Announcement

Course webpage
http://highenergy.phys.ttu.edu/~slee/2402/

Textbook
Modern Physics, 2/E
Randy Harris, University of California, Davis
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HW6 (due 4/9)
18, 20, 23, 32, 37, 38, 45, 47, 53, 60
Quiz 2 (4/9): Ch.6 & Ch.7

Schedule

<table>
<thead>
<tr>
<th></th>
<th>Tuesday</th>
<th>Thursday</th>
<th>Saturday</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ch.7</td>
<td>3/26</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ch.7,8</td>
<td>3/31</td>
<td>4/2</td>
<td></td>
</tr>
<tr>
<td>Ch.8</td>
<td>4/7</td>
<td>4/9</td>
<td></td>
</tr>
<tr>
<td>Ch.9</td>
<td>4/14</td>
<td>4/16</td>
<td></td>
</tr>
<tr>
<td>Ch.11,12</td>
<td>4/21</td>
<td>4/23</td>
<td></td>
</tr>
<tr>
<td>[Quiz.2: Ch.6/7]</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Presentations</td>
<td>9:00 – 12:30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4/28</td>
<td>4/30</td>
<td></td>
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</tr>
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<tr>
<td>5/5</td>
<td>5/9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[Summary]</td>
<td>Final Exam</td>
<td>4:300 - 7:00pm</td>
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</tbody>
</table>

Note.1: Term paper presentation (10 min. = 8+2 (Q&A))
Note.2: Term paper due (5/5)

Chapter. 7
QM in 3-dims & Hydrogen Atom

Outline:

• The Schrödinger Eq. in 3-Dimensions
• The 3D Infinite Well
• Energy Quantization & Spectral Lines in Hydrogen
• The Schrödinger Eq. for a Central Force
• Angular Behavior in a Central Force
• The Hydrogen Atom
• Radial Probability
• Hydrogen-like Atoms
Toward the Hydrogen Atom

Quantization of Angular Momentum

Angular momentum operator

\[ \hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}. \]

\[ \hat{L}_z^2 \Phi_{m_\ell}(\phi) = (m_\ell \hbar)^2 \Phi_{m_\ell}(\phi) \]

\[ \Phi_{m_\ell}(\phi) = e^{im_\ell \phi} \quad (m_\ell = 0, \pm 1, \pm 2, \pm 3, \ldots) \]

Angular Momentum Operator

Toward the Hydrogen Atom

We break it into pieces.

i.e. separation variables for a central force (see p247)

\[ L_z = m_\ell \hbar \quad (m_\ell = 0, \pm 1, \pm 2, \pm 3, \ldots) \]

Angular Momentum Operator

\[ \Phi \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Phi}{\partial r} \right) + \Phi \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \Phi \csc^2 \theta \frac{\partial^2 \Phi}{\partial \phi^2} \]

After canceling, we find that some of the variables are separate:

\[ \frac{1}{R} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\Theta} \csc \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi} \frac{\partial^2 \Phi}{\partial \phi^2} = \frac{-m^2}{\hbar^2} \]

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

i.e. separation variables for a central force (see p247)
**Toward the Hydrogen Atom - Separation of \( \theta \)**

Polar Equation

\[
\frac{1}{\Theta} \csc \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) - m_\ell^2 \csc^2 \theta \Theta(\theta) = C_\phi(\theta)
\]

or

\[
csc \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) - m_\ell^2 \csc^2 \theta \Theta(\theta) = C_\phi(\theta)
\]

Far more challenging equation than others we have seen :)

\[
m_{l}^2
\]

Solution is possible (non-divergent) only if:

\[
C_\phi \begin{array}{cccc}
0 & -2 & -6 & \ldots \\
\ell = 0, 1, 2, \ldots
\end{array}
\]

\[
m_\ell \begin{array}{cccc}
0, \pm 1, \pm 1, \pm 2 & \ldots & 0, \pm 1, \pm 2, \ldots, \pm \ell
\end{array}
\]

\( m \) and \( l \) are related!

