<table>
<thead>
<tr>
<th>Chapter</th>
<th>Reading</th>
<th>Questions/Problems, including Special labelled S1, S2,…</th>
</tr>
</thead>
<tbody>
<tr>
<td>1--Origins</td>
<td>All sections</td>
<td>Basics of classical physics &amp; challenges to it. Problem: Show that the exponential solutions to the e.m. wave equations in fact are valid solutions to it (see lecture slide)</td>
</tr>
<tr>
<td>3—Expts. Leading to quantum theory</td>
<td>Sections 3.1,3.3, 3.4, 3.5,3.6, 3.7,3.9 plus Section 14.8 on Accelerators, Synchrotrons, Linear Accelerators, pp. 533-536 (pp. 546-548), not including Fixed Target Accelerators</td>
<td>Probs. in Chap.3: 2,9,14,17,19,23, plus special part of 23: 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 (Use 20,000 volts),54 Probs. in Ch. 14- 31 and 34</td>
</tr>
<tr>
<td>2—Special relativity</td>
<td>Review entire chapter, but emphasis on 2.3, 2.5, 2.7, 2.8, 2.10-2.14, plus review from 12.6 on radioactive decay</td>
<td>Probs. in Chap. 2: 19, 25, 37, 51, 54,55,57,68,76, plus problem 12.26 (12.28)</td>
</tr>
<tr>
<td>12—Radioactive decay</td>
<td></td>
<td></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 lecture slides)</td>
<td>Probs. in Chap. 15: 2,4,9,11 (13),17 (21),24 (28)—plus for this problem, what is the frequency change due to velocity? Use equations in lecture for GPS.</td>
</tr>
<tr>
<td>4—Structure of the atom</td>
<td>4.1-4.6</td>
<td>Probs. in Chap. 4: 11,23-Use 410 nm,29,32,38</td>
</tr>
<tr>
<td>5—Wave properties of matter</td>
<td>All sections, plus supplementary reading on Fourier integrals</td>
<td>Probs. in Chap. 5: 1-Use 15°, 3, 10, 11, 12, 17, 19, 22, 25, 27, 28, 33, 40, 43, 45, 48 54(52), 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>All sections</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 and the kinetic energy operator,2,5,7,8,9,11,15,20,23,26,28,32 (34),37(39), 40(42),41(43),47(51),54(62)</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: 1,3,5,8,11,13,15,16,19(Do for a 4p state),20,29,32,35,38,46, plus S1: Show, using the full hydrogenic atom wave functions given in a lecture slide that, if you take the combinations $3d_{x^2}$+3$d_y$ and $3d_y$-3$d_x$, you get two of the real 3d orbitals, also shown in a lecture slide, and identify which ones.</td>
</tr>
</tbody>
</table>
### Question: 5
Probs. in Chap. 8: 1, 2, 4 (Do argon and krypton), 5, 7 (Do potassium, vanadium, selenium, zirconium, samarium, uranium), 11 (Do (a) $4s^2 4p^2$, (b) $4p^6 4d^1 5s^1$ and (c) $5s^2 4p^6 4f^1$), 12, 23 (Remember the dipole selection rules!), 24 (Do for 1.7 Tesla).

S1: Let $\hat{P}_{12}$ be the permutation operator for the labelling of two identical particles that occupy the same region in space, which is defined from $\hat{P}_{12} \psi (\vec{r}_1 , \vec{r}_2 ) = \psi (\vec{r}_2 , \vec{r}_1 )$. Now let $\hat{P}_{12}$ act on the following to determine which would be suitable choices for a wave function for two overlapping fermions (e.g. electrons, protons, or neutrons) or for two overlapping bosons (e.g., photons or pions) or for neither. Good wave functions must either be ant symmetric for fermions (-1 eigenvalue of $\hat{P}_{12}$) or symmetric for bosons (+1 eigenvalue of $\hat{P}_{12}$). Here, $\psi_{n/m_s,+} (\vec{r}_1 )$ represents particle 1 in spatial wavefunction $\psi_{n/m_s}$ and with spin up ($m_s = +1/2$), $\psi_{n/m_s,-} (\vec{r}_2 )$ represents particle 2 in spatial wavefunction $\psi_{n/m_s}$ and with spin down ($m_s = -1/2$), etc., etc. (See handout for further discussion.)

(a) $\psi (\vec{r}_1 , \vec{r}_2 ) = \psi_{100,+} (\vec{r}_1 ) \psi_{100,-} (\vec{r}_2 ) - \psi_{100,+} (\vec{r}_2 ) \psi_{100,-} (\vec{r}_1 )$

(b) $\psi (\vec{r}_1 , \vec{r}_2 ) = \psi_{100,+} (\vec{r}_1 ) \psi_{100,+} (\vec{r}_2 )$

(c) $\psi (\vec{r}_1 , \vec{r}_2 ) = \psi_{210,+} (\vec{r}_1 ) \psi_{21-1,-} (\vec{r}_2 ) - \psi_{21-1,-} (\vec{r}_1 ) \psi_{210,+} (\vec{r}_2 )$

(d) $\psi (\vec{r}_1 , \vec{r}_2 ) = \psi_{210,+} (\vec{r}_1 ) \psi_{21-1,-} (\vec{r}_2 )$.

