



# CH-110 Advanced General Chemistry I

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## Reminder: how to study for this class

- Solve exercises from the book! In addition to the ones we assign every week.
- Don't spend time reading or studying the slides. Start with exercises, go to slides to look for the appropriate material and formulas

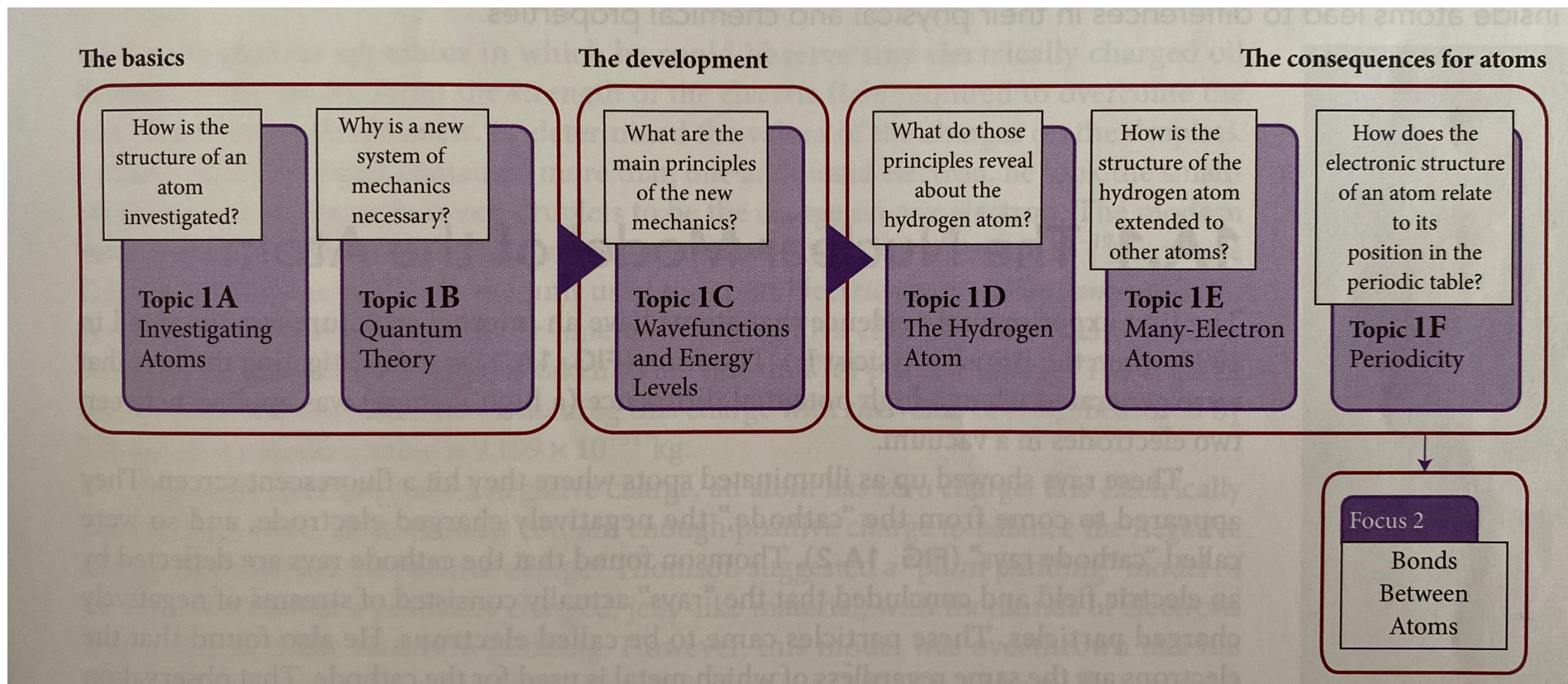
Image source: ChatGPT  
*Studying in Light*