\( l = \) a new quantum number

\[
\frac{1}{\Theta} \csc \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) - m_\ell^2 \csc^2 \theta \Theta(\theta) = C_\phi
\]

or

\[
csc \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta(\theta)}{d\theta} \right) - m_\ell^2 \csc^2 \theta \Theta(\theta) = C_\phi(\theta)
\]

Legendre Polynomials

\[
\Theta_{\ell,m_\ell}(\theta) = P_{\ell,m_\ell}(\cos \theta)
\]

\[
\ell = 0, 1, 2, \ldots
\]

\[
m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell
\]
Legendre Polynomials

<table>
<thead>
<tr>
<th>$\ell, m_\ell$</th>
<th>$P_{\ell,m_\ell} (\cos \theta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0, 0</td>
<td>1</td>
</tr>
<tr>
<td>1, 0</td>
<td>$\cos \theta$</td>
</tr>
<tr>
<td>1, 1</td>
<td>$\sin \theta$</td>
</tr>
<tr>
<td>2, 0</td>
<td>$\frac{1}{2}(3 \cos^2 \theta - 1)$</td>
</tr>
<tr>
<td>2, 1</td>
<td>$3 \cos \theta \sin \theta$</td>
</tr>
<tr>
<td>2, 2</td>
<td>$3 \sin^2 \theta$</td>
</tr>
<tr>
<td>3, 0</td>
<td>$\frac{1}{2}(5 \cos^3 \theta - 3 \cos \theta)$</td>
</tr>
<tr>
<td>3, 1</td>
<td>$\frac{3}{2}(5 \cos^2 \theta - 1) \sin \theta$</td>
</tr>
<tr>
<td>3, 2</td>
<td>$15 \cos \theta \sin^2 \theta$</td>
</tr>
<tr>
<td>3, 3</td>
<td>$15 \sin^3 \theta$</td>
</tr>
</tbody>
</table>

The meaning of $l$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

See Appendix G

$$\hat{L}^2 = -\hbar^2 \left[ \csc \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \csc^2 \theta \frac{\partial^2}{\partial \phi^2} \right]$$

Angular part of Schrodinger Eq.

$$\hat{L}^2 (\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi)) = \hbar^2 \ell (\ell + 1) (\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi))$$

Units of angular momentum

$$|L| = \sqrt{L^2} = \sqrt{\ell (\ell + 1)} \hbar$$  \hspace{1cm} ($\ell = 0, 1, 2, \ldots$)

$L \sim$ Magnitude of Angular Momentum

Angular part of Schrodinger Eq.

$$\hat{L}^2 (\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi)) = \hbar^2 \ell (\ell + 1) (\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi))$$

Angular part of Schrodinger Eq.

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Angular part of Schrodinger Eq.

$$\hat{L}^2 (\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi)) = \hbar^2 \ell (\ell + 1) (\Theta_{l,m_l}(\theta)\Phi_{m_l}(\phi))$$
Quantized so far:

\[ L_z = m_\ell \hbar \quad (m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell) \]

The projection of angular momentum to z-axis

\[ |L| = \sqrt{L^2} = \sqrt{\ell(\ell + 1)} \hbar \quad (\ell = 0, 1, 2, \ldots) \]

The magnitude of (orbital) angular momentum

\[ m_\ell = \text{MAGNETIC QUANTUM NUMBER} \]

\[ l = \text{ORBITAL QUANTUM NUMBER} \]

The Uncertainty Principle

Planar motion violates the uncertainty Principle!!

Angular Momentum Quantization

\[ |L| = \sqrt{L^2} = \sqrt{\ell(\ell + 1)} \hbar \]

\[ L_z = m_\ell \hbar \]

Angular probability densities for a central force
The Radial Part of Schrödinger Equation for Hydrogen Atom

\[ \frac{1}{R} \frac{d}{dr} \left( r \frac{dR}{dr} \right) + \left[ \frac{1}{\Theta} \csc \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \csc^2 \theta \frac{d}{d\theta} \right] m_\ell^2 = -r^2 \frac{m(E - U(r))}{\hbar^2} \]

\[ \frac{1}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \ell(\ell + 1) = -r^2 \frac{2m(E - U(r))}{\hbar^2} \]

Associated Laguerre Equation: \( R(r) = Ae^{-r/a_0} \), \( d^2R/dr^2 = R/a_0^2 \)

Energy quantization

\[ E = \frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2n^2} \]

(\( n = 1, 2, 3, \ldots \) and \( \ell = 0, 1, 2, \ldots, n - 1 \))

Quantum number \( \ell \) is limited to \( (n-1) \)

The principal quantum number \( n \)
Bohr Radius

\[ E = -\frac{\hbar^2}{2ma_0^2 n^2} \]

\[ a_0 = \frac{(4\pi\varepsilon_0)\hbar^2}{me^2} = 0.0529 \text{ nm} \]

How Small is “Small”?  

