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5.111 Principles of Chemical Science  
Fall 2008

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## 5.111 Lecture Summary #3

**Reading for today:** Section 1.2 (1.1 in 3<sup>rd</sup> ed), and Section 1.4 (1.2 in 3<sup>rd</sup> ed) with a focus on pgs 10-12 in the 4<sup>th</sup> ed or pgs 5-7 in the 3<sup>rd</sup> ed.

**Read for Lecture 4:** Section 1.5 (1.3 in 3<sup>rd</sup> ed) – The Wave-Particle Duality of Matter, and Section 1.6 (1.4 in 3<sup>rd</sup> ed) – The Uncertainty Principle.

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**Topics:**

- I. (Failure of) the classical description of an atom (continued from Lecture #2)
- II. Introduction to quantum mechanics: wave-particle duality
- III. Light as a wave, characteristics of waves
- IV. Light as a particle, the photoelectric effect

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### I. (FAILURE OF) THE CLASSICAL DESCRIPTION OF AN ATOM

**Coulomb's Force Law** to describe the  $F$  between the nucleus and electron in an H atom.

$$F(r) = \frac{-e^2}{4\pi\epsilon_0 r^2}$$

$e$  = absolute value of an electron's charge

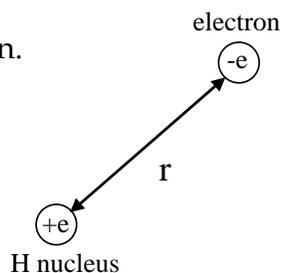
$r$  = distance between two charges

$\epsilon_0$  = permittivity constant of a vacuum ( $8.854 \times 10^{-12} \text{ C}^2\text{J}^{-1}\text{m}^{-1}$ )

Consider an H atom ( $Z=1$ ) with 1 electron and 1 proton.

When  $r \rightarrow \infty$        $F(r) = \underline{\hspace{2cm}}$

As  $r \rightarrow 0$        $F(r) = \underline{\hspace{2cm}}$



The closer the electron is to the nucleus, the larger the attractive force between the two charges.

- The Coulomb force law tells us the force ( $F$ ) as a function of  $r$ .
- The Coulomb force law does not tell us how  $r$  changes with \_\_\_\_\_.

There is a CLASSICAL EQUATION OF MOTION that tells us how the electron and nucleus move under influence of this Coulomb force: Newton's 2<sup>nd</sup> Law

$$F = ma$$

Force = mass times acceleration

We can rewrite  $F$  as a function of velocity,  $F = m(\underline{\hspace{2cm}})$  or distance,  $F = m(d^2r/dt^2)$ .

We can plug in the Coulomb force law for  $F$ , and solve the equation for any  $r_{\text{initial}}$ . If  $r_{\text{initial}}$  is  $10 \text{ \AA}$  ( $10^{-10} \text{ m}$ ), a typical distance for an H atom, the calculation indicates that

$$r = 0 \text{ at } t = \underline{\hspace{2cm}} \text{ sec!}$$

**This predicts that the electron should plummet into the nucleus in \_\_\_\_\_!**

What is wrong here?

It turns out that the **laws of classical mechanics** no longer work at this size scale.

Need a new kind of mechanics to describe this and other “unsettling” observations.

**QUANTUM MECHANICS** provides a single and comprehensive theory that explains the behavior of matter on an atomic (nanometer or smaller) scale.

## II. AN INTRODUCTION TO QUANTUM MECHANICS

- **Matter and radiation display both \_\_\_\_\_ and particle-like properties.**
- **Light consists of discrete packets of energy (called photons).**

We’ll briefly set aside our discussion of atomic structure (to be returned to in Lecture #5) to discuss these two sets of observations that are essential for understanding the atom.

