# Reading and problem assignments, for Quiz #2 and to the end of the quarter (see also website)

Physics 9D, Section B, Fadley—Assignments for Spring Quarter, 2010: Midterm coverage in red, Quiz No. 2 coverage in blue, until end of quarter in black. Note there is a second page!

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Reading</th>
<th>Questions/Problems</th>
</tr>
</thead>
<tbody>
<tr>
<td>1—Classical physics to 1900</td>
<td>All</td>
<td>None—a review of classical physics</td>
</tr>
<tr>
<td>2—Special relativity</td>
<td>All except 2.9, plus 12.6 on radioactive decay</td>
<td>Probs. in Chap. 2: 3,4,13,24,25,27,32,37,40, 51, 54,55,57,68,76,80,82,86,92, plus prob. 12.26</td>
</tr>
<tr>
<td>15—General relativity</td>
<td>15.1-15.4, 15.5—optional (relates to newspaper article in S.F. Chronicle of April 5, 2004 see slides)</td>
<td>Probs. in Chap. 15: 2,4,9,11,17,24: plus: What is the frequency change due to velocity? Use equations in lecture for GPS.</td>
</tr>
<tr>
<td>3—Expts. Leading to quantum theory</td>
<td>All sections, plus Section 14.8 on accelerators, pp. 533-537, not including “Fixed Target Accelerators”</td>
<td>Probs. in Chap. 3: 2,5,6,9,14,17,19,23: plus, Special part: If the emissivity of tungsten is 0.32 at this temperature, and the wire has a diameter of 0.01 cm, what length of wire would be necessary for a 60W bulb? 32,34,38,43,47,54 Probs. in Ch. 14: 31 and 34</td>
</tr>
<tr>
<td>4—Structure of the atom</td>
<td>All Sections</td>
<td>Probs. in Chap. 4: 2,3,5,6,11,16,22,23,29,32,37,38,48</td>
</tr>
<tr>
<td>5—Wave properties of matter</td>
<td>Sections 5.1-5.3 for midterm, remaining sections after, plus supplementary reading on Fourier integrals</td>
<td>Probs. in Chap. 5: 1,3,10, 11, 12, 17, 19, 22, for midterm, then 26, 27, 28, 33, 40, 43, 45, 48 54, plus Special Problems: S1-With reference to the website: <a href="http://www.falstad.com/fourier/index.html">http://www.falstad.com/fourier/index.html</a>, calculate the first two non-zero Fourier coefficients in the cosine+sine series representing a square wave, and show that they agree with the numbers given at this site. Why are there no cosine terms? S2- With reference to the supplementary reading on Fourier integrals, show that the final formula for g(ω) on p. 3 and plotted in 4.20 is correct.</td>
</tr>
<tr>
<td>6—Quantum theory</td>
<td>Sections 6.1-6.4, then all remaining sections —Quiz No. 2 coverage in blue—</td>
<td>Probs. in Chap. 6: S1-Show that the wave function for a free particle traveling to the right is an eigenfunction of the momentum operator $p$ and the kinetic energy operator $\hat{K}$, 2,5,7,8,9,11,15,20,23,26,28,32,37,40,41,47,54</td>
</tr>
<tr>
<td>7—The hydrogenic atom</td>
<td>All, plus supplementary reading on electronic transitions and selection rules (see link at website).</td>
<td>Questions: 1,2 Probs. in Chap. 7: 1,3,5,6,11,13,15,16,19,20(But do for $4p$ instead of $4p$) 29,32,35,38,46, plus Special prob2/Sem: Show, using the full hydrogenic atom wave functions given in a lecture slide that, if you take the combinations $3d_{x^2}$,$3d_{y^2}$ and $3d_{z^2}$ you get two of the real 3d orbitals, also shown in a lecture slide, and identify which ones.</td>
</tr>
<tr>
<td>8—Many-electron atoms &amp; the periodic table</td>
<td>Sections 8.1 and 8.2 only, plus supplementary reading on exchange symmetry or many-particle wave functions (see</td>
<td>Questions: 5 Probs. in Chap. 8: 1,2,4,5,7, 11,12,23 (Remember the dipole selection rules?) 24</td>
</tr>
</tbody>
</table>
The Hydrogenic Atom
Schroedinger Equation:
Spherical Polar Coordinates

Classically:
\[ \mathbf{L} = \mathbf{r} \times \mathbf{p} \]

is conserved

Quantum mechanically:
\[ \hat{H} \psi(r, \theta, \phi) = \hat{K} \psi(r, \theta, \phi) - \frac{Z e^2}{4 \pi \varepsilon_0 r} \psi = E \psi \]

Polar angle = \(\theta = \arccos(z/r)\)
Azimuthal angle = \(\phi = \arctan(y/x)\)

Converting to new coordinates

\[ \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi = -\cos \theta \left|_0^\pi \right. \times 2\pi = 4\pi \]
• Use separation of variables:

\[ \Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad \text{[ } \Theta(\theta) = f(\theta) \text{ & } \Phi(\phi) = g(\phi) \text{ in text } \]
Solving for the $\phi$ part = $\Phi(\phi)$:

"BOUNDARY" CONDITION IN $\phi$:

$$
\Phi(\phi) = \Phi(\phi + 2\pi)
$$

$$
e^{im_2\phi} = e^{im_2(\phi + 2\pi)} = e^{im_2\phi}e^{im_22\pi}
$$

$\Rightarrow m_2 = 0, \pm 1, \pm 2, \ldots$
Use separation of variables:

\[ \Psi(r, \Theta, \Phi) = R(r) \Theta(\Theta) \Phi(\Phi) \]

**Assumed Form**

Substitute, rearrange \( \phi \):

\[ \frac{d^2 \Phi}{d \phi^2} + C_\phi \Phi = 0 \Rightarrow \Phi(\phi) = A e^{\pm i C_\phi \phi} \]  \hspace{1cm} \text{(1)}

\[ C_\phi = m_z = 0, \pm 1, \ldots \]

\[ \Theta : \frac{1}{\sin \Theta} \left( \sin \Theta \frac{d}{d \Theta} \right) + \left( C_\Theta - \frac{m_z^2}{\sin^2 \Theta} \right) \Theta = 0 \] \hspace{1cm} \text{(2)}

\[ E_{\text{eff}}(r) \text{ IN MANY } e^- \text{ ATOM} \]

\[ R : \left[ -\frac{\hbar^2}{2 m_e} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{(n+1)^2 - \frac{E^2}{4 m_e r^2}}{2 m_e r^2} \right] R = ER \] \hspace{1cm} \text{(3)}

A "Radial Schrödinger Eqn."

\[ \hat{H}_{\text{radial}} R = ER \]

Solving for \( \Theta \) with (2) \( \Rightarrow \)

\[ \Theta_{n\lambda m} (\Theta) = \text{ASSOC. LEGENDRE POLYNOMIALS IN } (\cos \Theta) - \text{REAL} \]

\[ L = 0, 1, 2, 3, \ldots (n-1) \]

\[ m_\lambda = -L, -L+1, \ldots 0 \ldots L-1, L \]

Solving for \( R \) with (3) \( \Rightarrow \)

\[ R_{n\lambda m} (r) = \text{ASSOC. LAGUERRE FUNCTIONS IN } r; e^{-Zr/\alpha} - \text{REAL} \]

Changes for many-e\(^-\) atoms

The Bohr Formula!