S2: Show that the simple two-electron wave function for the ground state of He introduced in lecture is in fact normalized.
Converting to new coordinates

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

Quantum mechanically:

\[
\hat{K} = -\frac{\hbar^2}{2\mu} \nabla^2 = -\frac{\hbar^2}{2\mu} \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]
\]

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

\( \mu = \text{reduced mass} \)

\[
\mu = \frac{m_e}{1 + \frac{m_e}{M_n}}
\]

Classically:

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

\( L = r \times p \)

\( L \) is conserved

Center of mass

The Hydrogenic Atom
Schroedinger Equation:
Spherical Polar Coordinates

Hydrogenic Atom Sch. Eqn. is:

\[
\hat{H}\psi(r,\theta,\phi) = \hat{K}\psi(r,\theta,\phi) - \frac{Ze^2}{4\pi \varepsilon_0 r} \psi = E\psi
\]
Use separation of variables:

\[ \Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad [ \Theta(\theta) = f(\theta) \text{ & } \Phi(\phi) = g(\phi) \text{ in text} ] \]

**Assumed form**

Substitute, rearrange →

\[ \phi: \quad \frac{d^2 \Phi}{d\phi^2} + C_\phi \Phi = 0 \implies \Phi(\phi) = A e^{\pm iC_\phi \phi} \]

\[ \Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{\pm i m_\phi \phi} \quad (1) \text{ - complex} \]

\[ m_\phi = 0, \pm 1, \ldots \]
Solving for the $\phi$ part = $\Phi(\phi)$:

"Boundary" condition in $\phi$:

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

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

$$= 1$$

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

\[ \psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \]

Assumed form

Substitute, rearrange →

\[ \Phi(\phi) = \frac{1}{2\pi} e^{\pm im_\phi} \]

Complex

\[ C_\phi = m_\phi = 0, \pm 1, ... \]

\[ \Theta = \frac{1}{\sin \theta} \frac{d}{d\theta} (\sin \theta \frac{d \Theta}{d\theta}) + \left[ \frac{\Delta_\theta - \frac{m_\phi^2}{\sin^2 \theta} \right] \Theta = 0 \]

L(\ell + 1) \rightarrow Z_{\text{eff}}(r) \text{ in many e- atom}

\[ R = \left[ -\frac{\hbar^2}{2\mu} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{\ell(\ell + 1)}{2\mu r^2} - \frac{Ze^2}{4\pi \varepsilon_0 r} \right] R = ER \]

A "radial schrodinger eqn."

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

Changes for many-e- atoms

The Bohr Formula!

The same for many-e- atoms
The Bohr Formula!

\[ \Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad [ \Theta(\theta) = f(\theta) \text{ & } \Phi(\phi) = g(\phi) \text{ in text} ] \]

Assumed form:

1. \( \Phi(\phi) = A e^{\pm \text{i} m_\phi \phi} \)
2. \( \Theta(\theta) = \frac{1}{2 \pi} e^{\pm \text{i} m_\theta \theta} \)
3. \( R = -\frac{L(L+1)}{2m^2} \left( \frac{d^2}{dr^2} + \frac{2L+1}{r} \frac{d}{dr} \right) + \frac{\alpha^2 \text{e}^2}{4 \pi \text{\epsilon}_0 r} \) \( R = E \text{R} \)

The radial Schrödinger equation:

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

Solving for \( \Theta \) with 2:

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

Solving for \( R \) with 3:

\[ R_{nm}(r) = \text{ASSOC. LEGENDRE FUNCTIONS} \quad \text{also} \]
\[ (\text{POLYNOMIAL IN } \nu), e^{-\nu r}/r \text{ - REAL} \]

Changes for many-e\textsuperscript{-} atoms

The same for many-e\textsuperscript{-} atoms
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

\[
k_C \equiv \frac{1}{(4\pi\varepsilon_0)}
\]
GROUND STATE OF HYDROGENIC ATOM:

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

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

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

\[ r = a_0/Z \]

**MOST PROBABLE r = BOHR ORBIT RADIUS!**

\[ 4\pi r^2 dr \]

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

The atomic orbitals are complex if $m \neq 0$.

But we can make them real for convenience.

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

TABLE 6.1

<table>
<thead>
<tr>
<th>$n$</th>
<th>$\ell$</th>
<th>$m$</th>
<th>$\Phi(\phi)$</th>
<th>$\Theta(\theta)$</th>
<th>$R_{nm}(r)$</th>
<th>$\Psi_{nm}(r, \theta, \phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>$1 / \sqrt{2\pi}$</td>
<td>$1 / \sqrt{2}$</td>
<td>$2 \sqrt{2 \alpha_0} e^{-r/\alpha_0}$</td>
<td>$1 / \sqrt{\pi \alpha_0^2} e^{-r/\alpha_0}$</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>$1 / \sqrt{2\pi}$</td>
<td>$1 / \sqrt{2}$</td>
<td>$1 / 2 \sqrt{2 \alpha_0} e^{-r/2\alpha_0}$</td>
<td>$1 / 4 \sqrt{2 \pi \alpha_0^2} e^{-r/2\alpha_0}$</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>$\pm 1$</td>
<td>$1 / \sqrt{2\pi}$</td>
<td>$\sqrt{3} / 2 \sin \theta$</td>
<td>$1 / 2 \sqrt{6 \alpha_0^2} e^{-r/2\alpha_0}$</td>
<td>$1 / 8 \sqrt{3 \pi \alpha_0^2} e^{-r/2\alpha_0} \sin \theta e^{\pm i\phi}$</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>$1 / \sqrt{2\pi}$</td>
<td>$1 / \sqrt{2}$</td>
<td>$2 / 81 \sqrt{3 \alpha_0^2} e^{-r/3\alpha_0}$</td>
<td>$1 / 81 \sqrt{3 \pi \alpha_0^2} e^{-r/3\alpha_0} \sin \theta e^{\pm i\phi}$</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>$\pm 1$</td>
<td>$1 / \sqrt{2\pi}$</td>
<td>$\sqrt{6} / 2 \cos \theta$</td>
<td>$4 / 81 \sqrt{6 \alpha_0^2} e^{-r/3\alpha_0}$</td>
<td>$1 / 81 \sqrt{6 \pi \alpha_0^2} e^{-r/3\alpha_0} \cos \theta e^{\pm i\phi}$</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>$\pm 1$</td>
<td>$1 / \sqrt{2\pi}$</td>
<td>$\sqrt{10} / 4 (3 \cos^2 \theta - 1)$</td>
<td>$4 / 81 \sqrt{30 \alpha_0^2} e^{-r/3\alpha_0}$</td>
<td>$1 / 81 \sqrt{6 \pi \alpha_0^2} e^{-r/3\alpha_0} \sin \theta e^{\pm i\phi}$</td>
</tr>
</tbody>
</table>