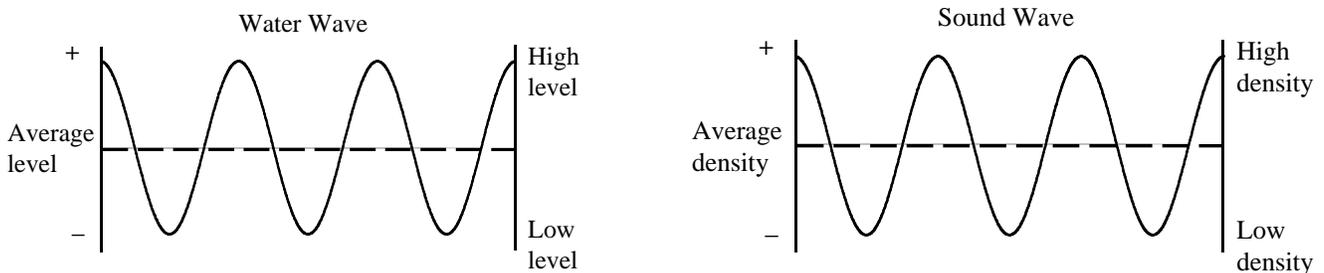
### THE WAVE-PARTICLE DUALITY OF MATTER AND RADIATION

Between 1887 and 1927 experiments were done that suggested the boundary between waves and particles is not rigid.

## III. LIGHT AS A WAVE, CHARACTERISTICS OF WAVES

We’ll begin by describing some general properties of waves, including water waves, sound waves and light (electromagnetic or EM) waves.

Waves have a periodic variation of some quantity.



amplitude: deviation from average level (can be a positive or negative value)

**Light** (\_\_\_\_\_ radiation) is the periodic variation of an electric field (and a perpendicular magnetic field).

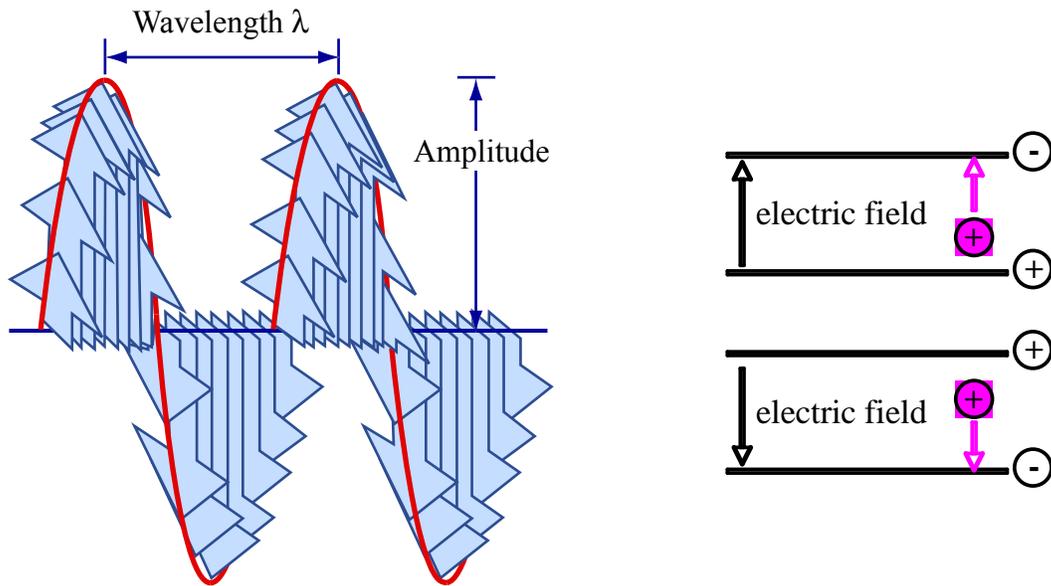


Figure by MIT OpenCourseWare.

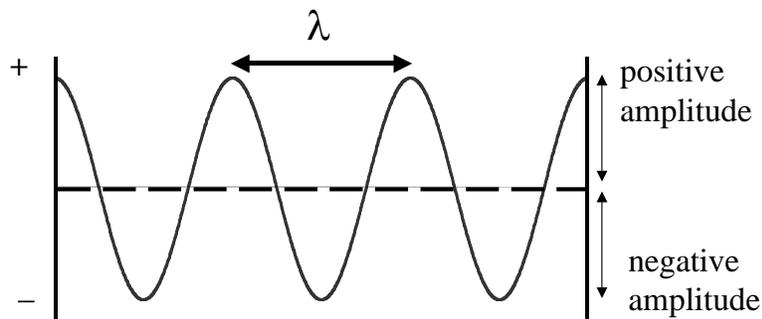
The electric field is the force field through which the Coulomb force operates.

