Recently:
1. Quantum tunneling
2. Schrödinger equation in 3-D
3. Hydrogen atom

Today:
1. Hydrogen atom (cont.)
2. Multi-electron atoms
3. Periodic table
4. Bonding (?)

Coming Up:
Finish bonding/banding...

Exam 3 – Next Thursday, 4/28
Lecture for Tuesday, 5/3

\[ \psi_{n\ell m}(r, \theta, \phi) = R_{\ell}(r)Y_{\ell m}(\theta, \phi) \]

<table>
<thead>
<tr>
<th>State</th>
<th>( r )</th>
<th>( \ell = 1 ), ( m \leq 0 )</th>
<th>( \ell = 1 ), ( m = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>0</td>
<td>dumbbell shaped</td>
<td>bagel shaped around z-axis (traveling wave)</td>
</tr>
</tbody>
</table>

\[ n = 2, \ell = 1, m = 0 \rightarrow \psi_{210} = \frac{1}{2\sqrt{5}} \frac{r}{a_0} e^{-2a_0r} \left( -\frac{r}{\sqrt{5}} \cos \theta \right) \]

\[ n = 2, \ell = 1, m = 1 \rightarrow \psi_{211} = \frac{1}{2\sqrt{6\pi}} \frac{r}{a_0} e^{-2a_0r} \left( -\frac{r}{\sqrt{6\pi}} \sin \theta \right) \]

Superposition applies:
- \( p_z \) (addition of \( m = 1 \) and \( m = -1 \))
- \( p_y \) (subtraction of \( m = 1 \) and \( m = -1 \))

Shapes of hydrogen wave functions:

In the 1s state, the most likely single place to find the electron is:

A) \( r = 0 \)
B) \( r = a_0 \)
C) Why are you confusing us so much?

\[ \psi \text{nlm} \]
Physics vs Chemistry view of orbits:

2p wave functions (Physics view) (n=2, l=1)

<table>
<thead>
<tr>
<th>m=1</th>
<th>m=0</th>
<th>m=-1</th>
</tr>
</thead>
</table>

Dumbbell Orbits (chemistry)

px = superposition (addition of m=-1 and m=+1)
py = superposition (addition of m=-1 and m=+1)

Chemistry: Shells – set of orbitals with similar energy

1s, 2s, 2p, 3s, 3p, 3d

n=1, 2, 3 … = Principle Quantum Number

E_n = -E_1 / n^2 (for Hydrogen, same as Bohr)

l=s, p, d, f … = Angular Momentum Quantum Number

l = 0, 1, 2, 3 (restricted to 0, 1, 2 … n-1)

|m| = 0, 1, 2, 3 = z-component of Angular Momentum (restricted to -l to l)

L_z = m\hbar

What is the magnitude of the angular momentum of the ground state of Hydrogen?

a. 0
b. \sqrt{2}\hbar
c. sqrt(2)\hbar
d. not enough information

Answer is a.
n=1 so l=0 and m=0 … Angular momentum is 0 …

According to Schrödinger:

| L | | L_n=1, l=0 | 0 |

\[ L \approx \sqrt{l(l+1)} \hbar \]

\[ |L_{n=1, l=0}| = \sqrt{0(0+1)} \hbar = 0 \]

\[ \vec{\mu} = -\frac{e}{2m_e} \vec{L} = 0 \] (S-state)

According to Bohr:

| L | | L_{n=1} | 1 \hbar |

\[ |L_{n=1}| = \hbar \]

\[ |L_{n=1}| = 1 \cdot \hbar = \hbar \]

\[ \vec{\mu}_B = -\frac{e}{2m_e} \vec{L} = -\frac{\hbar}{2m_e} \] (ground state)

Bohr magneton!!

\[ \mu_z = \pm \mu_B \neq 0!! \] (ground state)

Energy of a Current Loop in a Magnetic Field:

\[ \vec{\tau} = \vec{\mu} \times \vec{B} \]

\[ \tau = \mu B \sin(\phi) \]

\[ dU = -dW = -d\phi \]

\[ \Delta U = -\mu B \cos(\phi) = -\vec{\mu} \cdot \vec{B} \]

