

Reading for today: Section 1.5 and Section 1.6. (Same sections in 5th and 4th editions)

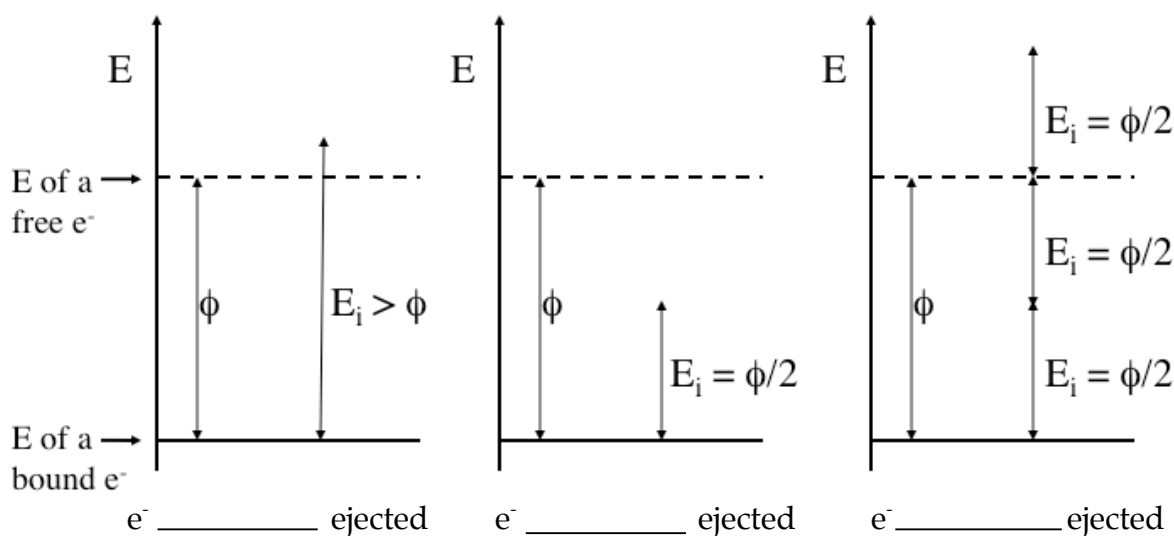
Read for Lecture #5: Section 1.3 – Atomic Spectra, Section 1.7 up to equation 9b – Wavefunctions and Energy Levels, Section 1.8 – The Principle Quantum Number. (Same sections in 5th and 4th editions)

Pre-lecture questions are a learning tool for you to test your knowledge of the material. They will not be graded on correctness, but rather on competition.

Topics: I. Light as a particle continued
II. Matter as a wave
III. The Schrödinger equation

I. LIGHT AS A PARTICLE CONTINUED

A) More on the Photoelectric Effect



Three photons, each with an energy equal to $\phi/2$ _____ eject an electron!

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 = 1.6022×10^{-19} J.

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

Metal surface: Zn, $\phi =$ _____

Incident light sources:

- UV lamp with a λ centered at 254 nm
- Red laser pointer ($\lambda = 700$ 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 ($\lambda = 254$ nm) and a red laser pointer ($\lambda = 700$ 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? $\lambda = 254$ nm

$E =$ _____ $\nu =$ _____ $E =$ _____

$E =$ _____ $E =$ _____

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

2) What is the energy per photon emitted by the red laser? $\lambda = 700$ nm

$E =$ _____

$E = \underline{(6.626 \times 10^{-34} \text{ Js})(2.998 \times 10^8 \text{ m/s})}$ $E =$ _____

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

$$\frac{1.00 \times 10^{-3} \text{ J}}{\text{s}} \times \underline{\hspace{2cm}} \times \underline{\hspace{2cm}} =$$

NOW LET'S TEST OUR PREDICTIONS WITH AN EXPERIMENT.

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!

$$p = hv/c \quad \text{and, since } c = v\lambda \quad \boxed{p = \underline{\hspace{2cm}}}$$

The experimental 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:

$$\begin{aligned} \text{wavelength of a particle} = \lambda &= \underline{\hspace{2cm}} & \begin{aligned} h &= \text{Planck's constant} \\ m &= \text{mass of the particle} \\ v &= \text{speed of the particle} \end{aligned} \\ \text{since linear momentum (p)} &= \underline{\hspace{2cm}} \end{aligned}$$

$$\text{de Broglie wavelength for matter waves} \quad \boxed{\lambda = h/p = \underline{\hspace{2cm}}}$$

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 (42 m/s) (Go Sox!)

$$\lambda = \underline{\hspace{2cm}} = \frac{6.626 \times 10^{-34} \text{ kgm}^2\text{s}^{-2}}{(\underline{\hspace{2cm}})(\underline{\hspace{2cm}})} \quad \text{Note: } J = \text{kg m}^2 \text{ s}^{-2}$$

$$\lambda = \underline{\hspace{2cm}} \quad \text{undetectably small!!!}$$

Now consider the λ of a gaseous electron (9×10^{-31} kg) traveling at 4×10^6 ms^{-1} :

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ kgm}^2\text{s}^{-2}}{(9 \times 10^{-31} \text{ kg}) \times (4 \times 10^6 \text{ ms}^{-1})}$$

$\lambda =$ _____ m = _____ Å. Compare this λ to the diameter of atoms (~ 0.5 - 4.0 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.