*The quantity $\alpha_0 = 4\pi \epsilon_0 \hbar^2 / me^2 = 5.3 \times 10^{-11}$ m is equal to the radius of the innermost Bohr orbit.

\[ e^{-r/\alpha_0} \rightarrow e^{-Zr/\alpha_0} \text{ for hydrogenic } Z \rightarrow Z_{\text{eff}}(r) \text{ in many-e}^{-} \text{ atoms} \]
And for a hydrogenic atom: atomic no. \( Z \), one electron

\[
\psi_{100} = \frac{1}{\sqrt{\pi}} \frac{(Z \beta^2)}{a_0} e^{-Zr/a_0}
\]

\[
\psi_{200} = \frac{1}{4\sqrt{2\pi}} \frac{(Z \beta^2)}{a_0} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}
\]

\[
\psi_{210} = \frac{1}{4\sqrt{2\pi}} \frac{(Z \beta^2) Zr}{a_0} e^{-Zr/2a_0} \cos \theta
\]

\[
\psi_{21\pm 1} = \frac{1}{8\sqrt{\pi}} \frac{(Z \beta^2) Zr}{a_0} e^{-Zr/2a_0} \sin \theta e^{\pm i\phi}
\]

\[
\psi_{300} = \frac{1}{81\sqrt{3\pi}} \frac{(Z \beta^2)}{a_0} \left(27 - 18 \frac{Zr}{a_0} + 2 \frac{Zr^2}{a_0^2}\right) e^{-Zr/3a_0}
\]

\[
\psi_{310} = \frac{1}{81\sqrt{\pi}} \frac{(Z \beta^2)}{a_0} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \cos \theta
\]

\[
\psi_{31\pm 1} = \frac{1}{81\sqrt{\pi}} \frac{(Z \beta^2)}{a_0} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \sin \theta e^{\pm i\phi}
\]

\[
\psi_{320} = \frac{1}{81\sqrt{6\pi}} \frac{(Z \beta^2)}{a_0} \frac{Zr^2}{a_0^2} e^{-Zr/3a_0} (3 \cos^2 \theta - 1)
\]

\[
\psi_{32\pm 1} = \frac{1}{81\sqrt{\pi}} \frac{(Z \beta^2)}{a_0} \frac{Zr^2}{a_0^2} e^{-Zr/3a_0} \sin \theta \cos \theta e^{\pm i\phi}
\]

\[
\psi_{32\pm 2} = \frac{1}{162\sqrt{\pi}} \frac{(Z \beta^2)}{a_0} \frac{Zr^2}{a_0^2} e^{-Zr/3a_0} \sin^2 \theta e^{\pm 2i\phi}
\]

These are written in terms of the parameter

\[
a_0 = \frac{\hbar^2}{\mu e^2} = 0.529 \times 10^{-8} \text{ cm}
\]
MAKING THE ATOMIC ORBITALS REAL (E.G., FOR CHEMICAL BONDING):

\[ \psi_{n\ell m}\alpha(r, \theta, \phi) = R_{n\ell}(r) \Theta_\ell(\theta) \frac{1}{2\pi} e^{im\phi} \]

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

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

EXAMPLE: 2p ORBITALS

\[ \psi_{2\ell 0} = \psi_{2p_0} = \psi_{2p_2} \propto r \cos \theta = z \quad \text{(ALREADY REAL)} \]
\[ \psi_{2\ell 1} = \psi_{2p_1} \propto r \sin \theta e^{i\phi} = r \sin \theta [\cos \phi + i \sin \phi] \]
\[ \psi_{2\ell -1} = \psi_{2p_{-1}} \propto r \sin \theta e^{-i\phi} = r \sin \theta [\cos \phi - i \sin \phi] \]

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

See special problem for Chap. 7
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: $Y_{\ell m_{\ell}}(\theta,\phi) =$ "spherical harmonics"

