Last time: Schrödinger Eqn for H atom is satisfied by a set of wavefns

\[ \psi_{n, l, m}(\vec{r}) \]

Where \( n = 1, 2, 3 \ldots \)
\( l = n-1, n-2 \ldots 0 \)
\( m = l, l-1 \ldots -l \)

When writing mathematical expressions for these wavefns, spherical coordinates are most convenient.

\[ \psi_{n, l, m}(\vec{r}) \text{ can be expressed as a product of an "r" function and a "}(\theta, \phi)\text{" function} \]

\[ \psi_{n, l, m}(\vec{r}) = R_{n, l}(r) Y_{l, m}(\theta, \phi) \]
Table 4.2: The first few spherical harmonics, $Y_n^m(\theta, \phi)$.

<table>
<thead>
<tr>
<th>$Y_n^m$</th>
<th>$Y_n^m(\theta, \phi)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Y_0^0$</td>
<td>$\frac{1}{4\pi} \frac{1}{\sqrt{2}}$</td>
</tr>
<tr>
<td>$Y_1^0$</td>
<td>$\frac{3}{4\pi} \frac{1}{\sqrt{2}} \cos \theta$</td>
</tr>
<tr>
<td>$Y_1^\pm$</td>
<td>$\frac{3}{8\pi} \frac{1}{\sqrt{2}} \sin \theta e^{\pm i\phi}$</td>
</tr>
<tr>
<td>$Y_2^0$</td>
<td>$\frac{5}{16\pi} \frac{1}{\sqrt{2}} (3 \cos^2 \theta - 1)$</td>
</tr>
<tr>
<td>$Y_2^\pm$</td>
<td>$\frac{15}{8\pi} \frac{1}{\sqrt{2}} \sin \theta \cos \theta e^{\pm i\phi}$</td>
</tr>
</tbody>
</table>

Table 4.6: The first few radial wave functions for hydrogen, $R_n(r)$.

\[
R_{10} = 2a^{-3/2} \exp\left(-\frac{r}{a}\right)
\]
\[
R_{20} = \frac{1}{\sqrt{2}} a^{-3/2} \left(1 - \frac{1}{2} \frac{r}{a}\right) \exp\left(-\frac{r}{2a}\right)
\]
\[
R_{21} = \frac{1}{\sqrt{24}} a^{-3/2} \frac{r}{a} \exp\left(-\frac{r}{2a}\right)
\]
\[
R_{30} = \frac{2}{\sqrt{27}} a^{-3/2} \left(1 - \frac{2}{3} \frac{r}{a} + \frac{2}{27} \left(\frac{r}{a}\right)^2\right) \exp\left(-\frac{r}{3a}\right)
\]
\[
R_{31} = \frac{1}{8\sqrt{6}} a^{-3/2} \left(1 - \frac{1}{6} \frac{r}{a}\right) \left(\frac{r}{a}\right) \exp\left(-\frac{r}{3a}\right)
\]
\[
R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2} \left(\frac{r}{a}\right)^2 \exp\left(-\frac{r}{3a}\right)
\]
\[
R_{40} = \frac{1}{4} a^{-3/2} \left(1 - \frac{3}{4} \frac{r}{a} + \frac{1}{8} \left(\frac{r}{a}\right)^2 - \frac{1}{192} \left(\frac{r}{a}\right)^3\right) \exp\left(-\frac{r}{4a}\right)
\]
\[
R_{41} = \frac{\sqrt{5}}{16\sqrt{3}} a^{-3/2} \left(1 - \frac{1}{4} \frac{r}{a} + \frac{1}{80} \left(\frac{r}{a}\right)^2\right) \frac{r}{a} \exp\left(-\frac{r}{4a}\right)
\]
\[
R_{42} = \frac{1}{64\sqrt{5}} a^{-3/2} \left(1 - \frac{1}{12} \frac{r}{a}\right) \left(\frac{r}{a}\right)^2 \exp\left(-\frac{r}{4a}\right)
\]
\[
R_{43} = \frac{1}{768\sqrt{35}} a^{-3/2} \left(\frac{r}{a}\right)^3 \exp\left(-\frac{r}{4a}\right)
\]
For example
\[ \psi_{1,0,0} = 2 a_0^{-3/2} e^{-r/a_0} \left( \frac{1}{4\pi} \right)^{1/2} \]

\[ \psi_{2,1,1} = \frac{1}{\sqrt{24}} a_0^{-3/2} \frac{5}{\pi} e^{-r/2a_0} \left( \frac{3}{8\pi} \right)^{1/2} \sin \theta \ e^{i\phi} \]