For an electron moving in a circular orbit: (old HW problem)

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

Stern-Gerlach Experiment with Silver Atoms (1922)

Ag = 4d^{10}5s^{1}

What was actually observed

Silver atoms

Inhomogeneous magnetic field

What gives??!
The Zeeman Effect: \[ \Delta U = -\mu B \cos(\phi) = -\vec{\mu} \cdot \vec{B} \]

Spectrum:
- With no external field
- External field ON

Helium (2 e⁻) in the excited state 1s²2p¹
- m = 0 states unaffected
- m = ±1 states split into \( \Delta E = \pm \mu_z B \)

The Anomalous Zeeman Effect: \[ \Delta U = -\mu B \cos(\phi) = -\vec{\mu} \cdot \vec{B} \]

Spectrum:
- With no external field
- External field ON

Hydrogen (1 e⁻) in the ground state: 1s¹
- m = 0 state splits into: \( \Delta E = \pm \mu_z B \)

For the orbital angular momentum of an electron:
- \( \mu_{z,orb} = -\frac{e}{2m_e} L_z = -\frac{e}{2m_e} m_z \hbar \)

What if there were an additional component of angular momentum?
- \( \mu_{z,spin} = -\frac{e}{m_e} S_z \quad S_z = \pm \hbar \)

\[ \implies \mu_{z,\text{tot}} = -\frac{e}{2m_e} (L_z + 2S_z) \]

\[ \implies \mu_{z,\text{tot}} = -\frac{e}{2m_e} (h + 2 \cdot 0) = -\frac{e}{2m_e} h \]

\[ \implies \mu_{z,\text{tot}} = -\frac{e}{2m_e} (0 + 2 \cdot \frac{h}{2}) = -\frac{e}{m_e} h \]

For the total angular momentum of an electron:
- \( \vec{J} = \vec{L} + \vec{S} \)

For the total magnetic moment due to the electron:
- \( \vec{\mu}_{\text{tot}} = -\frac{e}{2m_e} (\vec{L} + 2\vec{S}) \)

Bohr solved: \( \frac{p^2}{2m_e} + V(x) = E \)

Schrödinger solved: \[ \left[ \frac{\hat{p}^2}{2m_e} + V(x) \right] \Psi(x,t) = \hat{E} \Psi(x,t) \]

Dirac solved: \[ \left( \left( \frac{\hat{p}^2}{m_e^2} \right) \right) \Psi(x,t) = \hat{E} \Psi(x,t) \]

\[ n = 1, 2, 3 \ldots = \text{Principle Quantum Number} \]
\[ E_n = -\frac{E_e}{n^2} \quad (\text{for Hydrogen, same as Bohr}) \]

\[ l = 0, 1, 2, 3 \ldots = \text{Angular Momentum Quantum Number} \]
\[ m = -l, 0, l \quad (\text{restricted to } 0, 1, 2 \ldots n-1) \]

\[ \left| \vec{L} \right| = \sqrt{l(l+1)} \hbar \]

\[ m = -1, 0, 1, \ldots \text{z-component of Angular Momentum} \]

\[ L_z = mh \]

Dirac’s relativistic equation predicted the existence of antimatter!!!
**Energy Diagram for Hydrogen**

- \( n=1 \)  
  - 1s
- \( n=2 \)  
  - 2s  
  - 2p
- \( n=3 \)  
  - 3s  
  - 3p  
  - 3d

In HYDROGEN, energy only depends on \( n \), not \( l \) and \( m \).  
(NOT true for multi-electron atoms!)

An electron in hydrogen is excited to Energy = \(-13.6/9\) eV. How many different wave functions in H have this energy?

