>
<td>3 2 ( \pm 2 )</td>
<td>( \psi_{32 \pm 2} = \frac{1}{162\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \frac{Z^2r^2}{a_0^2} e^{-Zr/3a_0} \sin^2 \theta ) e( \pm 2i\phi )</td>
</tr>
</tbody>
</table>
Wave functions

- Shells
- Orthogonality
\[ \Theta^2_{\ell, m_\ell} (\theta) \]

- \( \ell = 0, m_\ell = 0 \)
- \( \ell = 3, m_\ell = 0 \)
- \( \ell = 3, m_\ell = \pm 1 \)
- \( \ell = 1, m_\ell = 0 \)
- \( \ell = 2, m_\ell = 0 \)
- \( \ell = 2, m_\ell = \pm 1 \)
- \( \ell = 3, m_\ell = \pm 1 \)
- \( \ell = 1, m_\ell = \pm 1 \)
- \( \ell = 2, m_\ell = \pm 2 \)
- \( \ell = 3, m_\ell = \pm 2 \)
- \( \ell = 3, m_\ell = \pm 3 \)
\[ \lvert \psi(r, \theta, \phi) \rvert^2 = R^2(r) \Theta^2(\theta) \]

\( (n, \ell, m_\ell) = (1, 0, 0) \)  
\text{1s}

\( (2, 0, 0) \)  
\( (2, 1, 0) \)  
\( (2, 1, \pm 1) \)  
\text{2s} \quad \text{2p}

\( (3, 0, 0) \)  
\text{3s}

\( (3, 1, 0) \)  
\( (3, 1, \pm 1) \)  
\text{3p}

\( (3, 2, 0) \)  
\( (3, 2, \pm 1) \)  
\( (3, 2, \pm 2) \)  
\text{3d}
\[ z-axis \]

\[ \theta \]

\[ x \quad y \]

\[
(2, 1, 0) \quad \quad (2, 1, \pm 1) \\
2p
\]

\[
(3, 1, 0) \quad \quad (3, 1, \pm 1) \\
3p
\]

\[
(3, 2, 0) \quad (3, 2, \pm 1) \quad (3, 2, \pm 2) \\
3d
\]
For a given \( n \), lower \( \ell \) is smaller rotational energy and larger radial, with more radial antinodes—a more elliptical orbit. The \( 3s \) has three radial antinodes.

Higher \( \ell \) is like a circular orbit at a single radius. The \( 3d \) has only one antinode.

\[ U(r) \propto \frac{1}{r} \]
Direct knockout reactions

- Atoms: \((e,2e)\) reaction
- Nuclei: \((e,e'p)\) reaction [and others like \((p,2p), (d,^3\text{He}), (p,d), \text{etc.}\)]
- Physics: transfer large amount of momentum and energy to a bound particle; detect ejected particle together with scattered projectile \(\rightarrow\) construct spectral function
- Impulse approximation: struck particle is ejected
- Other assumption: final state \(\sim\) plane wave on top of \(N-1\) particle eigenstate (more serious in practical experiments) but good approximation if ejectile momentum large enough
- If relative momentum large enough, final state interaction can be neglected as well
- \(\rightarrow\) PWIA = plane wave impulse approximation
- Cross section proportional to spectral function
(e,2e) data for atoms

• Start with Hydrogen

• Ground state wave function

\[ \phi_{1s}(p) = \frac{2^{3/2}}{\pi} \frac{1}{(1 + p^2)^2} \]

• (e,2e) removal amplitude

\[ \langle 0 | a_p | n = 1, \ell = 0 \rangle = \langle p | n = 1, \ell = 0 \rangle = \phi_{1s}(p) \]

Hydrogen 1s wave function “seen” experimentally
Electrons in atoms

• Atomic units (a.u.) --> standard usage
  - electron mass $m_e$ unit of mass
  - elementary charge $e$ unit of charge
  - length and time such that numerical values of $\hbar$ and $4\pi \varepsilon_0$ are unity
  - then atomic unit of length Bohr radius

    \[
    \text{a.u. (length)} = a_0 = \frac{4\pi \varepsilon_0 \hbar^2}{e^2 m_e} \approx 5.29177 \times 10^{-11} \text{ m}
    \]

  - and time \ a.u. (time) = $a_0 \frac{\alpha}{c} \approx 2.41888 \times 10^{-17} \text{ s}$

  - where \ $\alpha = \frac{e^2}{4\pi \varepsilon_0 \hbar c} \approx \frac{1}{137.036}$ is the fine structure constant

  - energy unit = Hartree \ $E_H = \frac{\hbar^2}{m_e a_0^2} \approx 27.2114 \text{ eV}$
Hamiltonian in a.u.