Probability Density and Normalization

\[ |\Psi(r, i)|^2 = |\psi(r, \theta, \phi)|^2 = (R(r)\Theta(\theta)\Phi(\phi))^* (R(r)\Theta(\theta)\Phi(\phi)) \]

\[ |\psi(r, \theta, \phi)|^2 = (R(r)\Theta(\theta))^2 \]

Total Prob. of finding electron somewhere in space must be “1”.  
Using the volume element in spherical polar coordinate (see 7-4), normalization condition becomes…

Quantum numbers

<table>
<thead>
<tr>
<th>Energy</th>
<th>( n )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>...</th>
<th>( n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \ell )</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>( m_\ell )</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>0</td>
<td>+1</td>
<td>0</td>
</tr>
</tbody>
</table>

Degeneracy

| | 1 | 4 | 9 | ... | \( n^2 \) |

\[ \frac{-\hbar^2}{2m} \frac{d}{dr} \left( r^2 \frac{d}{dr} R(r) \right) + \frac{\hbar^2}{2mr^2} \ell(\ell + 1) R(r) + U(r) R(r) = ER(r) \]

“accidental” degeneracy

Because of \( 1/r \)

Because of \( 1/r \)

Table 6.5 Radial Solutions of (6-26)

<table>
<thead>
<tr>
<th>( n, \ell )</th>
<th>( R_{n, \ell}(r) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 0</td>
<td>( \frac{1}{(1a_0)^{3/2}} 2e^{-r/2a_0} )</td>
</tr>
<tr>
<td>2, 0</td>
<td>( \frac{1}{(2a_0)^{3/2}} 2 \left( 1 - \frac{r}{2a_0} \right) e^{-r/2a_0} )</td>
</tr>
<tr>
<td>2, 1</td>
<td>( \frac{1}{(2a_0)^{3/2} \sqrt{3} a_0} e^{-r/2a_0} )</td>
</tr>
<tr>
<td>3, 0</td>
<td>( \frac{1}{(3a_0)^{3/2}} \left( 2 - \frac{4r}{3a_0} + \frac{4r^2}{27a_0^2} \right) e^{-r/3a_0} )</td>
</tr>
<tr>
<td>3, 1</td>
<td>( \frac{1}{(3a_0)^{3/2} 9a_0} \left( 1 - \frac{r}{6a_0} \right) e^{-r/3a_0} )</td>
</tr>
<tr>
<td>3, 2</td>
<td>( \frac{1}{(3a_0)^{3/2} 27 \sqrt{3} a_0^3} e^{-r/3a_0} )</td>
</tr>
</tbody>
</table>
Now, we can discuss where hydrogen’s e might be found

Traditional naming scheme

Spectroscopic notation

<table>
<thead>
<tr>
<th>Letter</th>
<th>s</th>
<th>p</th>
<th>d</th>
<th>f</th>
<th>g</th>
<th>h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value of ( \ell )</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
</tbody>
</table>

S: sharp, p: principle, d: diffuse, f: fundamental...

3d state: \( n=3 \) & \( l = 2 \)

2p state: \( n=2 \) & \( l = 1 \)

Electron Prob. Densities in the Hydrogen atom, through \( n = 3 \)

State are labeled using spectroscopic notation: \( n, l \)

2d state is possible? — No!!

Because, here, \( n=2 \), \( d =2 \);

Remember \( n > d \)

Experimental Evidence of Quantization:

Spectral Lines

experimentally observed hydrogen wavelengths

\[ \lambda = \frac{1}{R_H} \left( \frac{1}{\ell^2} - \frac{1}{n^2} \right) \quad (\ell = 3, 4, 5, \ldots) \]

Rydberg constant
Spectral Lines

Hydrogen’s energies & spectral lines:
A photon is emitted when the electron jumps downward.

Summary

Time-independent Schrödinger equation
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi(r) + U(r) \psi(r) = E \psi(r) \]

Hydrogen atom potential energy
\[ U(r) = -\frac{1}{4\pi\varepsilon_0} \frac{e^2}{r} \quad (6-9) \]

Hydrogen atom wave function
\[ \psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \]

Energy levels
\[ E = -\frac{m e^4}{2(4\pi \varepsilon_0)^2 \hbar^2 n^2} \quad (n = 1, 2, 3, \ldots) \]

Angular momentum
\[ |L| = \sqrt{\ell(\ell + 1)} \hbar \quad (\ell = 0, 1, 2, \ldots, n - 1) \]

Z angular momentum
\[ L_z = m_\ell \hbar \quad (m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell) \]