# Quantum Theory

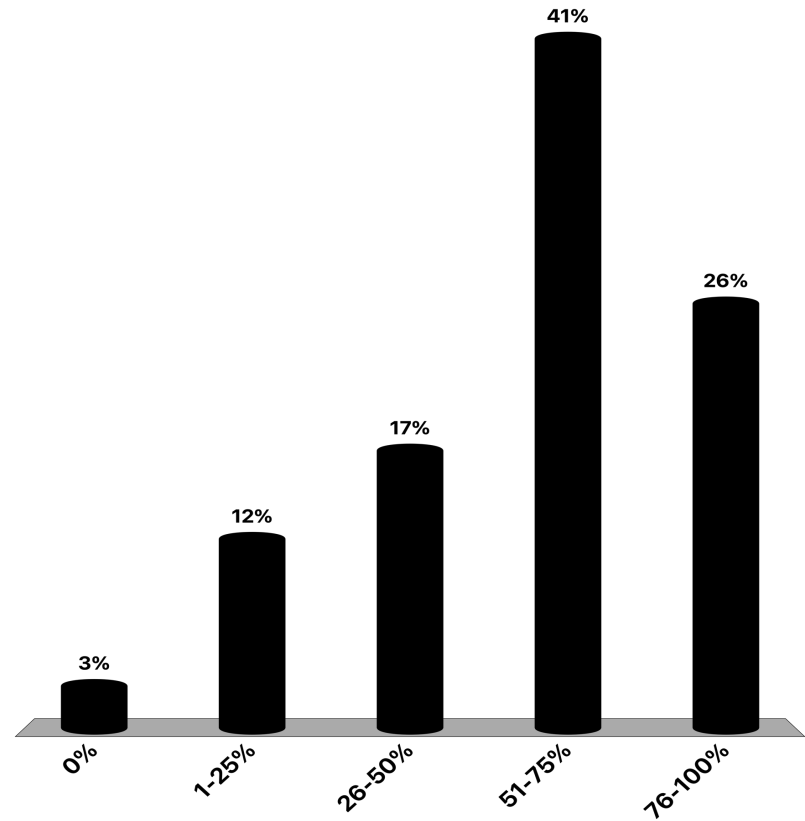
Topic 1B

# Overview Chapter 1 (Focus 1: Atoms)



Approximately what percentage of the material we've covered so far have you encountered in your previous studies?

- A. 0%
- B. 1-25%
- C. 26-50%
- D. 51-75%
- E. 76-100%



Topic 1B.1: Radiation, quanta, and photons

Topic 1B.2: Wave-particle duality

Topic 1B.3: The uncertainty principle

WHY DO YOU NEED TO KNOW THIS MATERIAL?

- The properties of electrons in atoms and molecules, which underlies the whole of **chemistry**, **can be understood only in terms of quantum mechanics.**

WHAT DO YOU NEED TO KNOW ALREADY?

- Concept of kinetic energy (Fundamentals A)
- Properties of electromagnetic radiation, specifically the **relationship between wavelength and frequency** (Topic 1A)

# Radiation, Quanta, and Photons

Topic 1B.1

# 1B.1 Radiation, quanta, and photons

## Recap last week

- Atomic spectrum of hydrogen:



- Empirical calculated by Ryberg:  $\nu = R \left( \frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$ ,  $n_1 = 1, 2, \dots, n_2 = n_1 + 1, n_1 + 2, \dots$
- No rainbow, but discrete lines!
- If electrons could have any energy, then they should emit any color.

## 1B.1 Radiation, quanta, and photons

### The answer

Electrons in atoms can only occupy discrete energy levels.

Electron energies in atoms are **quantized**.



Image source: ChatGPT

*Artsy rendition of electron energy quantization*

## 1B.1 Radiation, quanta, and photons

### Planck-Einstein equation

Energy is exchanged in discrete packets (*quanta*).

A photon of frequency  $\nu$  has energy:

$$E = h\nu$$

Important formula.  
Need to know how to apply.

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

**Interpretation:** Each spectral line in the atomic spectrum of hydrogen corresponds to photons of a specific energy ( $h\nu$ )

## 1B.1 Radiation, quanta, and photons

### The photoelectric effect

- **More evidence for quantization** came from photoelectric effect
- What was observed:
  1. Electrons emitted only if light frequency  $>$  threshold (depends on metal).
  2. Emission is immediate (independent of intensity).
  3. Electron kinetic energy  $\uparrow$  linearly with light frequency.