Note: JJ Thomson received a Nobel Prize for showing that an electron is a particle and GP Thomson received a Nobel Prize for showing that an electron is a wave

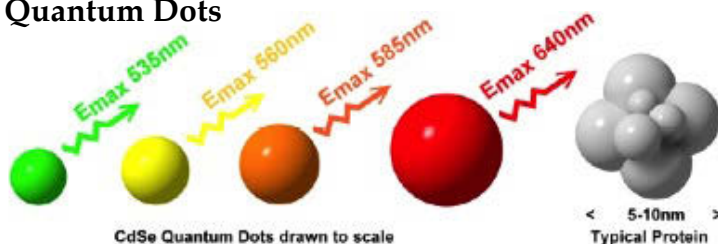
ELECTRONS HAVE BOTH WAVELIKE AND PARTICELIKE PROPERTIES.

In Their Own Words:

Research in the Bawendi laboratory includes the synthesis and application of quantum dots, semiconductor crystals of <10 nm in diameter. Quantum dots excited by UV radiation emit light of characteristic color that corresponds to the size and material of the quantum dot. Smaller dots emit bluer (higher E) light and larger dots emit redder (lower E) light.



Quantum Dots



Darcy Wanger, a graduate student in the Bawendi lab, discusses her research on quantum dots, which are being used in an ever-increasing number of biological and sensor applications. (Bawendi lab research webpage: <http://nanocluster.mit.edu/research.php>)

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III. THE SCHRÖDINGER EQUATION

The **Schrödinger Equation** is an equation of motion for particles (like electrons) that account for their wave-like properties.

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.

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

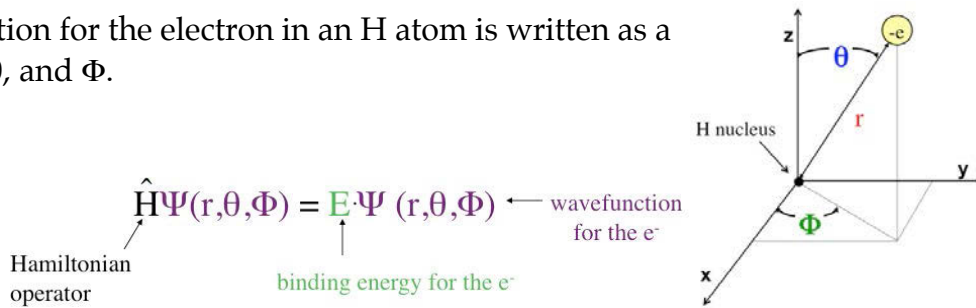
Schrödinger equation

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

$$E = \underline{\hspace{10em}}$$

$$\hat{H} = \underline{\hspace{10em}}$$

The wavefunction for the electron in an H atom is written as a function of r , θ , and Φ .



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...

COULOMB POTENTIAL ENERGY
$$U(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

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.

However, a complete quantum mechanical analysis of a multiatom system is still computationally intensive and improving quantum mechanical methods remains an active area of research.

BINDING ENERGIES (E_n) OF THE ELECTRON TO THE NUCLEUS

The Schrödinger equation for the H atom:

$$\hat{H}\Psi = E \cdot \Psi$$

$m = \underline{\hspace{2cm}} = \underline{\hspace{2cm}}$

$e = \underline{\hspace{2cm}}$

$\epsilon_0 =$ permittivity constant

$h =$ Planck's constant

$$\hat{H}\Psi = -\frac{1}{n^2} \frac{me^4 \cdot \Psi}{8\epsilon_0^2 h^2}$$

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

$\hat{H}\Psi =$ H atom orbital or wavefunction

The constants in this equation are can be combined into a single constant:

$$\frac{me^4}{8\epsilon_0^2 h^2} = R_H = \text{Rydberg's constant} = \underline{\hspace{2cm}}$$

The **binding energy** (E_n) of the electron to the nucleus for the **hydrogen atom**:

$$E_n = -\frac{1}{n^2} \frac{me^4}{8\epsilon_0^2 h^2} = \frac{-R_H}{n^2}$$

where $n = \underline{\hspace{2cm}}$ (a positive integer) = $\underline{\hspace{2cm}}$

KEY IDEA Binding energies are quantized!

The principal quantum number, n , comes out of solving the Schrödinger equation.

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5.111 Principles of Chemical Science
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