1. Single electron, hydrogen-like atoms

\[ E_n = -\frac{n^2 \hbar^2}{2m} \left( \frac{Z^2}{e^2} \right) + \left( -\frac{2\pi \hbar c}{\lambda} \right) \psi \]

\[ \psi_n = N P_l \psi_n^l e^{-\sqrt{2mE_n}/\hbar} r \psi_{n^l} \]

\[ n \geq 0 \]

\[ -m \leq L \leq m \]

Degeneracy: only \( n \) appears in \( E \)

\[ g_n = 2^n \]

2. Zeeman effect

Splitting of levels

\[ \Delta E = S d^3 \psi_n^l (-1)^\ell \psi_n \]

\[ \Delta E = \frac{e^2}{2M} B_2 L_z \psi_n \]

\[ (\pm) \frac{e^2}{2M} \psi_n L_z B_2 \]
Total Angular Momentum

\[ \hat{J} = \hat{L} + \hat{S} \]

\[ J = j \pm s \]

\[ \frac{1}{2} \gamma = \hbar (j + 1) \gamma \]

\[ J_z \gamma = \hbar m_j \gamma \]

Note:

- For a single electron
- \( j = \text{integer} \pm \frac{1}{2} \)
- Number states
- \(-j < m_j < j \)

\[ \sqrt{2j + 1} = 20 + 1 \pm 1 \]

Always even!
Electron with $L$, $S$:

\[ \frac{1}{2} j = L + S \]

"good" quantum number

\[ \begin{align*}
\frac{1}{2} y &= \hbar^2 y j(j+1) 4 \\
\frac{1}{2} z &= \hbar^2 z 2 y
\end{align*} \]

Total angular momentum:

\[ \vec{L} = \frac{\hbar}{2m} (\hat{l} + 2 S) \]

not postulated or proved but follows from old principles

\[ \vec{B} = B_\theta \hat{e}_\theta \]

\[ -\vec{\mu} \cdot \vec{B} = \frac{e \mu}{2m} (L_\theta + 2 S) \]

\[ \Rightarrow \Delta E = g_e \hbar z (\frac{e \hbar}{2m \omega}) B_\theta \]

\[ g_e = 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2 j (j+1)} \]
Many Electron Atoms

So now we know all about e.g.

\[ \text{He}^+ \]

\[ Z = 2 \]

next

\[ \text{He} \]

\[ Z = 2 \]

Ionization energy: nearly 25 eV!

but how can this be possible?

If both electrons share same orbital, OK:

\[ Z = 3 \]

\[ E_{1s} = 100 \text{ eV} \]

but

\[ \text{Li} \]

\[ Z = 3 \]

Ionization energy

\[ \pm 5.5 \text{ eV} \]

Why??
Figure 8.10 The low-lying atomic states of helium are shown. The ground state ($^1S_0$) is some 20 eV below the grouping of the lowest excited states. The level indicated by $^3P_{0,1,2}$ is actually three states ($^3P_0$, $^3P_1$, $^3P_2$), but the separations are too small to be indicated.

$(1s)^2$: two electrons in 1s-valence

1s2s 1 electron in 1s, 1 in 2s

1s2p 1, 1 in 2p

One of the electrons is progressively killed high and ionized with 2s-eV energy
Filling each shell \(2n^2\)

- \(n=1\): 2
- \(n=2\): 8
- \(n=3\): 18
- \(n=4\): 32
- \(n=5\): 50
- \(n=6\): 60

Closed shells are important. Elements in these shells are typically chemically unreactive.
\[ \begin{align*} 
\text{Li also understood!} \\
-4.5 \text{eV} & \quad (1s)^2 \quad (1s)^2 \quad 2p \\
& \quad (1s)^2 \quad 2p \\
& \quad (1s)^2 \quad 1s \quad 1s \\
\text{Pauli forbids} & \quad (1s)^3 \text{impossible!} \\
\text{PAULI PRINCIPLE} \\
\end{align*} \]

Pauli\textit{ forbids} 
\((1s)^3\) \textit{impossible}!

\[ 2p \text{-} (2\text{nd}) \text{- } \text{electron sees nearly a change} \ 3 - 2 = 1 \], thus

\[ \begin{align*} 
\text{we expect it is bound by} \\
E_{2p}^{2\text{p}} = -\frac{1}{2} \alpha^2 \frac{mc^2}{2} = \frac{1}{2} \approx 3.5 \text{eV} \\
\end{align*} \]

not bad for a approximation

\[ \begin{align*} 
\text{(obviously, screening not complete)} \\
\end{align*} \]
So the third electron must not go into the lowest atomic level.