We can characterize an electromagnetic wave in terms of:

**Amplitude** (a): the deviation from an average level

**Wavelength** ( $\lambda$ ): the \_\_\_\_\_ between successive maxima or minima

**Frequency** ( $\nu$ ): the number of \_\_\_\_\_ per unit time



We can also characterize electromagnetic radiation using the complete mathematical description for a wave:

$$E(x,t) = \underline{\hspace{10em}}$$

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

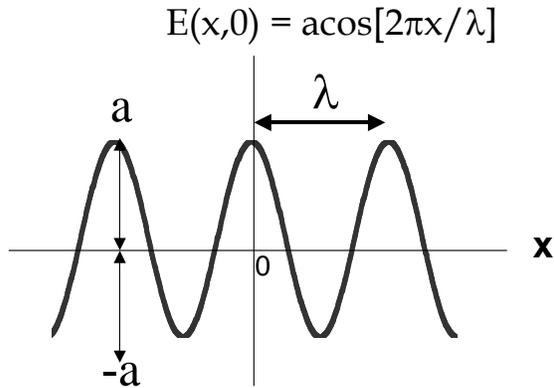
$$x = \underline{\hspace{10em}}$$

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

The EM wave is a function of two variables,  $x$  and  $t$ . For visualization, let's hold one variable constant and plot it as a function of the other variable. (So we will plot the wave at a fixed time as a function of position, or at a fixed position as a function of time.)

First we will examine an EM wave at a constant time.

At  $t = 0$



$a$  = maximum amplitude  
 $\lambda$  = wavelength (reported in units of length)

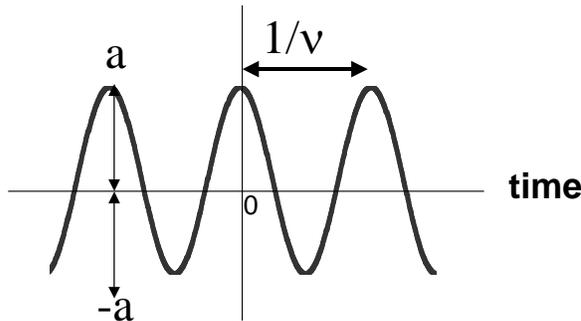
$E(x,0) = a$  (its maximum), when  $x =$  \_\_\_\_\_

Note: any time we see an equation of a wave, we automatically know its amplitude,  $a$ . We also know its maximum intensity: **intensity** = \_\_\_\_\_

We can also describe an EM wave at a constant position.

At  $x = 0$

$E(0,t) =$  \_\_\_\_\_



$a$  = maximum amplitude  
 $1/\nu$  = period = the time for 1 cycle to occur

- $E(0,t) = a$  (its maximum), when  $t = \dots -3/\nu, -2/\nu, -1/\nu, 0, 1/\nu, 2/\nu, 3/\nu \dots$
- Units of frequency ( $\nu$ ) : cycles per second = \_\_\_\_\_

**We can calculate the speed of a wave:**

Speed = distance traveled / time elapsed = \_\_\_\_\_ = \_\_\_\_\_

Electromagnetic radiation has a constant speed,  $c$  (the “speed of light”).

$\lambda \nu = c = 2.9979 \times 10^8 \text{ ms}^{-1}$

For any wavelength of light, the product of  $\lambda * \nu$  is always  $c$ .  $\lambda$  and  $\nu$  are NOT independent of each other. If you know  $\lambda$ , you can calculate  $\nu$ . If you know  $\nu$ , you can calculate  $\lambda$ .

The color of EM waves is determined by their wavelength:

RED has longest $\lambda$	$\sim 650 \text{ nm}$ ( $6.5 \times 10^{-7} \text{ m}$ )	and lowest $\nu$	$4.6 \times 10^{14} \text{ Hz}$
YELLOW	$\sim 580 \text{ nm}$ ( $5.8 \times 10^{-7} \text{ m}$ )		$5.2 \times 10^{14} \text{ Hz}$
GREEN	$\sim 520 \text{ nm}$ ( $5.2 \times 10^{-7} \text{ m}$ )		$5.8 \times 10^{14} \text{ Hz}$
BLUE has shortest $\lambda$	$\sim 460 \text{ nm}$ ( $4.6 \times 10^{-7} \text{ m}$ )	and highest $\nu$	$6.5 \times 10^{14} \text{ Hz}$

Visible light is only a small part of the entire electromagnetic spectrum:

radio waves	$\lambda = 1 \text{ m} - 10^8 \text{ m}$
microwaves	$\lambda = 10^{-3} \text{ m} - 1 \text{ m}$
infrared	$\lambda = 10^{-6} \text{ m} - 10^{-3} \text{ m}$
visible	$\lambda = 10^{-7} \text{ m} - 10^{-6} \text{ m}$
ultraviolet	$\lambda = 10^{-8} \text{ m} - 10^{-7} \text{ m}$
x-rays	$\lambda = 10^{-11} \text{ m} - 10^{-9} \text{ m}$
gamma-rays	$\lambda < 10^{-11} \text{ m}$

(You are not responsible for knowing specific wavelength or frequency ranges, but you should know the relative order of colors and types of waves.)