But we can make them real for convenience.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$2\ m_{\ell}$</th>
<th>$\Phi(\phi)$</th>
<th>$\Theta_{2m_{\ell}}(\theta)$</th>
<th>$R_{n\ell}(r)$</th>
<th>$Y_{nm_{\ell}}(r,\theta,\phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0 0</td>
<td>$\frac{1}{\sqrt{2\pi}}$</td>
<td>$\frac{1}{\sqrt{2}}$</td>
<td>$\frac{2}{a_0^{3/2}} e^{-r/a_0}$</td>
<td>$\frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0}$</td>
</tr>
<tr>
<td>2</td>
<td>0 0</td>
<td>$\frac{1}{\sqrt{2\pi}}$</td>
<td>$\frac{1}{\sqrt{2}}$</td>
<td>$\frac{1}{2\sqrt{2} a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$</td>
<td>$\frac{1}{4\sqrt{2} a_0^{3/2}} \left(2 - \frac{r}{a_0}\right) e^{-r/2a_0}$</td>
</tr>
<tr>
<td>2</td>
<td>1 0</td>
<td>$\frac{\sqrt{6}}{2\pi}$</td>
<td>$\frac{\sqrt{3}}{2}$</td>
<td>$\frac{r}{2\sqrt{6} a_0^2} e^{-r/2a_0}$</td>
<td>$\frac{1}{8\sqrt{6} a_0^3} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0}$</td>
</tr>
<tr>
<td>3</td>
<td>0 0</td>
<td>$\frac{1}{\sqrt{2\pi}}$</td>
<td>$\frac{1}{\sqrt{2}}$</td>
<td>$\frac{2}{81\sqrt{3} a_0^3} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0}$</td>
<td>$\frac{1}{81\sqrt{3} a_0^3} \left(27 - 18 \frac{r}{a_0} + 2 \frac{r^2}{a_0^2}\right) e^{-r/3a_0}$</td>
</tr>
<tr>
<td>3</td>
<td>1 0</td>
<td>$\frac{\sqrt{6}}{2\pi}$</td>
<td>$\frac{\sqrt{3}}{2}$</td>
<td>$\frac{r}{2\sqrt{6} a_0^2} e^{-r/2a_0}$</td>
<td>$\frac{1}{81\sqrt{6} a_0^3} \left(6 - \frac{r}{a_0}\right) e^{-r/3a_0}$</td>
</tr>
<tr>
<td>3</td>
<td>1 ±1</td>
<td>$\frac{\sqrt{6}}{2\pi} e^{\pm i\phi}$</td>
<td>$\frac{\sqrt{3}}{2} \sin \theta$</td>
<td>$\frac{4}{81\sqrt{6} a_0^3} \left(6 - \frac{r}{a_0}\right) e^{-r/3a_0}$</td>
<td>$\frac{1}{81\sqrt{6} a_0^3} \left(6 - \frac{r}{a_0}\right) e^{-r/3a_0}$</td>
</tr>
<tr>
<td>3</td>
<td>2 0</td>
<td>$\frac{\sqrt{10}}{4\pi} (3 \cos^2 \theta - 1)$</td>
<td>$\frac{\sqrt{15}}{4} \sin \theta \cos \theta$</td>
<td>$\frac{4}{81\sqrt{30} a_0^{3/2}} \left(3 \cos^2 \theta - 1\right) e^{-r/3a_0}$</td>
<td>$\frac{1}{81\sqrt{30} a_0^{3/2}} \left(3 \cos^2 \theta - 1\right) e^{-r/3a_0}$</td>
</tr>
<tr>
<td>3</td>
<td>2 ±1</td>
<td>$\frac{\sqrt{15}}{4\pi} e^{\pm i\phi}$</td>
<td>$\frac{\sqrt{15}}{4} \sin^2 \theta$</td>
<td>$\frac{4}{81\sqrt{30} a_0^{3/2}} \left(3 \cos^2 \theta - 1\right) e^{-r/3a_0}$</td>
<td>$\frac{1}{81\sqrt{30} a_0^{3/2}} \left(3 \cos^2 \theta - 1\right) e^{-r/3a_0}$</td>
</tr>
</tbody>
</table>

Radial node for $r = 2a_0$

Angular node for $\theta = 90^\circ$

Radial node for $r = 6a_0$

Angular nodes for $\cos^2 \theta = 1/3$

$\theta = 54.7^\circ$, $125.3^\circ$

*The quantity $a_0 = 4\pi\epsilon_0 r^2/m_e = 5.3 \times 10^{-11}$ m is equal to the radius of the innermost Bohr orbit.

Z→$Z_{\text{eff},n\ell}(r)$ in many-e⁻ atoms

---

**IS SAME FOR MANY e⁻ ATOMS**

**CHANGES FOR MANY e⁻ ATOMS**
Aside on use of spherical harmonics as a complete set, like sines, cosines in Fourier analysis:

Expanding the Earth’s gravitational field in (real) spherical harmonics

\[ V = \frac{GM}{r} \left( 1 + \sum_{n=2}^{n_{\text{max}}} \left( \frac{a}{r} \right)^n \sum_{m=0}^{n} P_{nm}(\sin \theta) \left[ \bar{C}_{nm} \cos m\phi + \bar{S}_{nm} \sin m\phi \right] \right) \]

\( n = 2 \) to 360, no \( n = 1 \) if center of mass at origin

Yields 130317 separate terms! Finally:

1 gal = 1 cm/s\(^2\) \( \approx \) 1/981 of mean gravitational accel.

Accurate to features of about 55 km in size
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 $a_0 = 4\pi\varepsilon_0\hbar^2/Ze^2 = 0.053$ nm is the radius of the first Bohr orbit.
**Radial Probability Density**

\[ P_{nl}(r) = r^2 |R_{nl}(r)|^2 \text{ vs. } r \]

**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:**

\( n - 2 \) zeroes (incl. origin)

\( P_{nl}'s \) grouped in \( K, L, M, \ldots \) "shells" 

\( n = 1, 2, 3, \ldots \)
The Radial Probability Density

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

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

\[ \text{Classical turning points: } E_n = -\frac{kZe^2}{r_c} \]

\[ \frac{r_e}{a_0} = 2n^2 \]

\[ \text{Gen. rule: always } n-2 \text{ zeroes in } P_{n\ell}(r) \text{ (incl. } r = 0) \]
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 3p₀ orbital has a spherical node (indicated by the dashed line) and a nodal plane (the xy plane). The 3dₓ²−ᵧ² orbital has two nodal cones; the 3dₓᵧ 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:

Contours of equal probability in $|\psi|^2$

See also:
http://www.orbitals.com/orb/index.html
Comparison of three QM potential-well problems in 1 dimension

**Radial Part of H Atom**

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

\[ U(r) = -\frac{kZe^2}{r} \]

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

\( \neq -\infty \)

**Rigid Box**

\[ E_n \propto n^2 \]

\( E = 0 \rightarrow E_0 \]

\( E_0 \neq 0 \)

Also cannot go to minimum!

