5.111 Principles of Chemical Science
Fall 2008

5.111 Lecture Summary #4

Reading for today: Section 1.5 (1.3 in *3rd ed*), Section 1.6 (1.4 in *3rd ed*)
Read for Lecture #5: Section 1.3 (1.6 in *3rd ed*) – Atomic Spectra, Section 1.7 up to
   equation 9b (1.5 up to eq. 8b in *3rd ed*) – Wavefunctions and Energy Levels,
   Section 1.8 (1.7 in *3rd ed*) – The Principle Quantum Number

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Topics: **I.** Light as a particle
                      A) the photoelectric effect
                      B) photon momentum
                 II. Matter as a wave
                 III. The Schrödinger equation

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I. LIGHT AS A PARTICLE

**A) The Photoelectric Effect (continued from Lecture #3)**
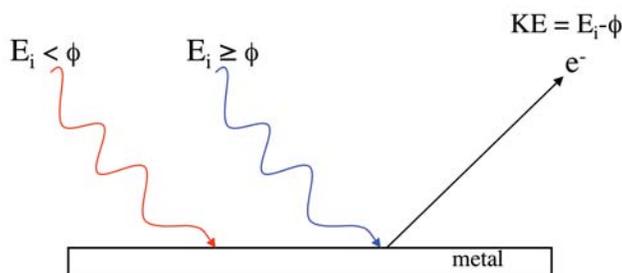
The energy of an incoming photon (E_i) must be equal to or greater than the workfunction (ϕ) of the metal in order to eject an electron.

e- _____ ejected   e- _____ ejected   e- _____ ejected
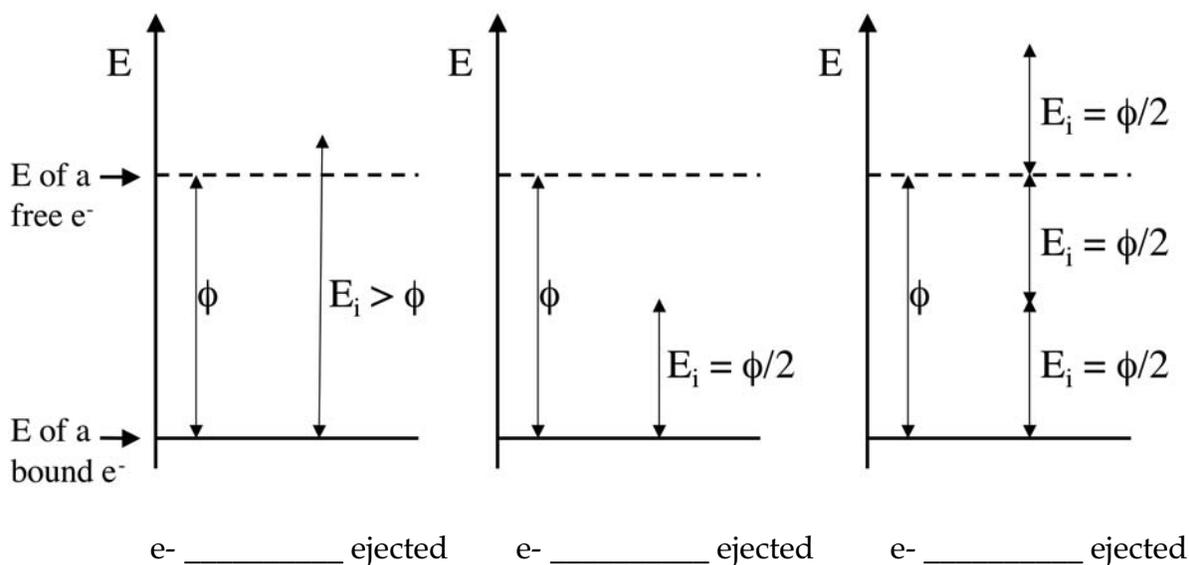
Three photons, each with an energy equal to $\phi/2$ will NOT eject an electron!

