Sparks

CH301

Quantum Mechanics

Waves? Particles? What and where are the electrons!?

UNIT 2 Day 3

LM 14, 15 & 16 + HW due Friday, 8:45 am
What are we going to learn today?

The Simplest Atom - Hydrogen

- Relate the empirical model to the theoretical model of the energy levels of electrons in H atom
- Solutions to the theoretical model predict electron configuration
Review Where We are Up to Now:

• Planck and Einstein established **wave-particle duality for light** via $E=nh$ and explanation of the photoelectric effect
  – From this also came quantization.

• De Broglie **extends the idea of wave-particle duality to matter**

• Rydberg and Bohr extends **quantization** by applying it to the hydrogen atom.
  – This explained spectra, a known phenomenon.
  – Didn’t work for multi-electron atoms

• Heisenberg’s **Uncertainty Principle** explains further complications about figuring out where the electrons are in an atom.
How do we deal with the new “wave/particle” things? **We need a new model!!**

Quantum Mechanics!

It doesn’t make sense!  
It shouldn’t!

You don’t live in a world of tiny particles with vanishingly small mass and momentum.

It is what it is.
The Schrödinger Equation allows us to solve for all possible wavefunctions and energies.

Wave functions – Tell us about “where” the electron is. (the probability of finding the particle at a given position)

Energies – Tell us about the energy of the electron
The Hydrogen Atom

Simplest of all atomic problems.
1 proton, 1 electron.

Function Machine (Schrödinger Equation)
That will give us the solutions

Put that into the Schrödinger Equation and solve

Wavefunctions and energies
The Hydrogen Atom

Infinite number of solutions
Which solution are we interested in?
LOWEST ENERGY
GROUND STATE ELECTRON CONFIGURATION

Function Machine
(Schrödinger Equation)
That will give us the solutions
Where is the Energy?

Two key ideas from Quantum Mechanics, systems are described by

**Energies** – Tell us about the energy of the electron

**Wave functions** – Tell us about “where” the electron is. (the probability of finding the particle at a given position)
DIAGRAM SOLUTIONS LOWEST ENERGY ELECTRON TO HIGHEST ENERGY ELECTRON
(Draw energy level diagram for hydrogen atom)
ENERGY

• Rydberg-from Bohr model:
  \[ \nu = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \]
  \( R = 3.29 \times 10^{15} \text{ Hz} \)

• Schrödinger calculated actual energy of the e\(^-\) in H using his wave equation with the proper expression for potential energy
  \[ E_n = -\frac{\hbar R}{n^2} = -2.18 \times 10^{-18} \text{ J/n}^2 \]
  \( n \) is principal quantum number which is an integer that labels the different energy levels

• e\(^-\) will climb up the energy levels until freedom – ionization \( n = \infty \)
IONIZATION VERSUS PHOTOELECTRIC EFFECT
Where is the particle?

Two key ideas from Quantum Mechanics, systems are described by:

- **Energies** – Tell us about the energy of the electron.
- **Wave functions** – Tell us about “where” the electron is. (the probability of finding the particle at a given position)
• Schrödinger replaced precise trajectory of a particle with a wave function.
• Born interpretation of the wave function - the probability of finding the particle in a region is proportional to the value of $\psi^2$.
• $\Psi^2 = \text{probability density} – \text{probability that a particle will be found in a region divided by the volume of the region}$
• $\psi^2 = 0$ indicates node
Electrons are they particles? Are they waves?

Neither!

They are strange quantum mechanical things that appear to us sometimes as being particles and sometimes as waves.
SOLUTIONS: Atomic Orbitals

• Apply wave function to $e^-$ in 3-D space, bound by nucleus.
• Solutions to these wave equations are called orbitals.
• Wave function squared gives the probability of finding the electron in that region in space.
• Each wave function is labeled by three quantum numbers,
  – $n$ – size and energy
  – $l$ – shape
  – $m_l$ – orientation
Atomic orbitals: defined by Quantum Numbers

- PRINCIPAL quantum number, $n$.
  - Describes the energy and approximate nuclear distance.
  - Shell
  - $n = 1, 2, 3, 4, ....$

- ANGULAR MOMENTUM quantum number, $\ell$.
  - Describes the shape of the orbital
  - orbitals of a shell fall into $n$ groups called subshells
  - $\ell = 0, 1, 2, .......(n-1)$
  - $\ell = s, p, d, f, .......$
Shapes are hard to draw

At the moment we really care about the wavefunction squared often called the probability density.