**Harmonic Oscillator**

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

\( U(x) = \frac{1}{2}Kx^2 \)

\( E_0 \)

\( E_0 \neq 0 \)

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, \( V(r) = \frac{Ze^2}{4\pi\varepsilon_0} \frac{1}{r} \)

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: \( \hat{L}^2 \psi_{n\ell m_r} = (\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2) \psi_{n\ell m_r} = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) \psi_{n\ell m_r} \)

\[
= \hbar^2 \ell (\ell + 1) \psi_{n\ell m_r}
\]

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

Z component of angular momentum: \( \hat{L}_z \psi_{n\ell m_r} = -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \psi_{n\ell m_r} = -i\hbar \frac{\partial}{\partial \phi} \psi_{n\ell m_r} = \hbar m_r \psi_{n\ell m_r} \)

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

E.g.—n = 3, \( \ell = 2 \) →”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

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

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

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

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

Operator \( \rightarrow \) Eigenvalue

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

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

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

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

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

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

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

and finally

Parity: \( \hat{R} \psi_{n\ell m_z}(\vec{r}) = \psi_{n\ell m_z}(\vec{r}^\prime) = (-1)^\ell \psi_{n\ell m_z}(\vec{r}) \)

Definition

\( r, \theta, \phi \rightarrow r, \pi - \theta, \phi + \pi \)
Some of the atomic orbitals, including radial dependence: Contours of equal probability in $|\psi|^2$

See also: [http://www.orbitals.com/orb/index.html](http://www.orbitals.com/orb/index.html)
# Degeneracy in the hydrogenic atom

<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>$n = 3$: $3s_0, 3p_x, 3p_y, 3p_z, 3d_{3z^2-r^2}, 3d_{x^2-y^2}, 3d_{xy}, 3d_{yz}, 3d_{xz}$</td>
<td>9</td>
</tr>
<tr>
<td>$n = \text{general}$</td>
<td>$n^2$</td>
</tr>
</tbody>
</table>
TRANSITIONS BETWEEN LEVELS AND SELECTION RULES:

\[ m, \bar{\Psi}_m(\vec{r}, t) = \psi_m(\vec{r}, \Theta, \Phi)e^{-iE_m t/\hbar} \]

\[ n, \bar{\Psi}_n(\vec{r}, t) = \psi_n(\vec{r}, \Theta, \Phi)e^{-iE_n t/\hbar} \]

X-POLARIZED

\[ \Delta \psi_m = E_n - E_m \]

During transition:

\[ \psi_n(\vec{r}, t) = a(t)\bar{\psi}_m + b(t)\bar{\psi}_n \]

\[ 1 \rightarrow 0 \quad \quad 0 \rightarrow 1 \]

Then

\[ = \int_{\text{all}} \bar{\psi} \times \psi \, dV \]

Only has non-zero oscillating + \( \ldots \)

Radiating part \( \propto \cos 2\pi v_{mn} t \)

If

\[ \langle x \rangle = \int_{\text{all}} \psi^n \times \psi_m \, dV \neq 0 \]

Intensity \( \propto \left| \int_{m \rightarrow n} \psi^n \times \psi_m \, dV \right|^2 \)

\( x = \text{"dipole operator"} \)

\[ \Rightarrow \text{"SELECTION RULES" OF:} \]

\[ l_{\text{FINAL}} = l_{\text{INITIAL}} \pm 1 \quad \text{or} \quad \Delta l = \pm 1 \]

\[ m_l, \text{FINAL} = m_l, \text{INITIAL}, m_l, \text{INITIAL} \pm 1 \quad \text{or} \quad \Delta m_l = 0, \pm 1 \]

See additional reading at website.
Allowed Transitions in the H Atom

Energy-level diagram for hydrogen showing transitions allowed by the selection rule $\Delta l = \pm 1$. In this diagram the vertical axis represents excitation energy above the ground state.
Bremsstrahlung
Copper, Molybdenum, 10-20 keV
Producing x-rays: the good old-fashioned way
+ Ze-

1s 2p 3p e-

Line Spectra + a continuum

50-100 keV

How are these measured?
How do the 2 aspects arise?
SPIN ANGULAR MOMENTUM: A LAST PROPERTY OF THE ELECTRON
THE STERN-GERLACH EXPERIMENT

Oven for Ag atoms \( \ldots 4d^{10} \) 5s\(^{-1} \)

Net Forces:

Two allowed orientations of magnetic moment \( \kappa \) - 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. \( s = \frac{1}{2} \)

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

\( s_z = \pm \hbar / 2 \)

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

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

= the Bohr magneton

= \( 9.274 \times 10^{-28} \) J / T
THE ELECTRON'S FINAL PROPERTY:
CHARGE = 1.602 X 10^{-19} C
MASS = 9.109 X 10^{-31} kg

+\ldots \quad \text{SPIN ANGULAR MOMENTUM:}
Quantum no. \, s = \frac{1}{2}

\begin{align*}
|\vec{s}| &= \hbar \sqrt{s(s + 1)} = \hbar \sqrt{3/4} \\
\hat{s}_z &= \pm \hbar / 2 \\
\text{SPIN MAGNETIC MOMENT:} \\
\hat{\mu}_s &= -\frac{e}{m_e} \hat{s} = -2 \mu_B \frac{\hat{s}}{\hbar}
\end{align*}

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

= the Bohr magneton

= 9.274 \times 10^{-28} \text{ J/T}
The atomic orbitals:

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

But we can make them real for convenience

With spin

e^{-r/na_0} \rightarrow e^{-Zr/na_0} \text{ for hydrogenic } Z \rightarrow Z_{\text{eff}}(r) \text{ in many-e\textsuperscript{-} atoms}

**TABLE 6.1**

**NORMALIZED WAVE FUNCTIONS OF THE HYDROGEN ATOM FOR n = 1, 2, AND 3**

<table>
<thead>
<tr>
<th>n</th>
<th>\ell</th>
<th>m_r</th>
<th>\phi</th>
<th>\Psi (r, \theta, \phi)</th>
<th>\text{R}(r)</th>
<th>\Psi_{n\ell m_r m_s} (r, \theta, \phi, \text{spin})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>±1</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>±1</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>±1</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>±1</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>±2</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>±1</td>
<td>0</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
<td>\frac{2}{a_0^2} e^{-r/na_0}</td>
<td>\frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a_0^3}} e^{-r/na_0}</td>
</tr>
</tbody>
</table>