The same for many-e\(^-\) atoms
GROUNDS STATE OF HYDROGENIC ATOM:

\[ \psi_{100} = R_{10}(r) Y_0^0(\theta, \phi) = \pi^{-1/2} \left( \frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} \]

\[ |\psi_{100}|^2 = \frac{Z^3}{\pi a_0^3} e^{-2Zr/a_0} \]

\[ P_{1s}(r) = (R_{10}(r))^2 r^2 \]

\[ r = a_0/Z \]

**Most probable r**

**Bohr orbit radius**

\[ E = E_{100} = \text{Bohr energy for } n = 1! \]
The atomic orbitals:

\[ Y_{\ell m} (\theta, \phi) = \text{"spherical harmonics"} \]

But we can make them real for convenience

**TABLE 6.1**

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \ell )</th>
<th>( m_\ell )</th>
<th>( \Phi (\phi) )</th>
<th>( \Theta (\theta) )</th>
<th>( R_{n\ell}(r) )</th>
<th>( Y_{n\ell m_\ell}(\rho, \theta, \phi) = \Phi \Theta \mathcal{Z}<em>{n\ell m</em>\ell} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{2}{a_0^2} e^{-r/a_0} )</td>
<td>( \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} )</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>( \frac{1}{\sqrt{2}} )</td>
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</tr>
<tr>
<td>2</td>
<td>1</td>
<td>( \pm 1 )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{2\sqrt{3}} \left(\frac{r}{a_0} \cos \theta \right) )</td>
<td>( \frac{1}{8\sqrt{\pi} a_0^{3/2}} \sin \theta e^{\pm i\theta} )</td>
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<td>0</td>
<td>0</td>
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<tr>
<td>3</td>
<td>1</td>
<td>( \pm 1 )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{81\sqrt{10}} a_0^{3/2} (3 \cos^2 \theta - 1) \frac{r^2}{a_0^2} e^{-r/3a_0} )</td>
<td>( \frac{1}{81\sqrt{\pi} a_0^{3/2}} (3 \cos^2 \theta - 1) \frac{r^2}{a_0^2} e^{-r/3a_0} )</td>
</tr>
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<td>( \frac{1}{81\sqrt{15}} a_0^{3/2} \left( \frac{r}{a_0} \cos \theta \right) )</td>
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<tr>
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<td>( \pm 1 )</td>
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<td>( \frac{1}{81\sqrt{15}} a_0^{3/2} \left( \frac{r}{a_0} \cos \theta \right) )</td>
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</tr>
<tr>
<td>3</td>
<td>2</td>
<td>( \pm 2 )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{\sqrt{2}} )</td>
<td>( \frac{1}{81\sqrt{15}} a_0^{3/2} \left( \frac{r}{a_0} \cos \theta \right) )</td>
<td>( \frac{1}{81\sqrt{\pi} a_0^{3/2}} \left( \frac{r}{a_0} \cos \theta \right) )</td>
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</tbody>
</table>

*The quantity \( a_0 = 4\pi e^2/m_e^2 = 5.3 \times 10^{-11} \text{ m} \) is equal to the radius of the innermost Bohr orbit.

**IS SAME FOR**

**CHANGES FOR**

\[ Z \rightarrow Z_{\text{eff},n\ell}(r) \text{ in many-e}^- \text{ atoms} \]
MAKING THE ATOMIC ORBITALS REAL (E.G., FOR CHEMICAL BONDING): 

\[ \psi_{n \ell m_\ell}(r, \theta, \phi) = R_{n \ell}(r) \Theta(\theta) \frac{1}{2\pi} \frac{e^{im_\ell \phi}}{\ell_{\text{max}}} \]

Complex       Real        Real        Complex

If \( m_\ell \neq 0 \)

So just take components of \( \pm m_\ell \) as:

\[ \psi_{n \ell(-\ell)}(r, \theta, \phi) = \begin{cases} 
\frac{1}{2} [\psi_{n \ell m_\ell} + \psi_{n \ell -m_\ell}] & \text{if } m_\ell \neq 0 \\
\frac{i}{2} [\psi_{n \ell m_\ell} - \psi_{n \ell -m_\ell}] & \text{if } m_\ell = 0 
\end{cases} \]

REAL

EXAMPLE: 2p ORBITALS

\[ \psi_{210} = \psi_{2p_0} = \psi_{2p_z} \propto r \cos \theta = z \quad \text{(already real)} \]

\[ \psi_{211} = \psi_{2p_1} \propto r \sin \theta e^{i\phi} = r \sin \theta [\cos \phi + i \sin \phi] \]

\[ \psi_{21-1} = \psi_{2p_{-1}} \propto r \sin \theta e^{-i\phi} = r \sin \theta [\cos \phi - i \sin \phi] \]

\[ \frac{1}{2} [\psi_{2p_1} + \psi_{2p_{-1}}] = \psi_{2p_x} \propto r \sin \theta \cos \phi = x \]

\[ \frac{-i}{2} [\psi_{2p_1} - \psi_{2p_{-1}}] = \psi_{2p_y} \propto r \sin \theta \sin \phi = y \]

\[ \frac{-i}{2} [\psi_{2p_1} - \psi_{2p_{-1}}] = \psi_{2p_z} \propto r \sin \theta \cos \phi = z \]
And the same thing for the d orbitals:

\[ \propto r^2 (3\cos^2 \theta - 1) = 3z^2 - r^2 \]

+ nodes for \( \cos \theta = 1/\sqrt{3} \)
\( \theta = 54.7^\circ, 125.3^\circ \)

See special problem for Chap. 7
The atomic orbitals:

\[ Y_\ell m_\ell (\theta, \phi) = \text{ "spherical harmonics"} \]

