Week 7/Tu: Lecture Units ‘16 & 17’

Unit 15: Wave properties of matter
-- electromagnetic transitions, Bohr
-- particle waves? deBroglie
-- standing waves

Unit 16: Electron standing waves
-- uncertainty, quantum numbers
-- properties of standing waves
-- shapes and nodes, labels
-- electron-electron repulsion

Unit 17: Electron orbitals
-- electron spin
-- periodicity of elements

Issues: Be sure to check your scores entered on CEMSCORES.chemistry.msu.edu
More on photoelectric effect

Homework #5 due this Saturday, Oct. 13th 8am
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Einstein contributed an important part to the modern understanding of electromagnetic radiation by explaining the photoelectric effect. Experiment: shine light onto a clean metal surface, observe e⁻’s depending on “color”

For example: potassium metal requires 2.0 eV of energy to remove an electron

What’s an “eV”? – electron Volt

\[ E_{\text{photon}} = h\nu = \frac{hc}{\lambda} \]

\[ 1 \text{ eV} = 1.602 \times 10^{-19} \text{ J} \]
Week 7/Tu: Example of Photoelectric Effect

Q: What is the maximum velocity of the electron ejected from a clean potassium surface by a 410 nm photon via the photoelectric effect?

Recall: K requires 2.0 eV of energy to remove an electron

Calculate: $E_{410 \text{nm}} = 4.84 \times 10^{-19} \text{J} = 3.02 \text{ eV}$

\[ \Delta E = E_{\text{photon}} \quad E_{\text{After}} = KE_{\text{electron}} + \text{BindingEnergy} \quad (\text{work function}) \]
We just had an example of an electron travelling at $6 \times 10^5$ m/s.

1) Calculate the de Broglie wavelength of this particle.

$$\lambda_{\text{deBroglie}} = \frac{h}{mv}$$

2) We can ask where is space is the electron? That is, how precisely can we measure its position?
Erwin Schroedinger gets most of the credit for solving the mathematical problem of a standing three dimensional wave for an electron in an atom. The formal mathematical equations are beyond the scope of this course (phew!) but we already have identified several features of the solutions called *Wavefunctions*. The mathematics results in quantized energy values – and has been called quantum mechanics.

1) An atom is a 3D spherical object so the wavefunction has to be a 3D object.
2) The wavelength (size) depends on the momentum (energy) of the electron.
3) The standing waves will be multiples of $\frac{1}{2}$ of a wavelength. Thus, we have a Principal Quantum Number, $n = 1, 2, 3 \ldots$ count $(\lambda/2)$’s.
4) The standing waves will have nodes that are 2D objects … planes or spheres. The number of nodes is one less than the number of $(\lambda/2)$.
5) We need to keep track of the # and type of nodes: planar nodes
6) Planes have orientations, need to keep track of direction of the plane
Electron standing wave, 3D object need to have 3 quantum numbers, that is, 3 labels for each of the wavefunctions.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>QN name</th>
<th>allowed values</th>
<th>Significance</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>principal</td>
<td>n = 1, 2, 3, …</td>
<td>$\lambda/2$, energy</td>
</tr>
<tr>
<td>l</td>
<td>“azimuthal”</td>
<td>$l = 0, 1, 2, \ldots$ (n-1)</td>
<td>planar nodes [angular momentum]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>s, p, d, …</td>
</tr>
<tr>
<td>$m_l$</td>
<td>magnetic</td>
<td>$-l \ldots -l, 0, l, \ldots +l$</td>
<td>orientation [direction, x y z]</td>
</tr>
</tbody>
</table>