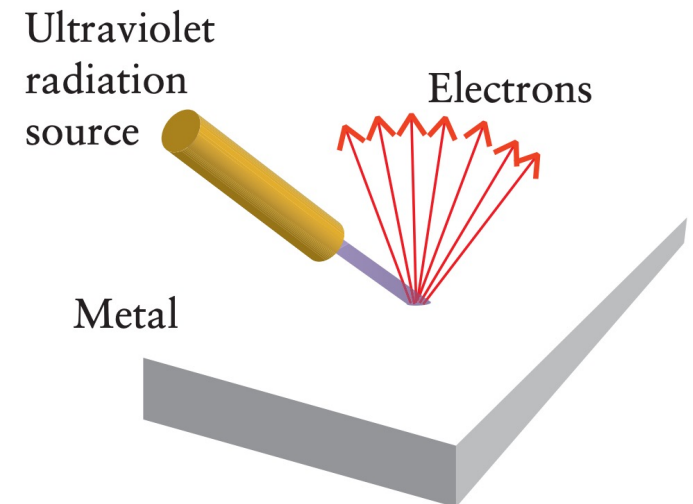


Figure 1.B3

## 1B.1 Radiation, quanta, and photons

### The photon (Einstein)

- Light consists of particles (*photons*), each with energy:

$$E = h\nu$$

- Photon energy  $\uparrow$  with frequency (UV > visible > IR).
- Intensity = number of photons, not energy per photon.
- **A photon is a packet of energy.**

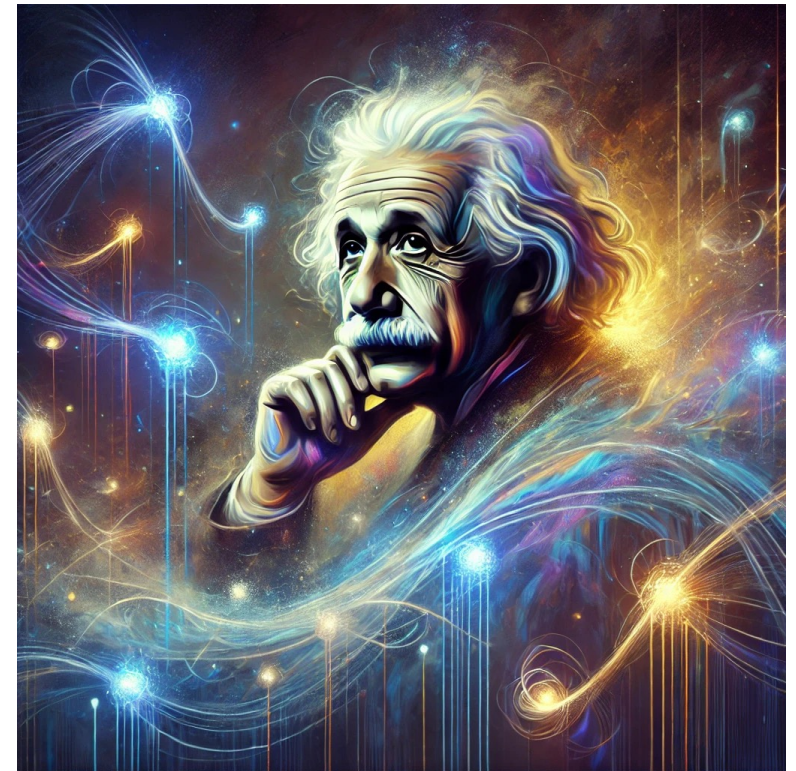


Image source: ChatGPT  
*Albert and the photon*

# 1B.1 Radiation, quanta, and photons

## The photon

**TABLE 1B.1 Photon Energy\***

Radiation type	Energy of photon/( $10^{-19}$ J)	Energy per mole of photons/( $\text{kJ} \cdot \text{mol}^{-1}$ )	Energy of photon/eV
X-rays and $\gamma$ -rays	$\geq 1.0 \times 10^3$	$\geq 6.0 \times 10^4$	$\geq 6.2 \times 10^2$
ultraviolet	5.7	340	3.6
visible light			
violet	4.7	280	2.9
blue	4.2	250	2.6
green	3.8	230	2.4
yellow	3.4	200	2.1
orange	3.2	190	2.0
red	2.8	170	1.8
infrared	2.0	120	1.3
microwaves and radio waves	$\leq 2.0 \times 10^{-3}$	$\leq 0.12$	$\leq 1.3 \times 10^{-3}$

\* Values are to 2 sf.

## 1B.1 Radiation, quanta, and photons

### Example 1B.2: Calculating the energy of a photon

What is (a) the energy of a single photon of blue light of frequency  $6.4 \times 10^{14}$  Hz; (b) the energy per mole of photons, in joules per mole, of this frequency?