But we can make them real for convenience

**TABLE 6.1**

NORMALIZED WAVE FUNCTIONS OF THE HYDROGEN ATOM FOR \( n = 1, 2, \) AND \( 3 \) (\( Z = 1 = \text{HYDROGEN} \))

<table>
<thead>
<tr>
<th>( n )</th>
<th>( 2 \ell m_\ell )</th>
<th>( \phi (\phi) )</th>
<th>( \Theta (\phi) )</th>
<th>( R_{\ell m_\ell} (r) )</th>
<th>( Y_{\ell m_\ell} (r, \theta, \phi) = \phi \Theta R_{\ell m_\ell} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0, 0</td>
<td>1</td>
<td>1</td>
<td>( \frac{2}{a_0} e^{-r/a_0} )</td>
<td>( \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} ) → Radial node for ( r = 2a_0 )</td>
</tr>
<tr>
<td>2</td>
<td>0, 0</td>
<td>( \frac{1}{\sqrt{2 \pi}} )</td>
<td>1</td>
<td>( \frac{1}{2 \sqrt{2} a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/a_0} )</td>
<td>( \frac{1}{4 \sqrt{2 \pi} a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0} ) → Angular node for ( \theta = 90^\circ )</td>
</tr>
<tr>
<td>2</td>
<td>0, ±1</td>
<td>( \frac{1}{\sqrt{2 \pi}} )</td>
<td>( \frac{1}{2} \sin \theta )</td>
<td>( \frac{1}{2 \sqrt{6} a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) e^{-r/2a_0} )</td>
<td>( \frac{1}{8 \pi a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) e^{-r/2a_0} ) sin ( \theta ) → Angular node for ( r = 6a_0 )</td>
</tr>
</tbody>
</table>
| 3 | 0, 0 | \( \frac{1}{\sqrt{2 \pi}} \) | 1 | \( \frac{1}{81 \sqrt{3} a_0^{3/2}} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0} \) | \( \frac{1}{8 \pi a_0^{3/2}} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0} \) sin \( \theta \) e\( ^{\pm i\phi} \) → Angular nodes for \( \cos^2 \theta = \frac{1}{3} \)
| 3 | 1, ±1 | \( \frac{1}{\sqrt{2 \pi}} \) | \( \frac{1}{2} \cos \theta \) | \( \frac{4}{81 \sqrt{6} a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \cos \theta \) e\( ^{-r/3a_0} \) | \( \frac{1}{8 \sqrt{3} a_0^{3/2}} \left(6 - \frac{r}{a_0}\right) \cos \theta \) e\( ^{-r/3a_0} \) sin \( \theta \) e\( ^{\pm i\phi} \) |
| 3 | 2, ±1 | \( \frac{1}{\sqrt{2 \pi}} \) | \( \frac{1}{2} \sin \theta \cos \theta \) | \( \frac{4}{81 \sqrt{30} a_0^{3/2}} \left(3 \cos^2 \theta - 1\right) \) e\( ^{-r/3a_0} \) | \( \frac{1}{8 \sqrt{3} a_0^{3/2}} \left(3 \cos^2 \theta - 1\right) \) e\( ^{-r/3a_0} \) sin \( \theta \) e\( ^{\pm i\phi} \) |

*The quantity \( a_0 = 4\pi e^2/mc^2 = 5.3 \times 10^{-11} \text{ m} \) is equal to the radius of the innermost Bohr orbit.

\[ Z \rightarrow Z_{\text{eff}, n\ell} (r) \text{ in many-e- atoms} \]
The Radial Parts $R_{n\ell}(r)$:

FIGURE 6.8 The variation with distance from the nucleus of the radial part of the electron wave function in hydrogen for various quantum states. The quantity $a_0 = 4\pi\varepsilon_0\hbar^2/m_e = 0.053$ nm is the radius of the first Bohr orbit.

- **n = 1**: Classical turning point
  - 1s

- **n = 2**:
  - 2p: node at $2a_0$

- **n = 3**:
  - 3p: node at $6a_0$

**General**: $n - l - 1$ nodes
**Radial Probability Density**

\[ P_n(r) = r^2 |R_{n\ell}(r)|^2 \text{ vs. } r \]

**Figure 6.9** The probability of finding the electron in a hydrogen atom at a distance between \( r \) and \( r + dr \) from the nucleus for the quantum states of Fig. 6.8.

**General:**

\( n - \ell \) zeroes (incl. origin)

\( P_{n\ell}'s \) grouped in \( K, L, M, \ldots \) "shells" when \( n = 1, 2, 3, \ldots \)
The Radial Probability Density

\[ P_{n\ell}(r) = r^2 R_{n\ell}(r)^2 : \]

\[ \frac{a_0}{Z^3} P(r) \]

\[ \frac{a_0}{Z^3} P(r) \]

\[ \frac{a_0}{Z^3} P(r) \]

Classical Turning Points:

\[ E_n = -\frac{k^2 e^2}{r_c} \]

General Rule:

Always \( n-\ell \) zeroes in \( P_{n\ell} \) (incl. \( r=0 \))
The hydrogenic atom- putting it all together in three dimensions:

Figure 6.12 Shapes of some hydrogen-atom orbitals. The 2s orbital has a spherical node, which is not visible; the 3s orbital has two such nodes. The 3p_\alpha orbital has a spherical node (indicated by the dashed line) and a nodal plane (the xy plane). The 3d_{z^2} orbital has two nodal cones; the 3d_{x^2-y^2} orbital has two nodal planes. Note that the view shown is not the same for the various orbitals.
Some of the atomic orbitals: including radial dependence

Total No e- = 2

1s $n=1$, $l=0$
2s $n=2$, $l=0$
2p $n=2$, $l=1$
3s $n=3$, $l=0$
3p $n=3$, $l=1$
3d $n=3$, $l=2$

$3z^2-r^2$, $x^2-y^2$, $yz$, $zx$, $xy$
Comparison of three QM potential-well problems in 1 dimension

Radial Part of H Atom

\[ E_n \propto \left(\frac{1}{n^2}\right) \]

[Graph showing energy levels for different states]

Rigid Box

\[ E_n \propto n^2 \]

[Graph showing energy levels for different states]

Harmonic Oscillator

\[ E_n \propto (n + \frac{1}{2}) \]

[Graph showing energy levels for different states]