The # of electrons ejected from the surface of a metal is proportional to the _____ of photons absorbed by the metal (assuming $E_i \geq \phi$), and <u>not</u> the energy of the photons.
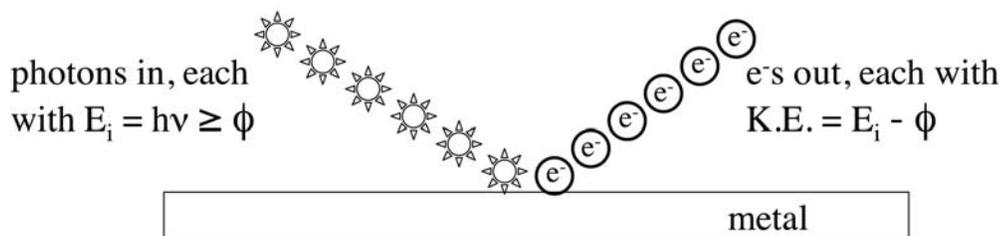
- Thus, the **intensity** (I) of the light (energy/sec) is proportional to the # of photons ejected/sec.
- High intensity means more _____ and NOT more _____.

Unit of intensity (I) : W = _____

Terminology tips to help solve problems involving photons and electrons:

- **photons:** also called light, electromagnetic radiation, etc.
  - may be described by _____, _____, or _____
- **electrons:** also called photoelectrons.
  - may be described by _____, _____, or λ (see part II of today's notes)
- **eV** is a unit of energy = 1.6022 x 10^{-19} J.

NOW FOR AN IN-CLASS DEMO OF THE PHOTOELECTRIC EFFECT:

Metal surface: Zn, ϕ = _____
Incident light sources:
  - UV lamp with a λ centered at 254 nm
  - Red laser pointer (λ = 700 nm)

First, let's solve the following problems to determine if there is sufficient energy in a single photon of UV or of red light to eject an electron from the surface of the Zn plate. For calibration, we'll also calculate the # of photons in a beam of light.

Consider our two light sources: a UV lamp (λ = 254 nm) and a red laser pointer (λ = 700. nm).

1) What is the energy per photon emitted by the UV lamp?
2) What is the energy per photon emitted by the red laser pointer?
3) What is the total number of photons emitted by the laser pointer in 60 seconds if the intensity (I) = 1.00 mW?

1) What is the energy per photon emitted by the UV lamp? λ = 254 nm

E = _____   ν = _____   E = _____

E = _____   E = _____

The UV lamp _____ have enough energy per photon to eject electrons from the surface of a zinc plate (ϕ of Zn = 6.9 x 10^{-19} J).

2) What is the energy per photon emitted by the red laser? λ = 700. nm

E = _____

E = __(6.626 x10^{-34} Js)(2.998 x 10^8 m/s)__   E = _____

_____

The red laser _____ have enough energy per photon to eject electrons from the surface of a zinc plate (ϕ of Zn = 6.9 x 10^{-19} J).

3) What is the total number of photons emitted by the red laser in 60 seconds if the intensity (I) of the laser is 1.00 mW?

1.00 mW = 1.00 x 10^{-3} J/s

$\dfrac{1.00 \times 10^{-3} \text{ J}}{\text{s}}$ x _____ x _____ =

The intensity of a light _____ related to the energy of its photons. Intensity is related to the **number** of photons.
     LIGHT IS BOTH A WAVE AND A MASSLESS PARTICLE. Einstein taught us that both descriptions (wave and particle) can coexist without a contradiction.

B) PHOTON MOMENTUM

If light is a stream of particles, each of those particles must have a momentum. Using relativistic equations of motion, Einstein showed that a photon has momentum p, even though it has zero mass!

$$p = h\nu/c \qquad \text{and, since } c = \nu\lambda \qquad \boxed{p = \underline{\hspace{1cm}}/\underline{\hspace{1cm}}}$$

Observation of photon momentum (Arthur Compton, 1927 Nobel Prize) is another piece of evidence for the particle-like behavior of light.

II. MATTER AS A WAVE

1924 Louis de Broglie (PhD thesis and 1929 Nobel Prize!) postulated that just as light has wave-like and particle-like properties, **matter (electrons) must also be both particle-like and a wave-like.** Using Einstein's idea that the momentum of a photon $(p) = h/\lambda$, de Broglie suggested:

wavelength of a particle = **$\lambda = h/p$**　　　　h = Planck's constant
　　　　　　　　　　　　　　　　　　　　　　m = mass of the particle
　　　　　　　　　　　　　　　　　　　　　　v = speed of the particle
mv = linear momentum (p) so **$\lambda = h/(mv)$**

de Broglie wavelength for matter waves 　　$\boxed{\lambda = h/p = h/(mv)}$

Let's do a sample calculation to think about why matter waves hadn't previously been observed.