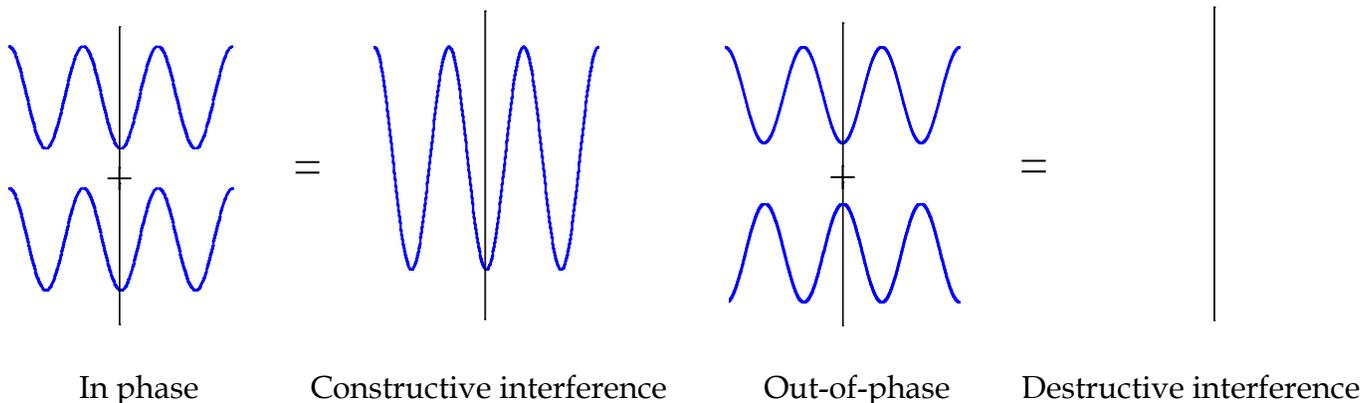
**MIT Chemistry Research Example:**

Research in the **Bawendi laboratory** includes the synthesis and application of **quantum dots**, semiconductor crystals of  $<10 \text{ nm}$  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 frequency) light and larger dots emit redder (lower frequency) light. Quantum dots are being used and designed for an ever-increasing number of biological and sensor applications.

Bawendi lab research webpage: <http://nanocluster.mit.edu/research.php>

Tech interview with Prof. Bawendi: <http://www-tech.mit.edu/V128/N35/bawendi.html>

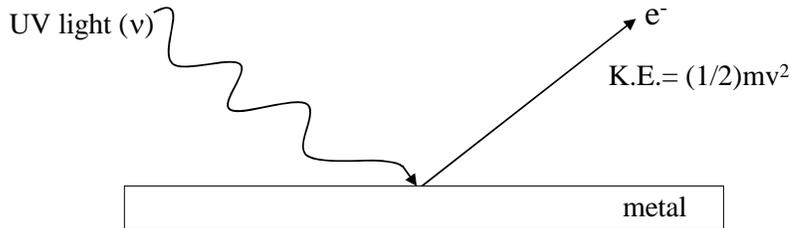
**Waves have the property of superposition**



## IV. LIGHT AS A PARTICLE

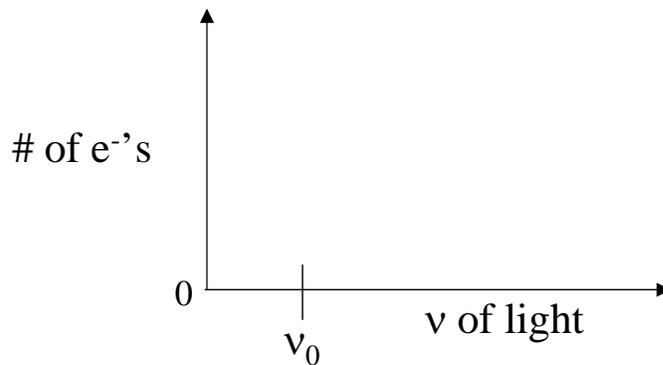
### The Photoelectric Effect

A beam of light hitting a metal surface can eject electrons.