**Also Cannot Go To Minimum!**

**Zero-Point Energies \( \neq 0 \)**
EIGENFUNCTION PROPERTIES OF THE ATOMIC WAVEFUNCTIONS

Energy: Hydrogenic atom – $\hat{H}\psi_{n\ell m_r} = E_n\psi_{n\ell m_r}$, $E_n$ from Bohr formula, $V(r) = \frac{Ze^2}{4\pi\varepsilon_0} \frac{1}{r}$

Operator $\rightarrow$ Eigenvalue

Many-electron atom – $\hat{H}\psi_{n\ell m_r} = E_{n\ell}\psi_{n\ell m_r}$,

$E_{n\ell}$ from solution of radial Schrödinger with

$$V_{\text{eff}}(r) = \frac{Z_{\text{eff},n\ell}(r)e^2}{4\pi\varepsilon_0} \frac{1}{r}$$

Square of angular momentum: $\hat{L}^2\psi_{n\ell m_r} = \hbar^2 (\ell + 1)\psi_{n\ell m_r}$

→ Always measure same value: $\Delta(\hat{L}^2) = 0$

Z component of angular momentum: $\hat{L}_z\psi_{n\ell m_r} = \hbar m_\ell\psi_{n\ell m_r}$

→ Always measure same value: $\Delta(L_z) = 0$

E.g.—$n = 3$, $\ell = 2 \rightarrow “3d”$
Quantization of space:
The (randomly) precessing vector model:

- $L_x, L_y, L_z$ cannot all be constant: violates uncertainty principle
- Only $L^2$ (or $|L|$) and $L_z$ constant

$L_z = \hbar m_z, m_z = \pm 2, \pm 1, 0, -1, -2$

$L^2 = \hbar^2 L(2+1) = \hbar^2 2(3)$

$|L| = \hbar \sqrt{L}$
EIGENFUNCTION PROPERTIES OF THE ATOMIC WAVEFUNCTIONS

Energy: Hydrogenic atom – \( \hat{H}_n^m = E_n^m \psi_n^m \), \( E_n \) from Bohr formula, \( V(r) = \frac{Ze^2}{4\pi\varepsilon_0 r} \)

Operator \rightarrow \text{Eigenvalue}

Many-electron atom – \( \hat{H}_{n\ell m} = E_{n\ell m} \psi_{n\ell m} \),
\( E_{n\ell} \) from solution of radial Schroedinger with

\[
V_{\text{eff}}(r) = \frac{Z^2_{\text{eff}, n\ell}(r) e^2}{4\pi\varepsilon_0 r}
\]

Square of angular momentum: \( \hat{L}^2 \psi_{n\ell m} = \hbar^2 \ell(\ell + 1) \psi_{n\ell m} \)

\( \rightarrow \) Always measure same value: \( \Delta(\hat{L}^2) = 0 \)

Z component of angular momentum: \( \hat{L}_z \psi_{n\ell m} = \hbar m \psi_{n\ell m} \)

\( \rightarrow \) Always measure same value: \( \Delta(L_z) = 0 \)

E.g. — \( n = 3, \ell = 2 \rightarrow \text{“}3d\text{”} \)

and finally

Parity = evenness or oddness: \( \hat{\Pi} \psi_{n\ell m}(\vec{r}) = \psi_{n\ell m}(-\vec{r}) \)

\( = (-1)^\ell \psi_{n\ell m}(\vec{r}) \)
Degeneracy in the hydrogenic atom (without spin)

<table>
<thead>
<tr>
<th>States</th>
<th>Degeneracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n = 1 ): 1s_0</td>
<td>1</td>
</tr>
<tr>
<td>( n = 2 ): 2s_0, 2p_{+1}, 2p_0, 2p_{-1} \ or 2s_0, 2p_x, 2p_y, 2p_z</td>
<td>4</td>
</tr>
<tr>
<td>( n = 3 ): 3s_0, 3p_x, 3p_y, 3p_z, \ or 3d_{3z^2-r^2}, 3d_{x^2-y^2}, 3d_{xy}, 3d_{yz}, 3d_{xz}</td>
<td>9</td>
</tr>
<tr>
<td>( n = \text{general} )</td>
<td>( n^2 )</td>
</tr>
</tbody>
</table>
TRANSITIONS BETWEEN LEVELS AND SELECTION RULES:

\[ m, \Phi_m(r,t) = \psi_m(r,\theta,\phi)e^{-iE_m t/\hbar} \]

\[ n, \Phi_n(r,t) = \psi_n(r,\theta,\phi)e^{-iE_n t/\hbar} \]

\[ \Delta \Phi(r,t) = a(t)\Phi_m + b(t)\Phi_n \]

1 \rightarrow 0, \quad 0 \rightarrow 1
Many transitions are not allowed: selection rules important.
ALLOWED TRANSITIONS IN X-RAY EMISSION:

\[ n = 5 \quad n = 4 \quad n = 3 \quad n = 2 \]

\[ N_{\alpha} \quad N_{\beta} \quad M_{\alpha} \quad M_{\beta} \quad L_{\alpha} \quad L_{\beta} \quad L_{\gamma} \]

\[ L \quad M \quad N \quad O \]

ALLOTTED: \( \Delta L = -1 \)

FORBIDDEN:

\[ \Delta L = 2 \quad 2s \rightarrow 1s \quad 3s \rightarrow 1s \quad 3d \rightarrow 1s \]

+ a continuum

Line Spectra

Bremsstrahlung
SPIN ANGULAR MOMENTUM: A LAST PROPERTY OF THE ELECTRON
THE STERN-GERLACH EXPERIMENT

- **Oven for Ag atoms**
  - Filled: \( 4d^{10}5s^1 \)
- **Oven for H atoms**
  - Source: \( 1s^2 \)
- **Collimator**
- **Magnet**
- **Collector plate**
- **Beam of silver atoms or H atoms**
- **Inhomogeneous magnetic field**
- **Class plate**
- **Classical pattern**
- **Actual pattern**

**Net forces:**
- \( B(z_2) > B(z_1) \)
- \( \uparrow \) for positive spin
- \( \downarrow \) for negative spin

**Two allowed orientations of magnetic moment \( \mathbf{\kappa} = \text{spin angular momentum} \)**
THE ELECTRON’S FINAL PROPERTY:
CHARGE = 1.602 X 10^{-19} C
MASS = 9.109 X 10^{-31} kg

SPIN ANGULAR MOMENTUM:
Quantum no. s = ½

\[ |\vec{S}| = \hbar \sqrt{s(s+1)} = \hbar \sqrt{3/4} \]

\[ S_z = \pm \hbar / 2 \]