- a. 1
- b. 3
- c. 6
- d. 9
- e. 10

Answer is d:

With the addition of spin, we now have 18 possible quantum states for the electron with \( n=3 \)

**Schroedinger finds quantization of energy and angular momentum:**

\[ E_n = -\frac{\hbar^2}{8m} \left( \frac{1}{n^2} \right) \]

- I. The energy of the ground state solution is **same**
- II. The orbital angular momentum of the ground state solution is **different**
- III. The location of the electron is **different**

- a. same, same, same  
- b. same, same, different  
- c. same, different, different  
- d. different, same, different  
- e. different, different, different

Bohr got energy right, but he said orbital angular momentum \( L = n \hbar \), and thought the electron was a point particle orbiting around nucleus.

**How does Schroedinger model of atom compare with other models? Why is it better?**

- **Schroedinger model:**  
  - Gives correct energies.  
  - Gives correct orbital angular momentum.  
  - Describes electron as 3D wave.  
  - Quantized energy levels result from boundary conditions.  
  - Schroedinger equation can generalize to multi-electron atoms.

- **Bohr model:**  
  - Postulates fixed energy levels  
  - Gives correct energies.  
  - Doesn’t explain WHY energy levels fixed.  
  - Describes electron as point particle moving in circle.

- **deBroglie model:**  
  - Also gives correct energies.  
  - Explains fixed energy levels by postulating electron is standing wave, not orbiting particle.  
  - Only looks at wave around a ring: basically 1D, not 3D

- **Both models:**  
  - Gets angular momentum wrong.  
  - Can’t generalize to multi-electron atoms.

**Schroedinger’s solution for multi-electron atoms**

What’s different for these cases?  
Potential energy (V) changes!  
(Now more protons AND other electrons)

\[ V(q_i) = k q_i \text{ proton} + k q_i \text{ other} + \text{ other interactions} \]

Need to account for all the interactions among the electrons  
Must solve for all electrons at once! (use matrices)

**Gives very difficult to solve ... huge computer programs!**

**Solutions change:**

- wave functions change  
  - higher Z \( \rightarrow \) more protons \( \rightarrow \) electrons in 1s more strongly bound \( \rightarrow \) radial distribution quite different  
  - general shape (p-orbital, s-orbital) similar but not same

- energy of wave functions affected by Z (\# of protons)
  - higher Z \( \rightarrow \) more protons \( \rightarrow \) electrons in 1s more strongly bound (more negative total energy)
A brief review of chemistry

Electron configuration in atoms:
How do the electrons fit into the available orbitals?
What are energies of orbitals?

Will the 1s orbital be at the same energy level for each atom? Why or why not? What would change in Schrödinger’s equation?
No. Change number of protons ... Change potential energy in Schrödinger’s equation ... 1s held tighter if more protons.

Can Schrödinger make sense of the periodic table?

For a given atom, Schrödinger predicts allowed wave functions and energies of these wave functions.

1869: Periodic table (based on chemical behavior only)
1897: Thompson discovers electron
1909: Rutherford model of atom
1913: Bohr model

Why would behavior of Li be similar to Na?
a. because shape of outer most electron is similar.
b. because energy of outer most electron is similar.
c. both a and b.
d. some other reason
In case of Na, what will energy of outermost electron be and WHY?
- a. much more negative than for the ground state of H
- b. somewhat similar to the energy of the ground state of H
- c. much less negative than for the ground state of H

Wave functions for sodium
- Li (3 e's)
- Na (11 e's)

Sodium has 11 protons.
- 2 electrons in 1s
- 2 electrons in 2s
- 6 electrons in 2p
- Left over: 1 electron in 3s

Electrons in 1s, 2s, 2p generally closer to nucleus than 3s electron, what effective charge does 3s electron feel pulling it towards the nucleus?
- Close to 1 proton... 10 electrons closer in shield (cancel) a lot of the nuclear charge.

In case of Na, what will energy of outermost electron be and WHY?
- a. much more negative than for the ground state of H
- b. somewhat similar to the energy of the ground state of H
- c. much less negative than for the ground state of H

Schrodinger predicts wave functions and energies of these wave functions.

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