*The quantity \( a_0 = 4\pi\varepsilon_0 \hbar^2/m_e^2 = 5.3 \times 10^{-11} \text{ m} \) is equal to the radius of the innermost Bohr orbit.
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&lt;sub&gt;0&lt;/sub&gt;</td>
<td>Not</td>
<td>2</td>
</tr>
<tr>
<td>$n = 2$: 2s&lt;sub&gt;0&lt;/sub&gt;, 2p&lt;sub&gt;0&lt;/sub&gt;, 2p&lt;sub&gt;0&lt;/sub&gt;, 2p&lt;sub&gt;-1&lt;/sub&gt;, or 2p&lt;sub&gt;x&lt;/sub&gt;, 2p&lt;sub&gt;y&lt;/sub&gt;, 2p&lt;sub&gt;z&lt;/sub&gt;</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>$n = 3$: 3s&lt;sub&gt;0&lt;/sub&gt;, 3p&lt;sub&gt;x&lt;/sub&gt;, 3p&lt;sub&gt;y&lt;/sub&gt;, 3p&lt;sub&gt;z&lt;/sub&gt;, or 3d&lt;sup&gt;3z^2-r^2&lt;/sup&gt;, 3d&lt;sub&gt;x^2-y^2&lt;/sub&gt;, 3d&lt;sub&gt;xy&lt;/sub&gt;, 3d&lt;sub&gt;yz&lt;/sub&gt;, 3d&lt;sub&gt;xz&lt;/sub&gt;</td>
<td>9</td>
<td>18</td>
</tr>
<tr>
<td>$n = general$</td>
<td>$n^2$</td>
<td>$2n^2$</td>
</tr>
</tbody>
</table>
ORBITAL ANGULAR MOMENTUM → ORBITAL MAGNETIC MOMENT

CLASSICAL

\[ \mu = iA \]

CURRENT LOOP

(a)

(b)
ORBITAL ANGULAR MOMENTUM $\Rightarrow$ ORBITAL MAGNETIC MOMENT

CLASSICAL

$\mu = iA$

with: the Bohr magneton $\mu_B \equiv \frac{e\hbar}{2m_e}$

CURRENT LOOP

$\mu_L = -\frac{e}{2m_e} \bar{L} = -\mu_B \frac{\bar{L}}{\hbar}$

$|\vec{\mu}_L| = iA = \frac{ev}{2\pi} \cdot \pi r^2$

$= \left(\frac{e}{2m_e}\right) |\vec{L}|$

$\vec{L} = r \times \vec{p}$

$|\vec{L}| = rmv$
Quantization of Space and the Zeeman Effect

Classical interaction of magnetic moment and B field:
(Young and Freedman, Ch. 27, Purcell, pp. 413-421)

\[ E = \text{potential energy} \]
\[ = -\vec{\mu} \cdot \vec{B} = -\mu B \cos \phi \]
∴ Lowest energy for \( \vec{\mu} \) 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 $|L|)$ + $L_z$ constant

$\mathbf{L} = \hbar m_L, m_L = \pm 2, \pm 1, 0, -1, -2$

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

$|\mathbf{L}| = \hbar \sqrt{L}$
Classical interaction of magnetic moment and B field:
(Young and Freedman, Ch. 27, Purcell, pp. 413-421)

\[ E = \text{potential energy} = -\vec{\mu} \cdot \vec{B} = -\mu B \cos \phi \]

\[ \therefore \text{Lowest energy for } \vec{\mu} \text{ parallel to } \vec{B} \]
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.
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.

\[ \hat{H} \psi = \hat{K} \psi + \hat{V} \psi + \hat{H}_{S-O} \psi = E \psi \]

\[ E_{S-O} = -\hat{r} \cdot \hat{\mathbf{B}}_L \]

\[ E_{S-O} \propto C + \hat{S} \cdot \hat{L} \]

ADDS TO \( \hat{A} \) IN SCHROD. EQN.
Spin-orbit coupling and a new angular momentum $J$

$H_{S-O}$ 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.
Spin-orbit coupling and a new angular momentum \( J \)

with:
\[
J_z = \sum m_j \cdot j, \quad j = 0, \pm 1, \pm 2, \ldots
\]

Eigenfunctions:
\[
|j, m_j \rangle
\]

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 \( j = 1 \). Notice that there are now an even number of orientations possible, not the odd number familiar from the space quantization of \( L \) alone.

Good quantum nos. if \( E_s \) strong

\[
2j + 1 \text{ degeneracy}
\]

Processingle model

Again

Processing model
EIGENFUNCTION PROPERTIES OF THE ATOMIC WAVEFUNCTIONS

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

Many-electron atom – \( \hat{H} \phi_{n\ell m}\ell = E_{n\ell} \phi_{n\ell m}\ell \), \( E_{n\ell} \) from solution of radial Schroedinger 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: \( \hat{L}^2 \psi_{n\ell m}\ell = (\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2) \psi_{n\ell m}\ell = -\hbar^2 \left( \frac{\partial^2}{\partial\theta^2} \cot\theta + \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right) \psi_{n\ell m}\ell \)

\[= \hbar^2 \ell (\ell + 1) \psi_{n\ell m}\ell\]

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

Z component of angular momentum: \( \hat{L}_z \psi_{n\ell m}\ell = -i\hbar (x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}) \psi_{n\ell m}\ell = -i\hbar \frac{\partial}{\partial\phi} \psi_{n\ell m}\ell = \hbar m_\ell \psi_{n\ell m}\ell\)

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

E.g. – \( n = 3, \ell = 2 \rightarrow "3d" \)
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.*

$Fe (Z=26) - 2p_{3/2}$

$2p \quad \Delta E_{SO} = 13.1 \text{ eV}$
LINE SPECTRA OF DIFFERENT SOURCES:

Atomic hydrogen

Sodium

Helium

Neon

Mercury

Molecular hydrogen = H₂

The Sun: blackbody emission plus absorption

WHY LINES?