SPIN MAGNETIC MOMENT:
\[ \vec{\mu}_s = -\frac{e}{m_e} \vec{S} = -2 \mu_B \vec{s} \]

with \( \mu_B = \frac{e\hbar}{2m_e} \)

= the Bohr magneton

= 9.274 x 10^{-28} J / T
The atomic orbitals:

$$\Psi_{n \ell m_z, m_s}(r, \theta, \phi, \text{spin}) = \Psi_{n \ell m_z}(r, \theta, \phi) \times [\alpha(\uparrow) \text{ or } \beta(\downarrow)]$$

**Complex, if \( m \neq 0 \)**

**But we can make them real for convenience**

**Matching for many \( e^- \) atoms**

**Changing for many \( e^- \) atoms**

**Z \( \rightarrow \) \( Z_{\text{eff, } n \ell}(r) \) in many-\( e^- \) atoms**
## Degeneracy in the hydrogenic atom with spin

<table>
<thead>
<tr>
<th>States</th>
<th>Degeneracy without spin</th>
<th>Degeneracy with spin</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n = 1$: $1s_0$</td>
<td>Not</td>
<td>2</td>
</tr>
<tr>
<td>$n = 2$: $2s_0$, $2p_{+1}, 2p_0, 2p_{-1}$, or $2s_0$, $2p_x, 2p_y, 2p_z$</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>$n = 3$: $3s_0$, $3p_x, 3p_y, 3p_z$, or $3d_{3z^2-r^2}, 3d_{x^2-y^2}, 3d_{xy}, 3d_{yz}, 3d_{xz}$</td>
<td>9</td>
<td>18</td>
</tr>
<tr>
<td>$n = \text{general}$</td>
<td>$n^2$</td>
<td>$2n^2$</td>
</tr>
</tbody>
</table>
ORBITAL ANGULAR MOMENTUM $\rightarrow$ ORBITAL MAGNETIC MOMENT

\[
\mu = iA
\]

\[
\vec{\mu}_L = -\frac{e}{2m_e} \vec{L} = -\mu_B \frac{\vec{L}}{\hbar}
\]

\text{with: } \mu_B \equiv \frac{e\hbar}{2m_e} \equiv \text{the Bohr magneton}
Classical interaction of magnetic moment and B field:
(Young and Freedman, Ch. 27)

\[ E = \text{potential energy} \]

\[ = -\mu \cdot \vec{B} = -\mu B \cos \phi \]

\[ \therefore \text{Lowest energy for } \mu \text{ parallel to } \vec{B} \]
Quantization of space:
The (randomly) precessing vector model:

- $L_x, L_y, L_z$ cannot all be constant: violates uncertainty principle
- Only $L^2$ (or $|L|$) and $L_z$ constant

\[ L_z = \hbar m_e, \quad m_e = +2, +1, 0, -1, -2 \]
\[ L^2 = \hbar^2 L(L+1) \]
\[ = \hbar^2 2(3) \]
\[ |L| = \hbar \sqrt{6} \]
Classical interaction of magnetic moment and B field:
(Young and Freedman, Ch. 27)

\[ E = \text{potential energy} = -\vec{\mu} \cdot \vec{B} = -\mu B \cos \phi \]
\[ \therefore \text{Lowest energy for } \vec{\mu} \text{ parallel to } \vec{B} \]
A FINAL (RELATIVISTIC) ATOMIC INTERACTION: SPIN-ORBIT COUPLING

(a) An electron circles an atomic nucleus, as viewed from the frame of reference of the nucleus. (b) From the electron's frame of reference, the nucleus is circling it. The magnetic field the electron experiences as a result is directed upward from the plane of the paper. The interaction between the electron's spin magnetic moment and this magnetic field leads to the phenomenon of spin-orbit coupling.

\[ \hat{H}_\psi = \hat{\kappa}_s \psi + \hat{\nu}_s \psi + \hat{H}_{s-o} \psi = E \psi \]

\[ E_{s-o} = -\frac{\mu_s \cdot \vec{B}_L}{2} \]

\[ E_{s-o} \propto + \frac{\vec{s} \cdot \vec{L}}{} \]

ADDS TO \( \hat{A} \) IN SCHROED. EQN.
\( \hat{H}_{S=0} \) couples \( \vec{S} \) and \( \vec{L} \) to new "conserved" \( \vec{J} \):

Figure 8.12 (a) A vector model for determining the total angular momentum \( J = L + S \) of a single electron. (b) The allowed orientations of the total angular momentum \( J \) for the states \( j = \frac{1}{2} \) and \( j = \frac{3}{2} \). Notice that there are now an even number of orientations possible, not the odd number familiar from the space quantization of \( L \) alone.

\[
\sqrt{\frac{2}{3}} \hat{J}_z \sqrt{j(j+1)}
\]

with: \( j = \{ \frac{3}{2}, \frac{5}{2}, \ldots \} \)

\[
\hat{J}_z = \hat{n} \hat{m}_j
\]

with: \( m_j = -j, -j+1, \ldots +j \)

\( 2j+1 \) degeneracy

\( \psi_{nl,s=\frac{1}{2},j,m_j} \) → "nLj" notation

Good quantum nos. if \( E_{S=0} \) strong.
SPIN-ORBIT SPLITTING IN HYDROGEN 2p (SMALL!):

Figure 8.11 The 2p level of hydrogen is split by the spin-orbit effect into a doublet separated by the spin-orbit energy $\Delta E = 5 \times 10^{-5}$ eV. The higher energy state is the one for which the spin angular momentum of the electron is "aligned" with its orbital angular momentum. The 1s level is unaffected, since no magnetic field arises for orbital motion with zero angular momentum.

But larger in inner shells of heavy atoms: E.g.

Fe (Z=26) - $2p_3/2$ and $2p_1/2$

$\Delta E_{SO} = 43.1$ eV

$\Delta E \approx 2\mu B = 23 \times 10^{-5}$ eV

$B_L = \frac{\mu_B}{2r} \frac{eV}{2\pi}$

$\mu_B = \text{Bohr magneton}$

$= \frac{e\hbar}{2m}$

$= \frac{9.3 \times 10^{-24}}{2\pi} \text{J/T} 

\approx 8.4 \times 10^{14}$ Hz

Tesla

$= 4\pi \times 10^{4}$ Gauss

$= 2.1 \times 10^{-9}$ T

$\mu_0 = 4\pi \times 10^{-7}$ N/A²

$\Rightarrow \Delta E_{SO} = 4.7 \times 10^{-5}$ eV is correct
LINE SPECTRA OF DIFFERENT SOURCES:

**Atomic hydrogen**

**Sodium**

**Helium**

**Neon**

**Mercury**

**Molecular hydrogen = \( H_2 \)**

The Sun: blackbody emission plus absorption

**WHY LINES?**

Sodium- D-line emiss.