Radial probability density is the probability of finding the electron at some distance from the nucleus
Hydrogen Like atoms

Below is a plot of the radial distribution of He\(^+\), and H (both have only 1 electron)
Which is He\(^+\)?
Classify the solutions

Classify our wavefunction solutions based upon both

Energy - principle quantum number n

“Shape” - angular momentum quantum number l
Shapes are hard to draw

How do we draw three dimensional functions?

It is hard.

http://winter.group.shef.ac.uk/orbitron/
s orbital – actually 1s is “easy” to draw
s-orbitals
Solutions Shapes (where is the electron?)

These are the $n = 2$ solutions, which one of these is not like the others?
• MAGNETIC quantum number, \( m_\ell \).
  – indicates the **orientation** of the angular momentum around the nucleus
  – distinguishes different *orbitals* within a subshell
  – The number of values of \( m_\ell \) gives you the number of orbitals for a given subshell.
  – \( m_\ell = \) integers from \(-\ell\) through 0 to \(+\ell\).
  – there are \( 2\ell + 1 \) values of \( m_\ell \) for a given value of \( \ell \).
p-orbitals

Probability distribution of p orbital

3 different orientations of p subshell, denoted by the three values of $m_l$
A cross section of the electron probability distribution for a 3p orbital.
d-orbitals

Probability distribution of d orbital

5 different orientations of d orbitals denoted by 5 different values of $m_l$.
f-orbitals

7 different orientations of f orbitals denoted by the seven different values for $m_l$. 
The location of an electron in a H atom is described by a wave function known as an atomic orbital, each orbital is designated by a set of three quantum numbers and fall into shells and subshells.
Ground state for H

- Picture shows the difference in energy levels for the first 3 energy levels available for an electron in the H atom. Show the ground state vs an excited state location on the diagram.
Electronic Configuration and Quantum Numbers for H

State the ground state electron configuration and the associated quantum numbers for H.
Electronic Configuration and Quantum Numbers for H

The three quantum numbers for an electron in a hydrogen atom in a certain excited state are \( n=4, \ l=2, \ m_l=-1 \). In what type of orbital is the electron located?
What are all the possible quantum numbers for an electron located in a 2d orbital of a H atom?
DEFINITIONS:
quantum numbers – orbital notation

- The location of an electron in a H atom is described by a wave function known as an atomic orbital, each orbital is designated by a set of three quantum numbers and fall into shells and subshells.
Electronic Configuration of many electron atom

- $Z$ denotes the nuclear charge and hence the # of e- in an atom
- Potential energy of electrons in a many electron atom is more complex than the simple H atom
- Too difficult to solve exactly
- Loss of degeneracy in shells
- Outer electrons are shielded from nucleus
- Need to add 4$^{th}$ quantum number, $m_s$, spin quantum number
4\textsuperscript{th} Quantum Number

- $m_s$ - spin magnetic quantum number - indicates the spin on the electron, the electron can spin one of two directions up or down
- Pauli Exclusion Principle: In a given atom no two electrons can have the same set of four quantum numbers.
- An orbital can hold only two electrons, and they must have opposite spin.
What Did We Learn Today?

LIGHT CAN BE USED TO PROBE THE ENERGY OF ELECTRONS IN MATTER

Developed a physical model that predicts the energy of electron in H atom – QUANTUM

ELECTRONS IN ATOMS HAVE DISCRETE ENERGIES

ELECTRONS CAN BE DESCRIBED BY WAVE FUNCTIONS THAT CAN BE CLASSIFIED BY QUANTUM NUMBERS
Learning Outcomes

Understand QM is a model and that solutions to the Schrödinger equation yield wave functions and energies

Understand that the wave function can be used to find a radial distribution function that describes the probability of an electron as a function of distance away from the nucleus

List, define and describe the three quantum numbers for the H-atom wave functions and know what possible combinations of quantum numbers are allowed.

Define the atomic orbital names based on quantum numbers