¿Por qué líneas?
From Serway, Moses, and Moyer—"Modern Physics"
Bremsstrahlung
Copper, Molybdenum,..
10-20 keV
Producing x-rays:
the good old-fashioned way
+\[1s \rightarrow 2p, j = \frac{3}{2}\]
+\[1s \rightarrow 2p, j = \frac{1}{2}\]
Line Spectra
+a continuum

Spin-orbit splitting in high-resolution x-ray spectra
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 $\hat{P}_{12} = \text{permutation operator} \rightarrow \vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2$

and eigenvalues of $\pm 1$

Finally, all particles in two classes:

FERMIIONS: (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

$$s = 0, 1, 2, \ldots$$

$$\hat{P}_{12} \psi = +1 \psi$$

→the Exchange Interaction
→Hund’s 1st rule & magnetism

Probability of finding two electrons at the same point in space with the same spin (↑↑ or ↓↓) is zero: “the Fermi Hole”
Antisymmetry and the Pauli Exclusion Principle:

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

Simple normalized antisymmetric trial wave function is

$$\psi(\vec{r}_1, \vec{s}_1; \vec{r}_2, \vec{s}_2)$$

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

interchanging labels via permutation operator $\hat{P}_{12}$ gives

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

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

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

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

Also, if we try to put both electrons in 1s with spin-up (↑), first term always cancels second term, and $\psi = 0$! Therefore, we have the Pauli Exclusion Principle→
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 Schroedinger Eqn. with* $Z_{eff}$)

- **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)
A really accurate first wave function for He: Hyllerass, 1927-30, hand calculation and minimization of total energy:

If we take the nuclear charge to be $+Ze$ instead of $+2e$, we can treat helium-like ions such as $H^-$, $Li^+$, $Be^{2+}$. The Hamiltonian operator is

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{r_{12}}$$

(9.49)

How can we improve our variational result? We might try a function that had the general form of (9.77), i.e., a product of two functions, one for each electron:

$$\varphi = g(1)g(2)$$

(9.88)

However, we could try a variety of functions $g$ in (9.88), instead of the single exponential used in (9.77). A systematic procedure for finding the function $g$ that gives the lowest value of the variational integral will be discussed in Section 11.1. This procedure shows that for the best possible choice of $g$ in (9.88), the variational integral equals $-77.9$ eV, which is still in error by 1.4 percent. We might ask why (9.88) does not cause the variational integral to converge to the true ground-state energy, no matter what form we try for $g$. The answer is that when we write the trial function as the product of separate functions for each electron, we are making an approximation. Because of the $e^2/r_{12}$ term in the Hamiltonian, the Schroedinger equation for helium is not separable, and the true ground-state wave function cannot be written as the product of separate functions for each electron. To reach the true ground-state energy, we must go beyond a function of the form (9.88).

The Bohr model gave the correct energies for the hydrogen atom but failed when applied to helium. Hence in the early days of quantum mechanics, it was important to show that the new theory could give an accurate treatment of helium. The pioneering work on the helium ground state was done by Hyllerass in the years 1928-1930. He used variational functions that contained the interelectronic distance $r_{12}$ explicitly. This provides an effective way of taking into account the effects of one electron on the motion of the other. One function Hyllerass used is

$$\varphi = N [e^{-\xi r_1} e^{-\xi r_2} (1 + br_{12})]$$

(9.89)

where $N$ is the normalization constant and $\xi$ and $b$ are the variational parameters. Since

$$r_{12} = [(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2]^{1/2}$$

(9.90)

the function (9.89) goes beyond the simple product form (9.88). Minimization of the variational integral with respect to the parameters gives $\xi = 1.849$, $b = 0.364$, and a ground-state energy of $-78.7$ eV, in error by 0.3 eV. The $1 + br_{12}$ term makes the wave function larger for large values of $r_{12}$; this is as it should be, because the repulsion between the electrons makes it energetically more favorable for the electrons to avoid each other. A more complicated function used by Hyllerass is

$$\varphi = e^{-\xi r_1} e^{-\xi r_2} \sum_{i,j,k} c_{ijk} (r_1 + r_2) (r_1 - r_2) r_{12}^3$$

(9.91)

where the summation is over nonnegative integral values of $i$, $j$, and $k$. Using a function containing six terms in the sum, Hyllerass obtained an energy only 0.01 eV above the true ground-state energy.

Hyllerass's work has been extended by others. Pekeris\textsuperscript{3} used a function of the form (9.91) containing 1078(!) terms. The calculations involved a determinant of order 1078 and were carried out on an electronic computer. Pekeris found a ground-

The Hydrogenic Atom
Schroedinger Equation:
Spherical Polar Coordinates

Classically:
\[ \vec{L} = \vec{r} \times \vec{p} \]
is conserved
\[ \mu = \text{reduced mass} \]
\[ \mu = \frac{m_e}{1 + \frac{m_e}{M_n}} \]

Quantum mechanically:
\[ \hat{K} = -\frac{\hbar^2}{2\mu} \nabla^2 = -\frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \]
\[ \hat{L}^2 = \frac{\hat{p}_r^2}{2\mu} = \frac{\hat{L}^2}{2\mu r^2} \]

Polar angle = \( \theta = \text{arc cos}(z/r) \)
Azimuthal angle = \( \phi = \text{arc tan}(y/x) \)

\[ \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi = -\cos \theta \int_0^r r \times 2\pi = 4\pi \]

Converting to new coordinates
Intraatomic electron screening in many-electron atoms--a simple model

In many-electron atoms:
For a given n, s feels nuclear charge more than p, more than d, more than f

Lifts degeneracy on ℓ in hydrogenic atom

\[ k_c = \frac{1}{4\pi\varepsilon_0} \]
Intraatomic electron screening in many-electron atoms--a self-consistent Q.M. calculation

Plus radial one-electron functions:

\[ P_{n\ell}(r) \equiv rR_{n\ell}(r) \]
The shell structure of an Ar atom, as measured and calculated.