Sodium- D-line absorp.
Spin-orbit splitting in spectroscopy: the sodium doublet

EXAMPLE 8.4  The Sodium Doublet

The famed sodium doublet arises from the spin–orbit splitting of the sodium $3p$ level, and consists of the closely spaced pair of spectral lines at wavelengths of 588.995 nm and 589.592 nm. Show on an energy level diagram the electronic transitions giving rise to these lines, labeling the participating atomic states with their proper spectroscopic designations. From the doublet spacing, deduce the magnitude of the spin–orbit energy.

Solution  The outer electron in sodium is the first electron to occupy the $n = 3$ shell, and it would go into the lowest energy subshell, the $3s$ or $3S_{1/2}$ level. The next highest levels belong to the $3p$ subshell. The $2(2\ell + 1) = 6$ states of this subshell are grouped into the $3P_{1/2}$ level with two states, and the $3P_{3/2}$ level with four states. The spin-orbit effect splits these levels by the spin–orbit energy. The outer electron, once it is excited to either of these levels by some means (such as an electric discharge in the sodium vapor lamp), returns to the $3S_{1/2}$ level with the emission of a photon. The two possible transitions $3P_{3/2} \rightarrow 3S_{1/2}$ and $3P_{1/2} \rightarrow 3S_{1/2}$ are shown in Figure 8.13. The emitted photons have nearly the same energy, but differ by the small amount $\Delta E$ representing the spin–orbit splitting of the initial levels. Since $E = \frac{hc}{\lambda}$ for photons, $\Delta E$ is found as

$$\Delta E = \frac{hc}{\lambda_2} - \frac{hc}{\lambda_1} = \frac{hc(\lambda_2 - \lambda_1)}{\lambda_1 \lambda_2}$$

For the sodium doublet, the observed wavelength difference is

$$\lambda_2 - \lambda_1 = 589.592 \text{ nm} - 588.995 \text{ nm} = 0.597 \text{ nm}$$

Using this with $hc = 1240 \text{ eV} \cdot \text{nm}$ gives

$$\Delta E = \frac{(1240 \text{ eV} \cdot \text{nm})(0.597 \text{ nm})}{(589.592 \text{ nm})(588.995 \text{ nm})} = 2.13 \times 10^{-3} \text{ eV}$$

Exercise 2 Using the spin–orbit interaction energy calculated in Example 8.4, deduce a value for the magnetic field strength at the site of the orbiting $3p$ electron in sodium.

Answer  $B = 18.38 \text{ T}$, a large field by laboratory standards.

From Serway, Moses, and Moyer—"Modern Physics"
What properties do wave functions of overlapping (thus indistinguishable) particles have?—electrons as example:

\[ \psi = \psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2), \text{ including spin of both electrons} \]

But labels can’t affect any measurable quantity.

E.g. – probability density:

\[ |\psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2)|^2 = |\psi(\vec{r}_2, \vec{s}_2; \vec{r}_1, \vec{s}_1)|^2 \]

Therefore

\[ \psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2) = \pm 1 \psi(\vec{r}_2, \vec{s}_2; \vec{r}_1, \vec{s}_1) \]

\[ = \hat{P}_{12} \psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2) \]

with \( \hat{P}_{12} \) = permutation operator \( \rightarrow \vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2 \)

and eigenvalues of \( \pm 1 \)

Finally, all particles in two classes:

**FERMIONS** (incl. e⁻'s): \( \psi \) antisymmetric

\[ s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots \]

\[ \hat{P}_{12} \psi = -1 \psi \]

**BOSONS** (incl. photons): \( \psi \) symmetric

\[ s = 0,1,2,... \]

\[ \hat{P}_{12} \psi = +1 \psi \]

Probability of finding two electrons at the same point in space with the same spin (\( \uparrow \uparrow \) or \( \downarrow \downarrow \)) is zero: “the Fermi Hole”

→the Exchange Interaction

→Hund’s 1st rule & magnetism
Antisymmetry and the Pauli Exclusion Principle:

Try Helium, 2 electrons in ground state 1s wave functions, “1s²”

Simple normalized antisymmetric trial wave function is

\[
\psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2) = \frac{1}{\sqrt{2}} \left[ \phi_{1s}(\vec{r}_1, \vec{s}_1 = \uparrow)\phi_{1s}(\vec{r}_2, \vec{s}_2 = \downarrow) - \phi_{1s}(\vec{r}_1, \vec{s}_1 = \downarrow)\phi_{1s}(\vec{r}_2, \vec{s}_2 = \uparrow) \right]
\]

interchanging labels gives

\[
\psi(\vec{r}_2, \vec{s}_2; \vec{r}_1, \vec{s}_1) = \frac{1}{\sqrt{2}} \left[ \phi_{1s}(\vec{r}_2, \vec{s}_2 = \uparrow)\phi_{1s}(\vec{r}_1, \vec{s}_1 = \downarrow) - \phi_{1s}(\vec{r}_2, \vec{s}_2 = \downarrow)\phi_{1s}(\vec{r}_1, \vec{s}_1 = \uparrow) \right]
\]

\[
= -\psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2), \text{ as required}
\]

Can’t tell which electron is spin up--indistinguishable

Also, if we try to put both electrons in 1s with spin-up (\(\uparrow\)), first term always cancels second term, and \(\psi = 0\)! Therefore, we have the Pauli Exclusion Principle \(\rightarrow\)
Thus, in a many-electron system:

- Anti-symmetry of total wave function implies:
  
  **Pauli Exclusion Principle:**
  
  No two electrons can have all the same quantum nos. $n, \ell, m_\ell, m_s$
  
  or, if spin-orbit split
  $n, \ell, j, m_j$

- Electronic structure determined by filling $n, \ell$ (or $n, \ell, j$) levels from lowest to highest energy ($E_{n,\ell}$ from radial Schrödinger Eqn. with $Z_{\text{eff}}$ depending on $n$ and $\ell$)

- Partially filled subshells $n, \ell$ (or $n, \ell, j$) have their lowest energy when a maximum no. of electrons have parallel spins
  = highest total spin angular momentum $= \vec{S}$ (Hund’s First Rule), and then they couple to yield highest total orbital angular momentum $= \vec{L}$ (Hund’s Second Rule)
The Hydrogenic Atom
Schroedinger Equation:
Spherical Polar Coordinates