Consider a 5 oz (0.142 kg) baseball crossing home plate at 94 mph (___m/s) (Go Sox!)

$$\lambda = \underline{\hspace{1.5cm}} = \frac{6.626\times10^{-34}\ \text{kgm}^2\text{s}^{-2}\text{s}}{(\qquad\quad)(\qquad\quad)} \qquad \text{Note: J = kg m}^2\ \text{s}^{-2}$$

$$\lambda = \underline{\hspace{3cm}} \qquad\qquad \text{undetectably small!!!}$$

Now consider the **λ of a gaseous electron** (9×10^{-31} kg) traveling at 1×10^5 ms^{-1}:

$$\lambda = \frac{h}{mv} = \frac{6.626\times10^{-34} \text{ kgm}^2\text{s}^{-2}\text{s}}{(9\times10^{-31} \text{ kg}) \times (1\times10^5 \text{ ms}^{-1})}$$

λ = _____ m = _____ Å. Compare this λ to the diameter of atoms (1-10 Å)!

Clinton Davisson and **Lester Germer** (1925) **diffracted electrons** from a Ni crystal and observed the resulting interference patterns, thus verifying wave behavior of e$^-$'s.

G.P. Thomson had a similar discovery. He showed that electrons that passed through a very thin gold foil produced a diffraction pattern. Thomson shared the 1937 Nobel Prize with Davisson for demonstrating that

ELECTRONS HAVE BOTH WAVELIKE AND PARTICELIKE PROPERTIES.

If particles like e$^-$'s have wave properties what is the equation of motion for an e$^-$?

III. THE SCHRÖDINGER EQUATION

Microscopic particles, like electrons, whose λ's are on the order of their environment do not obey classical equations of motion. Electrons must be treated like waves to describe their behavior.

1927 Erwin Schrödinger wrote an equation of motion for particles (like electrons) that account for their wave-like properties.
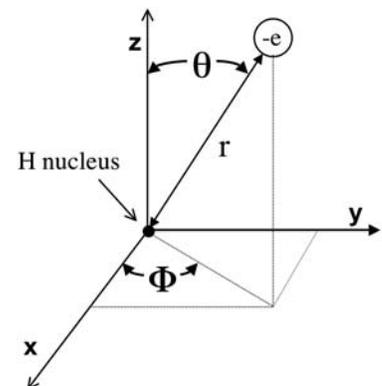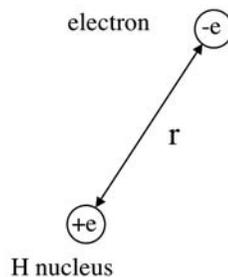
Schrödinger equation

$$\hat{H}\Psi = E\cdot\Psi \qquad\qquad \Psi = \text{wavefunction (describes the particle)}$$

$$E = \text{_____}$$

$$\hat{H} = \text{_____}$$

For the H atom, where the potential energy is a function of one distance variable, r, it simplifies the equation to use spherical polar coordinates. The wavefunction for the electron in an H atom is written as a function of r, θ, and Φ.

$$\Psi(r, \theta, \Phi)$$

The Schrödinger equation for the H atom:

$$\hat{H}\Psi(r,\theta,\Phi) = E\cdot\Psi(r,\theta,\Phi) \quad \longleftarrow \quad \text{wavefunction for the } e^-$$

Hamiltonian operator   binding energy for the e^-

where

$$\hat{H} = \frac{-\hbar^2}{2m_e}\left(\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{d^2}{d\phi^2}\right) + U(r)$$

The U(r) term is the potential energy of interaction between the e^- and nucleus.

The potential energy of interaction is the Coulomb interaction…

<div align="center">COULOMB POTENTIAL ENERGY</div>

$$U(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$$

The Schrödinger equation is to quantum mechanics like Newton's equations of motion are to classical mechanics.

Classical mechanics fails in the realm of microscopic particles- need a more complete mechanics- classical mechanics is "contained" within quantum mechanics.

What does solving the Schrödinger equation mean?

- Finding _____ , binding energies of electrons

- Finding _____ , wavefunctions or orbitals

Unlike classical mechanics, the Schrödinger equation correctly predicts (within 10^{-10} %!) experimentally observed properties of atoms.

For the hydrogen atom

$$\hat{H}\Psi = -\frac{1}{n^2}\frac{me^4}{8\varepsilon_0^2 h^2}\cdot\Psi$$

H atom orbital or wavefunction

$E \equiv$ binding energy of the electron to the nucleus