• Most of atomic physics can be understood on the basis of

\[ H_N = \sum_{i=1}^{N} \frac{p_i^2}{2} - \sum_{i=1}^{N} \frac{Z}{|r_i|} + \frac{1}{2} \sum_{i \neq j}^{N} \frac{1}{|r_i - r_j|} + V_{mag} \]

• for most applications \( V_{mag} \Rightarrow V_{so}^{eff} = \sum_{i} \zeta_i \ell_i \cdot s_i \)

• Relativistic description required for heavier atoms
  - binding sizable fraction of electron rest mass
  - binding of lowest s state generates high-momentum components

• Sensible calculations up to Kr without \( V_{mag} \)

• Shell structure well established
Shell structure

- Simulate with
  \[ H_0^N = \sum_{i=1}^{N} H_0(i) \]

- with
  \[ H_0(i) = \frac{p_i^2}{2} - \frac{Z}{r_i} + U(r_i) \]

- even without auxiliary potential \( \Rightarrow \) shells
  - hydrogen-like: \( (2\ell + 1) \ast (2s + 1) \) degeneracy
  - but \( \varepsilon_n = -\frac{Z^2}{2n^2} \) does not give correct shell structure (2,10,28...)
  - degeneracy must be lifted
  - how?
Effect of other electrons in neutral atoms

- Consider effect of electrons in closed shells for neutral Na
- Large distances: nuclear charge screened to 1
- Close to the nucleus: electron “sees” all 11 protons
- Approximately:

\[ \varepsilon_{2s} < \varepsilon_{2p} \]
\[ \varepsilon_{3s} < \varepsilon_{3p} < \varepsilon_{3d} \]

- "Far away" orbits: still hydrogen-like!
Example: Na

- Fill the lowest shells
- Use schematic potential
  \[ H_0 |n\ell m_\ell m_s \rangle = \varepsilon_{n\ell} |n\ell m_\ell m_s \rangle \]
- Ground state: fill lowest orbits according to Pauli
  \[ |300m_s, 211\frac{1}{2}, 211 - \frac{1}{2}, ..., 100\frac{1}{2}, 100 - \frac{1}{2} \rangle \equiv |\Phi_0(Na)\rangle \]
- Excited states?
Closed-shell atoms

• Neon

• Ground state

\[ |\Phi_0(\text{Ne})\rangle = |211\frac{1}{2}, 211 - \frac{1}{2}, \ldots, 100\frac{1}{2}, 100 - \frac{1}{2}\rangle \]

• Excited states

\[ |n\ell \ (2p)^{-1}\rangle = a_{n\ell}^\dagger a_{2p} |\Phi_0(\text{Ne})\rangle \]

• operators: see later

• Note the H-like states

• Splitting?

• Basic shell structure of atoms understood \(\Rightarrow\) IPM
Periodic table

[Graph showing ionization energy vs. atomic number with points for He, Ne, Ar, Kr, Xe, and Rn labeled.]
Level sequence (approximately)
(e,2e) data for atoms

- Start with Hydrogen
- Ground state wave function \[ \phi_{1s}(p) = \frac{2^{3/2}}{\pi} \frac{1}{(1 + p^2)^2} \]
- (e,2e) removal amplitude

\[ \langle 0 | a_p | n = 1, \ell = 0 \rangle = \langle p | n = 1, \ell = 0 \rangle = \phi_{1s}(p) \]

Hydrogen 1s wave function “seen” experimentally
Helium

- IPM description is very successful
- Closed-shell configuration $1s^2$
- Reaction more complicated than for Hydrogen
- DWIA (distorted wave impulse approximation)

\[ S = \int dp \left| \langle \Psi_{n-1}^N | a_p | \Psi_0^N \rangle \right|^2 \]

agreement with IPM! $\rightarrow 1$

Other closed-shell atoms

- Spectroscopic factor becomes less than 1
- Neon $2p$ removal: $S = 0.92$ with two fragments each 0.04
- IPM not the whole story: fragmentation of sp strength
- Summed strength: like IPM
- IPM wave functions still excellent
- Example: Argon $3p$ $S = 0.95$
- Rest in 3 small fragments

![Differential cross section](image)
Argon spectroscopic factors

- s strength also in the continuum: Ar^{++} + e
- note vertical scale
- red bars: 3s fragments exhibit substantial fragmentation

Diagram showing the spectroscopic factors for Ar with vertical scale and energy level transitions labeled.
Conventional current is opposite electron motion.

Two right-hand rules:
\[ \mu = IA \]
\[ L = r \times p \]
<table>
<thead>
<tr>
<th>Subshell $n\ell$</th>
<th>1s</th>
<th>2s</th>
<th>2p</th>
<th>3s</th>
<th>3p</th>
<th>4s</th>
<th>3d</th>
<th>4p</th>
<th>5s</th>
<th>4d</th>
<th>5p</th>
<th>6s</th>
<th>4f</th>
<th>5d</th>
<th>6p</th>
<th>7s</th>
<th>5f</th>
<th>6d</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n + \ell$</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>4</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>7</td>
<td>7</td>
<td>7</td>
<td>7</td>
<td>7</td>
<td>8</td>
</tr>
<tr>
<td>Number of electrons $2(2\ell + 1)$</td>
<td>2</td>
<td>2</td>
<td>6</td>
<td>2</td>
<td>6</td>
<td>2</td>
<td>10</td>
<td>6</td>
<td>2</td>
<td>10</td>
<td>6</td>
<td>2</td>
<td>14</td>
<td>10</td>
<td>6</td>
<td>2</td>
<td>14</td>
<td>10</td>
</tr>
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