Each wavefunction, called an orbital, can be uniquely identified (n, l, $m_l$)
Quantum numbers or labels for each of the wavefunctions:

\[ n = 1 \]

must have \((n-1) = 0\) nodes  \(1s\)  \(l = 0\) only possibility
Quantum numbers or labels for each of the wavefunctions:

\[ n = 2 \]
must have \((2-1)=1\) nodes

\[ \begin{align*}
    l &= 0 \\
    m_l &= 0
\end{align*} \]

\[ 2s , \quad 2p \]

\[ \begin{align*}
    l &= 1 \\
    m_l &= -1, 0, +1
\end{align*} \]

\[ p_x, \quad p_y, \quad p_z \]

\[ n = 1 \quad l = 0 \]
must have \((1-1)=0\) nodes

\[ \begin{align*}
    l &= 0 \\
    m_l &= 0
\end{align*} \]

\[ 1s \]

\[ l = 0 \text{ only possibility, } m_l = 0 \]
Quantum numbers or labels for each of the wavefunctions:

- $n = 3$  
  $3s$, $l = 0$, $m_l = 0$  
  $3p$, $l = 1$  
  must have $(3-1) = 2$ nodes

- $n = 2$  
  must have $(2-1) = 1$ nodes
  $2s$, $l = 0$  
  $m_l = 0$
  $2p$, $l = 1$  
  $m_l = -1, 0, +1$

- $n = 1$  
  $l = 0$  
  must have $(1-1) = 0$ nodes
  $1s$, $l = 0$  
  only possibility, $m_l = 0$
In hydrogen atom, the energy only depends on “n” the Principal QN

\[
\Sigma (2l+1) = n^2
\]

total # orbitals

<table>
<thead>
<tr>
<th>n = 1, 2, …</th>
<th>l = 0, 1, … (n-1)</th>
<th>( \Sigma (2l+1) = n^2 )</th>
<th>total # orbitals</th>
</tr>
</thead>
<tbody>
<tr>
<td>n = 2: 2s 2p(_x) 2p(_y) 2p(_z)</td>
<td>1+3 = 4</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>n = 1: 1s</td>
<td>= 1</td>
<td>1</td>
<td></td>
</tr>
</tbody>
</table>
In hydrogen atom, the energy only depends on “n” the Principal QN

<table>
<thead>
<tr>
<th>n</th>
<th>Orbitals</th>
<th>( \Sigma (2l+1) = n^2 )</th>
<th>total # orbitals</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1s</td>
<td>= 1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2s 2p(_x) 2p(_y) 2p(_z)</td>
<td>1+3 = 4</td>
<td>5</td>
</tr>
<tr>
<td>3</td>
<td>3s 3p((3)) 3d(<em>{xy}) 3d(</em>{yz}) 3d(<em>{xz}) 3d(</em>{x^2-y^2})</td>
<td>1+3+5 = 9</td>
<td>14</td>
</tr>
</tbody>
</table>
In hydrogen atom, the energy only depends on “n” the Principal QN

<table>
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<tr>
<th>n</th>
<th>1, 2, …</th>
<th>l = 0, 1, … (n-1)</th>
<th>( \Sigma (2l+1) = n^2 )</th>
<th>total # orbitals</th>
</tr>
</thead>
<tbody>
<tr>
<td>n = 4: 4s 4p (3) 4d (5) 4f (7)</td>
<td>1+3+5+7 = 16</td>
<td>25</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n = 3: 3s 3p (3) 3d_xy 3d_yz 3d_z^2 3d_xz 3d_x^2-y^2</td>
<td>1+3+5 = 9</td>
<td>14</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n = 2: 2s 2p_x 2p_y 2p_z</td>
<td>1+3 = 4</td>
<td>5</td>
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<td></td>
</tr>
<tr>
<td>n = 1: 1s</td>
<td>= 1</td>
<td>1</td>
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</table>

We have no energy dependence on “l” for one electron in these orbitals

The Periodic Table indicates the special cases are: \( Z = 2, 10, 18, 36, 54 \)

→ looks like we missed something, at least a factor of two!
In hydrogen atom, the energy only depends on “n” the Principal QN.

An energy level diagram shows the relative energies of the orbitals. (fill up from the bottom)

Recall the Energy values from Bohr: \( E_n = -\frac{\hbar c}{n^2} \)
More than one electron: there is repulsion between the two electrons due to their having the same electrical charge.

With many electrons, the energy depends on “n” and also slightly on “l”.

The order becomes mixed between n = 3 & 4 but don’t worry, the Periodic Table shows the pattern.