The \( r \)-dependence

\[ r e^{-r/a_0} \]

multiply straight line with \( e^{-r/a_0} \)

The \( \theta \)-dependence

<table>
<thead>
<tr>
<th>( \theta = 0 )</th>
<th>( \theta = \pi/2 )</th>
<th>( \theta = \pi )</th>
</tr>
</thead>
</table>

Magnitude increases at the "equator"

The \( \phi \)-dependence

\( \phi \) determines the complex phase angle of \( \psi_{2,1,1} \)
MORE DISCUSSION OF THE COMPLEX PHASE ANGLE

You may be familiar with the "de Broglic wavelength" of an electron

\[ \lambda_{db} = \frac{h}{p} \quad \text{Planck's constant} \]

\[ p \quad \text{momentum of electron.} \]

Large momentum, short wavelength (and vice versa)

Q: What physical quantity oscillates over the course of one wavelength?

A: The complex phase angle of the wave function.

For example, \[ \psi(\vec{r}) = A e^{\frac{2\pi i}{\lambda_{db}} x} \]

\[ \text{normalization constant} \]

\[ \text{describes an electron moving in the } x\text{-direction with momentum exactly } \frac{h}{\lambda_{db}}. \]

\[ \text{Momentum} \quad \text{Equivalent} \quad \text{The rate that phase changes through space} \]

\[ \text{This concept will come up again & again.} \]
ORBITAL ANGULAR MOMENTUM
OF H-ATOM WAVE FUNCTIONS

Consider \( \psi_{2,1,1}(\vec{r}) \)

The complex phase angle depends on the \( \phi \) coor.

\[ \psi_{2,1,1} \propto e^{i\phi} \]

If \( \phi \) changes by \( 2\pi \)

then phase angle changes by \( 2\pi \).

\( \lambda_{dB} \) depends on the radius of the orbit around the proton. If orbit radius is \( r \)

then \( \lambda_{dB} = 2\pi r \).

From classical mechanics, orbital angular momentum is

\[ L = mv r = pr \]

In this case, \( p = \frac{\hbar}{\lambda_{dB}} \)

Therefore \( L = \frac{\hbar}{2\pi} r = \frac{\hbar}{2\pi} = \frac{\hbar}{r} \)

\( \psi_{2,1,1} \) has one quanta of angular mom

independent of \( r \)!
The wave functions with higher energy have more kinetic energy which means more curvature.

\[
\left| \frac{\hbar^2}{2m} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) \right| \text{ is bigger.}
\]

The curvature can come from the \( r \)-dependence of the wavefunction, or the angular dependence, or both.
Radial component of H-atom wavefunctions, $R_{nl}(r)$

Increase angular momentum

$l = 0$  $l = 1$  $l = 2$

Focus on the $n=3$ orbitals

$R_{3,0}$ puts all curvature in the $r$-direction ($\psi_{0,0}$ is constant)

$R_{3,1}$ has less curvature in $r$-direction (more curvature in $\theta$ & $\phi$)

$R_{3,2}$ has minimal curvature in $r$-direction (no nodes) Most curvature in $\theta$ & $\phi$ directions.
Also notice that s-orbitals ($l=0$) are maximal at $r=0$, while all other orbitals have nodes at $r=0$.

Why? Giving an $e^-$ orbital angular momentum is equivalent to changing $V(r)$.

$$V_{\text{effective}}(r)$$

$\begin{align*}
\text{l=0, } &\text{ } V \propto \frac{1}{r} \\
\text{l=1} & \\
\text{l=2} &
\end{align*}$$