Classically:

\[ V(r) = -\frac{Ze^2}{4\pi \varepsilon_0 r} \]

\[ \vec{L} = \vec{r} \times \vec{p} \]

is conserved

Quantum mechanically:

Polar angle = \( \theta = \text{arc cos}(z/r) \)

Azimuthal angle = \( \phi = \text{arc tan}(y/x) \)

Converting to new coordinates

Classically:

\[ \oint_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi = -\cos \theta \bigg|_0^\pi \times 2\pi = 4\pi \]

The Hydrogenic Atom
Schroedinger Equation:
Intraatomic electron screening in many-electron atoms—a self-consistent Q.M. calculation

Plus radial one-electron functions:

\[ P_{n\ell}(r) = rR_{n\ell}(r) \]
In many-electron atoms:
For a given n, s feels nuclear charge more than p, more than d, more than f

Lifts degeneracy on \( \ell \) in hydrogenic atom

\[
k_c = \frac{1}{(4\pi\varepsilon_0)}
\]
Ar--Evidence for shell structure
The radial probability distribution of all of the electrons in Argon, as derived from electron diffraction experiments and quantum-mechanical theory.

The shell structure of an Ar atom, as measured and calculated:

\[ K = L = 1s^2 \text{ } 2s^2 \text{ } 2p^6 \]

\[ M = 3s^2 \text{ } 3p^6 \]
ALLOWED TRANSITIONS IN X-RAY EMISSION:

\[ \begin{align*}
\text{O} & \quad n=5 \\
\text{N} & \quad n=4 \\
\text{M} & \\
\text{L} & \quad n=2 \\
\text{K} & \quad n=1
\end{align*} \]

\[ \begin{align*}
\text{allowed: } \Delta L &= -1 \\
\text{forbidden: } \Delta L &= \pm 2
\end{align*} \]

\[ \begin{align*}
K_\alpha & \quad L_\alpha, L_\beta, L_\gamma \\
K_\beta & \\
K_\gamma & \\
K_\delta & \\
3d & \quad n=3 \\
3s & \quad n=2 \\
2s & \quad n=1
\end{align*} \]

\[ \begin{align*}
(6 \text{ e}^-) & \rightarrow (5 \text{ e}^-) \\
(2 \text{ e}^-) & \rightarrow (1 \text{ e}^-) \text{ with hole}
\end{align*} \]

Bremsstrahlung:

\[ \begin{align*}
(2 \text{ e}^-) & \rightarrow (1 \text{ e}^-) \text{ with hole}
\end{align*} \]
Why lines?

Why similar systematics to hydrogen, but with $Z_{\text{eff}}$?

$Z_{\text{eff}} = Z - \text{no. inner e- screening} \approx Z - 7 - 2 = Z - 9$

$Z_{\text{eff}} = Z - \text{no. inner e- screening} \approx Z - 1$

Understood now!

Atomic number = $Z$

Square root of x-ray frequency
Filling the Atomic Orbitals:

<table>
<thead>
<tr>
<th>Orbital</th>
<th>n</th>
<th>l</th>
<th>m = 0</th>
<th>m = 1</th>
<th>m = 2</th>
<th>Maximum Occupation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>1</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>2s</td>
<td>2</td>
<td>0</td>
<td></td>
<td></td>
<td>x2</td>
<td>8</td>
</tr>
<tr>
<td>2p</td>
<td>2</td>
<td>1</td>
<td></td>
<td>+</td>
<td>-</td>
<td>6</td>
</tr>
<tr>
<td>3s</td>
<td>3</td>
<td>0</td>
<td></td>
<td></td>
<td>x2</td>
<td>10</td>
</tr>
<tr>
<td>3p</td>
<td>3</td>
<td>1</td>
<td></td>
<td>+</td>
<td>x2</td>
<td>18</td>
</tr>
<tr>
<td>3d</td>
<td>3</td>
<td>2</td>
<td></td>
<td>+</td>
<td>x2</td>
<td>+ 14 for nf</td>
</tr>
</tbody>
</table>

Total Degeneracy = 2

Filling the Atomic Orbitals:

Maximum Occupation = Degeneracy 2
### Transition Metals

Periodic Table, with the Outer Electron Configurations of Neutral Atoms in Their Ground States

The notation used to describe the electronic configuration of atoms and ions is discussed in all textbooks of introductory atomic physics. The letters s, p, d, . . . signify electrons having orbital angular momentum 0, 1, 2, . . . in units \( \hbar \); the number to the left of the letter denotes the principal quantum number of one orbit, and the superscript to the right denotes the number of electrons in the orbit.