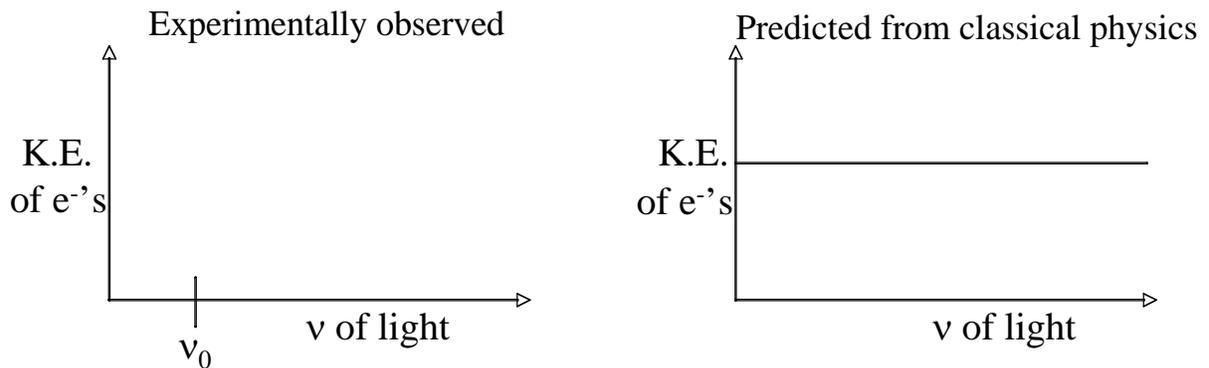
The frequency,  $\nu$ , of the incoming light must be equal to some threshold frequency,  $\nu_0$ , for an electron to be emitted. The  $\nu_0$  value depends on the identity of the metal.

At a constant intensity, the frequency of the light has no effect on the number of electrons ejected, as long as the frequency is above  $\nu_0$ . (Below  $\nu_0$ , no electrons are emitted.)

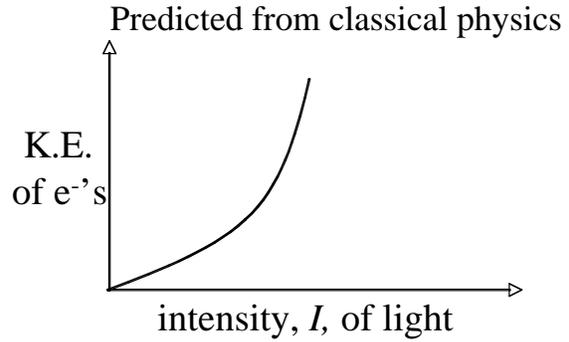
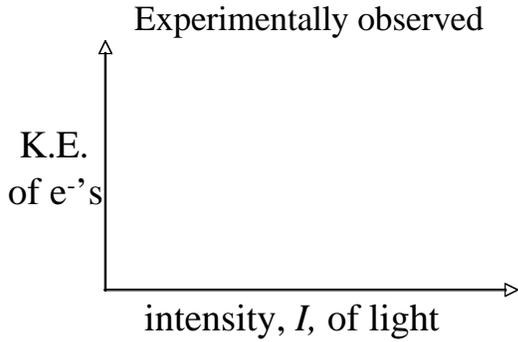


**The following (very surprising!) observations were made:**

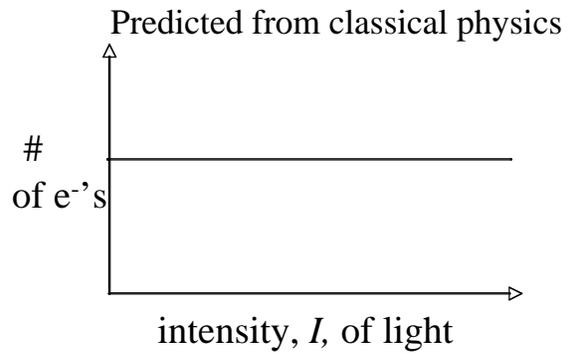
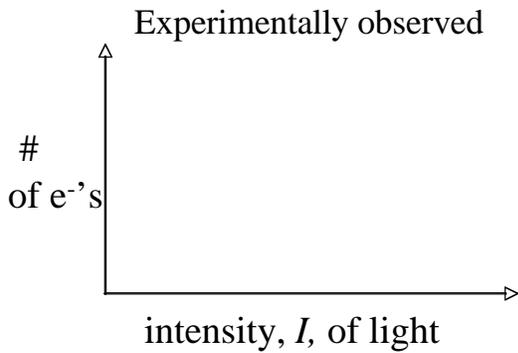
The kinetic energy, K.E., of ejected electrons was measured as function of the frequency of the incident light:



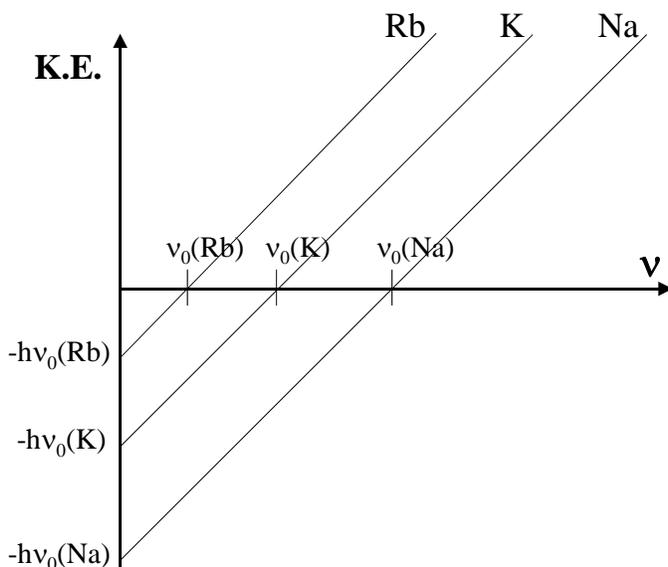
The kinetic energy, K.E., of the ejected electrons was measured as a function of intensity of the incident light.



The # of electrons ejected was measured as a function of intensity of the incident light.



These data were in direct opposition to the predictions of classical mechanics. In 1905 Einstein analyzed plots of K.E. as a function of frequency for different metals and found that all of the data fit into a linear form



$$y = mx + b$$

$$\text{slope (m)} = 6.626 \times 10^{-34} \text{ Js}$$

$$\text{y-intercept (b)} = (6.626 \times 10^{-34} \text{ Js})\nu_0$$

$$\text{Planck's constant} = h = 6.626 \times 10^{-34} \text{ Js}$$

Einstein could rewrite the equation of the line:

$$y = mx + b$$

$$\text{K.E} = \text{_____} - \text{_____}$$

$h\nu =$  the energy of the incident light  $= E_i$

Einstein postulated (1905)

- 1) The energy of a photon is proportional to its frequency!!!

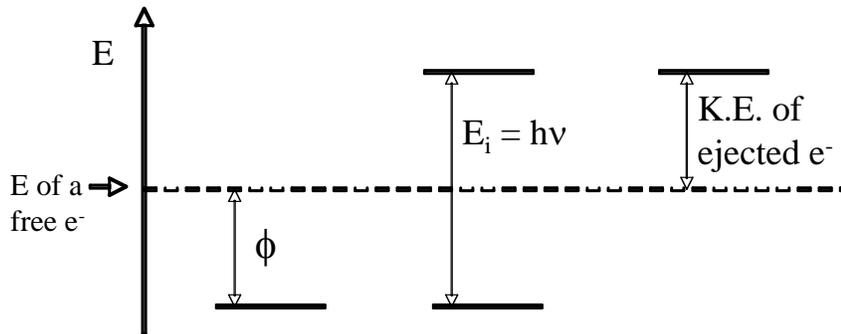
$$E = h\nu$$

- 2) Light is made up of energy "packets" called "photons"

This provided a new model for the photoelectric effect:

$h\nu = E_i =$  energy of the incident photon

$h\nu_0 = \text{_____} =$  energy required to eject an  $e^-$  from the surface of a metal.



We can describe this mathematically:

$$\text{K.E.} = \text{_____} \quad \text{or} \quad E_i = \text{_____}$$

(Note: these are just different forms of the equation  $\text{K.E} = h\nu - h\nu_0$ )