$K = L = 1s^2 \ 2s^2 2p^6$

$M = 3s^2 3p^6$

The radial probability distribution of all of the electrons in Argon, as derived from electron diffraction experiments and quantum-mechanical theory.
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>
Degeneracy in the a real atom with spin

**States**

- **$n = 1$:** $1s_0$
  
- **$n = 2$:** $2s_0$
  
  - $2p_{+1}, 2p_0, 2p_{-1}, \text{ or}$
  
  - $2p_x, 2p_y, 2p_z$

- **$n = 3$:** $3s_0$
  
  - $3p_x, 3p_y, 3p_z$
  
  - $3d_{x^2-r^2}, 3d_{x^2-y^2}, 3d_{xy}, 3d_{yz}, 3d_{xz}$

- **$n = 4$:** $4s_0$
  
  - $4p_x, 4p_y, 4p_z$
  
  - $4d_{x^2}, 4d_{y^2}, 4d_{xy}, 4d_{yz}, 4d_{xz}$
  
  - $4f_y^3, 4f_x^3, 4f_z^3, 4f_x(z-y), 4f_y(z-x), 4f_z(x-y), 4f_{xyz}$

- **$n$ total:** $2n^2$
Figure 7.13 The sequence of quantum states in an atom. Not to scale.
Seeing the energy levels with the photoelectric effect → "photoelectron spectroscopy" or "photoemission"

Gold: Z = 79: 1s^2 2s^2 2p^6 3s^2 3p^6 3d^10 4s^2 4p^6 4d^10 4f^1 5s^2 5p^6 5d^10 6s^1
Bremsstrahlung
Copper, Molybdenum, ...
10-20 keV
Producing x-rays:
the good old-fashioned way
+ Ze
1s
2p
3p
Line Spectra
+a continuum
50-100 keV
How are these measured?
How do the 2 aspects arise?

Hole
(2 e⁻) → (1 e⁻ with hole)

Line Spectra
+ a continuum

Bremsstrahlung

(6 e⁻) → (7 e⁻ with hole)
Why lines?

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

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

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

Understood now!

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

- **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**
  - $n=3$, $l=2$

Maximum Occupation = Degeneracy

Total:

- $2s^2$ + $2p^6$ + $3s^2$ + $3p^6$ + $3d^{10}$ + 14 for nf
FIGURE 7.13  The sequence of quantum states in an atom. Not to scale.
### 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 \( s, p, d, \ldots \) signify electrons having orbital angular momentum 0, 1, 2, \ldots 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>Periodic Table</th>
<th>Ground States</th>
<th>Transition Metals</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>He</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>B</strong></td>
<td>( 2s^2 )</td>
<td></td>
</tr>
<tr>
<td><strong>C</strong></td>
<td>( 2s^22p^2 )</td>
<td></td>
</tr>
<tr>
<td><strong>N</strong></td>
<td>( 2s^22p^3 )</td>
<td></td>
</tr>
<tr>
<td><strong>O</strong></td>
<td>( 2s^22p^4 )</td>
<td></td>
</tr>
<tr>
<td><strong>F</strong></td>
<td>( 2s^22p^5 )</td>
<td></td>
</tr>
<tr>
<td><strong>Ne</strong></td>
<td>( 2s^22p^6 )</td>
<td></td>
</tr>
<tr>
<td><strong>Al</strong></td>
<td>( 3s^2 )</td>
<td></td>
</tr>
<tr>
<td><strong>Si</strong></td>
<td>( 3s^23p^2 )</td>
<td></td>
</tr>
<tr>
<td><strong>P</strong></td>
<td>( 3s^23p^3 )</td>
<td></td>
</tr>
<tr>
<td><strong>S</strong></td>
<td>( 3s^23p^4 )</td>
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</tr>
<tr>
<td><strong>Cl</strong></td>
<td>( 3s^23p^5 )</td>
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</tr>
<tr>
<td><strong>Ar</strong></td>
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</tr>
<tr>
<td><strong>K</strong></td>
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</tr>
<tr>
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</tr>
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<tr>
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<td></td>
</tr>
</tbody>
</table>

- **4f** Filling...
- **6s** Filling...
- **5d** Filling...
- **5f** Filling...

### Rare Earths

- **Ce**
- **Pr**
- **Nd**
- **Pm**
- **Sm**
- **Eu**
- **Gd**
- **Tb**
- **Dy**
- **Ho**
- **Er**
- **Tm**
- **Yb**
- **Lu**

### Actinides

- **Ac**
- **Th**
- **Pa**
- **U**
- **Np**
- **Pu**
- **Am**
- **Cm**
- **Bk**
- **Cf**
- **Es**
- **Fm**
- **Md**
- **No**
- **Lr**

**Exceptions**

- **4f** Filling...
- **5d** Filling...
- **6s** Filling...

- **5f** Filling...
- **6s** Filling...
- **6d** Filling...

- **7f** Filling...

- **8s** Filling...

\[ \begin{align*}
\text{Exceptions:} & & \text{Exceptions:} \\
\text{5f} & & \text{6d} \\
\text{7f} & & \text{8s} \\
\end{align*} \]
SOME PERIODIC PROPERTIES:
(plus see www.webelements.com)
From www.webelements.com, with much more:
Hund’s First Rule: highest total spin angular momentum