<table>
<thead>
<tr>
<th>Element</th>
<th>Configuration</th>
<th>Element</th>
<th>Configuration</th>
<th>Element</th>
<th>Configuration</th>
<th>Element</th>
<th>Configuration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>1s² 2s¹</td>
<td>Be</td>
<td>1s² 2s²</td>
<td>Na</td>
<td>3s² 3p¹</td>
<td>Mg</td>
<td>3s² 3p²</td>
</tr>
<tr>
<td>K</td>
<td>4s² 4p¹</td>
<td>Ca</td>
<td>4s² 4p²</td>
<td>Sc</td>
<td>3d³ 4s²</td>
<td>Ti</td>
<td>3d² 4s²</td>
</tr>
<tr>
<td>V</td>
<td>3d³ 4s²</td>
<td>Cr</td>
<td>3d⁴ 4s¹</td>
<td>Mn</td>
<td>3d⁵ 4s²</td>
<td>Fe</td>
<td>3d⁶ 4s²</td>
</tr>
<tr>
<td>Co</td>
<td>3d⁷ 4s²</td>
<td>Ni</td>
<td>3d⁸ 4s²</td>
<td>Cu</td>
<td>3d⁹ 4s²</td>
<td>Zn</td>
<td>3d¹⁰ 4s²</td>
</tr>
<tr>
<td>Ga</td>
<td>4s² 4p³</td>
<td>Ge</td>
<td>4s² 4p⁴</td>
<td>As</td>
<td>4s² 4p⁵</td>
<td>Se</td>
<td>4s² 4p⁶</td>
</tr>
<tr>
<td>Br</td>
<td>4s² 4p⁷</td>
<td>Kr</td>
<td>4s² 4p⁸</td>
<td>Rb</td>
<td>5s² 5p¹</td>
<td>Sr</td>
<td>5s² 5p²</td>
</tr>
<tr>
<td>Y</td>
<td>4d² 5s²</td>
<td>Zr</td>
<td>4d³ 5s²</td>
<td>Nb</td>
<td>4d⁴ 5s²</td>
<td>Mo</td>
<td>4d⁵ 5s²</td>
</tr>
<tr>
<td>Tc</td>
<td>4d⁶ 5s²</td>
<td>Ru</td>
<td>4d⁷ 5s²</td>
<td>Rh</td>
<td>4d⁸ 5s²</td>
<td>Pd</td>
<td>4d⁹ 5s²</td>
</tr>
<tr>
<td>Ag</td>
<td>4d¹⁰ 5s²</td>
<td>Cd</td>
<td>4d¹¹ 5s²</td>
<td>In</td>
<td>4d¹² 5s²</td>
<td>Sn</td>
<td>4d¹³ 5s²</td>
</tr>
<tr>
<td>Sb</td>
<td>4d¹⁴ 5s²</td>
<td>Te</td>
<td>4d¹⁵ 5s²</td>
<td>Pb</td>
<td>4d¹⁶ 5s²</td>
<td>Bi</td>
<td>4d¹⁷ 5s²</td>
</tr>
<tr>
<td>Po</td>
<td>4d¹⁸ 5s²</td>
<td>At</td>
<td>4d¹⁹ 5s²</td>
<td>Rn</td>
<td>4d²⁰ 5s²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fr</td>
<td>5d² 6s²</td>
<td>Ra</td>
<td>5d² 6s²</td>
<td>Ac</td>
<td>5d² 6s²</td>
<td>Ce</td>
<td>4f⁵ 5d² 6s²</td>
</tr>
<tr>
<td>Pr</td>
<td>4f⁶ 5d² 6s²</td>
<td>Nd</td>
<td>4f⁷ 5d² 6s²</td>
<td>Pm</td>
<td>4f⁸ 5d² 6s²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sm</td>
<td>4f⁹ 5d² 6s²</td>
<td>Eu</td>
<td>4f⁹ 5d² 6s²</td>
<td>Gd</td>
<td>4f⁹ 5d² 6s²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tb</td>
<td>4f¹⁰ 5d² 6s²</td>
<td>Dy</td>
<td>4f¹¹ 5d² 6s²</td>
<td>Ho</td>
<td>4f¹² 5d² 6s²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Er</td>
<td>4f¹³ 5d² 6s²</td>
<td>Tm</td>
<td>4f¹⁴ 5d² 6s²</td>
<td>Yb</td>
<td>4f¹⁵ 5d² 6s²</td>
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<tr>
<td>Lu</td>
<td>4f¹⁶ 5d² 6s²</td>
<td>Th</td>
<td>5f² 6d² 7s²</td>
<td>Pa</td>
<td>5f² 6d² 7s²</td>
<td></td>
<td></td>
</tr>
<tr>
<td>U</td>
<td>5f³ 6d² 7s²</td>
<td>Np</td>
<td>5f⁴ 6d² 7s²</td>
<td>Pu</td>
<td>5f⁵ 6d² 7s²</td>
<td></td>
<td></td>
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<tr>
<td>Am</td>
<td>5f⁶ 6d² 7s²</td>
<td>Cm</td>
<td>5f⁷ 6d² 7s²</td>
<td>Bk</td>
<td>5f⁸ 6d² 7s²</td>
<td></td>
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</tr>
<tr>
<td>Cf</td>
<td>5f⁹ 6d² 7s²</td>
<td>Es</td>
<td>5f¹⁰ 6d² 7s²</td>
<td>Fm</td>
<td>5f¹¹ 6d² 7s²</td>
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<td></td>
</tr>
<tr>
<td>Md</td>
<td>5f¹² 6d² 7s²</td>
<td>No</td>
<td>5f¹³ 6d² 7s²</td>
<td>Lr</td>
<td>5f¹⁴ 6d² 7s²</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Notes:**
- The rare earths (RARE EARTHS) and actinides (ACTINIDES) are exceptions to the typical electronic configurations.
- The configuration \( d^{10} \) is half-filled, making it more stable.
SOME PERIODIC PROPERTIES:
(plus see www.webelements.com)
From www.webelements.com, with much more:
Hund's First Rule: highest total spin angular momentum
The quantum mechanics of covalent bonding in molecules: \( \text{H}_2^+ \) with one electron

\[
\varphi_- = \varphi_{\text{antibonding}} \\
\approx \varphi_{1sa} - \varphi_{1sb}
\]

\[
\varphi_+ = \varphi_{\text{bonding}} \\
\approx \varphi_{1sa} + \varphi_{1sb}
\]

**FIGURE 10.2** The net potential energy curve, showing the equilibrium separation and binding energy.

**FIGURE 8.4** (a) Potential energy of an electron in the electric field of two nearby protons. The total energy of a ground-state electron in the hydrogen atom is indicated. (b) Two nearby protons correspond quantum-mechanically to a pair of boxes separated by a barrier.
1. Hydrogen

Symmetry: $D_{ooh}$

### Bonding

$\phi_{bonding}^{MO} \approx \phi_{1sa} + \phi_{1sa}$

### Anti-Bonding

$\phi_{anti}^{MO} \approx \phi_{1sa} - \phi_{1sa}$

$\varepsilon_{positive}$ (unoccupied)

$\varepsilon = 0.2656$ a.u. = +7.21 eV

$\varepsilon_{negative}$ (occupied)

$\varepsilon = -0.5944$ a.u. = -16.16 eV

(Compare - 13.61 for H atom 1s)
THE ELECTRONS IN CARBON MONOXIDE:

- Symmetry: C_{nv}

- $\phi_{j}^{\text{MO}}(\mathbf{r}) = \sum_{\text{Atoms A Orbitals } i} c_{A_{i}j} \Phi_{A_{i}}^{\text{AO}}(\mathbf{r})$

- Carbon Monoxide

- 6\,e: 8\,e

- Bonding 3\sigma
  - \(2\,e = 5.210\) (3)

- Bonding 4\sigma
  - \(2\,e = 10.98\) (4)

- Non/Weakly Bonding 4\sigma
  - \(2\,e = 20.00\) a.u. (1 a.u. = 27.2 eV) (4)

- Bonding 5\sigma
  - \(1\,e = 0.1268\) (5, 6)

- Bonding 1\pi
  - \(1\,e = 0.6544\) (6)

- Anti-Bonding 2\pi
  - \(1\,e = 0.2755\) (10)

- Isocontours of 14.1\%

- 5\sigma

- 1\pi_x

- 1\pi_y

- Atomic orbital makeup

- G1s Core
  - (2)

- G1s Core
  - (4)