**Must Know** ➞ Pauli Exclusion Principle

No two electrons in an atom may have the same set of quantum numbers.

But then why did Helium have two electrons in its orbital?

Each electron has an intrinsic property called **spin** and can come in two states with quantum numbers:

\[ + \uparrow \quad - \downarrow \]
<table>
<thead>
<tr>
<th>$n$</th>
<th>$\ell$</th>
<th>Subshell</th>
<th>Subshell Capacity</th>
<th>Total Electrons in All Subshells</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1$s$</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>2$s$</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2$p_x$</td>
<td>6</td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>3$s$</td>
<td>2</td>
<td>12</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>3$p_y$</td>
<td>6</td>
<td>18</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>4$s$</td>
<td>2</td>
<td>20</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>3$d$</td>
<td>10</td>
<td>30</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>4$p$</td>
<td>6</td>
<td>36</td>
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<tr>
<td>5</td>
<td>0</td>
<td>5$s$</td>
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<td>38</td>
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<tr>
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<td>2</td>
<td>4$d$</td>
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<td>48</td>
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<tr>
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<td>1</td>
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<tr>
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<tr>
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<td>4$f$</td>
<td>14</td>
<td>70</td>
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<td>10</td>
<td>80</td>
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<tr>
<td>6</td>
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<td>6</td>
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<tr>
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<tr>
<td>5</td>
<td>3</td>
<td>5$f$</td>
<td>14</td>
<td>102</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>6$d$</td>
<td>10</td>
<td>112</td>
</tr>
</tbody>
</table>
The atomic number and element symbol are given in the top of each box. The electron configuration for each element is specified by giving the values of the principal quantum numbers \( n \), the angular momentum quantum numbers \( l \) (s, p, d, or f), and the number of electrons outside closed shells. The configuration of some of the closed shells is given on the left.

Dmitri Ivanovich Mendeleev (1834-1907)
Developed the periodic table of elements.
Could you please review the important differences and similarities between the Bohr model and the Schroedinger wave model?

Thanks,

Shona Eroto

<table>
<thead>
<tr>
<th>Similarities</th>
<th>Differences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Angular momentum quantized</td>
<td>Bohr Model ( N = 1, 2, 3, \ldots ) ( 0 \leq \ell &lt; n ) (-\ell \leq M \leq \ell)</td>
</tr>
<tr>
<td>Quantized orbits</td>
<td>Schroedinger Wave Mechanics</td>
</tr>
<tr>
<td>Atomic size explained by internal electron mass and fine structure constant ( h)</td>
<td>Radial wave function also explains electron delocalization due to uncertainty principle</td>
</tr>
<tr>
<td>Sharp orbit size ( R = \frac{n^2 a_0}{\ell} )</td>
<td>Pauli Principle and degeneracy/states come together to understand atomic structure</td>
</tr>
<tr>
<td>No rules for number of ( \ell ) in an orbit</td>
<td>[ \sum \ell = \ell^2 = 0, \pm 2 \ell ] for an electron to understand these waves</td>
</tr>
</tbody>
</table>

Subject: question for bonus?
Date: Tue, 1 May 2001 19:58:33 EDT
From: Skrote1@sol.com
To: rafelski@physics.arizona.edu
Atomic structure \(Z > 1\!\)

Schrödinger Atom like Bohr Atom except: orbits are 'uncertain'

\[ r_n \rightarrow P(r) = r^{2} \frac{14}{(n^2)} \]

As \(Z\) increases, the size of orbit decreases \(\propto \frac{1}{Z}\) but the electron screening.

Also: for states with nodes, several maxima, e.g., \(3p\) behaves as \(1P\) \(\rightarrow 3p\) \((l=1)\)

\(\Rightarrow 3p\) sees many electron-electron Coulomb repulsions in \(3d\)

\(\Rightarrow 3s\) sees min in \(3p\)