#### SOLVE

(a) From  $E(1 \text{ photon}) = h\nu$ ,

$$E(1 \text{ photon}) = (6.626 \times 10^{-34} \text{ J}\cdot\text{s}) \times (6.4 \times 10^{14} \text{ Hz}) = 4.2 \times 10^{-19} \text{ J}$$

(b) From  $E(\text{per mole of photons}) = N_{\text{A}}E$ ,

$$\begin{aligned} E(\text{per mole of photons}) &= (6.022 \times 10^{23} \text{ mol}^{-1}) \times (4.2 \times 10^{-19} \text{ J}) \\ &= 2.5 \times 10^5 \text{ J mol}^{-1}, \text{ or } 250 \text{ kJ mol}^{-1} \end{aligned}$$

To derive the energy in part (a), we have used  $1 \text{ Hz} = 1 \text{ s}^{-1}$ , so  $\text{J}\cdot\text{s} \times \text{Hz} = \text{J}\cdot\text{s} \times \text{s}^{-1} = \text{J}$ .

## 1B.1 Radiation, quanta, and photons

### The work function ( $\Phi$ ) of a metal

- Work function ( $\Phi$ ): minimum energy to eject an electron (in eV).
- Photon must have  $h\nu \geq \Phi$ .
- If  $h\nu > \Phi$ :

$$E_{\text{photon}} = h\nu = \Phi + \frac{1}{2} m_e v^2$$

- Commonly expressed in eV (**electronvolt**), defined as the kinetic energy acquired by an electron when it is accelerated through a potential difference of 1 V:
- $1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$

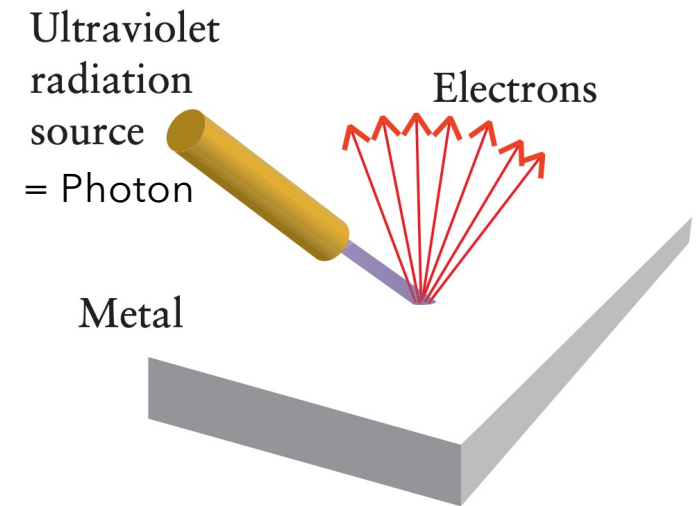


Figure 1.B3

# 1B.1 Radiation, quanta, and photons

## Einstein's photoelectric equation

$\frac{1}{2}m_e v^2$	=	$h\nu$	-	$\Phi$
$\underbrace{\hspace{1.5cm}}$		$\underbrace{\hspace{1.5cm}}$		$\underbrace{\hspace{1.5cm}}$
Kinetic energy of ejected electron		Energy supplied by photon		Energy required to eject photon

Important formula.  
Need to know how to apply.

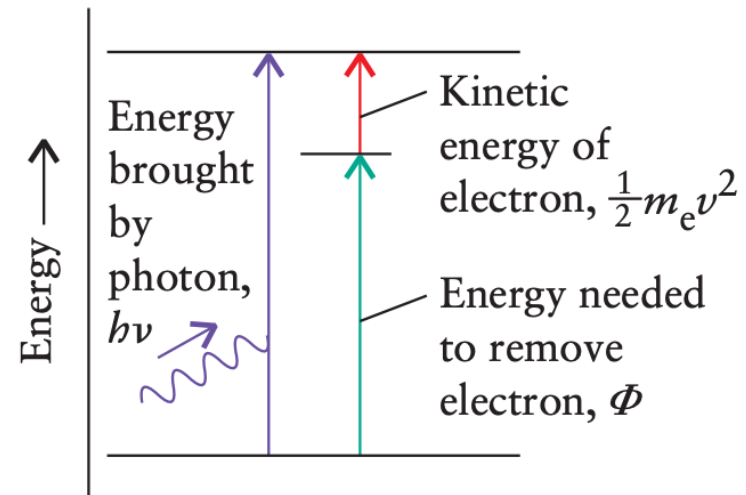
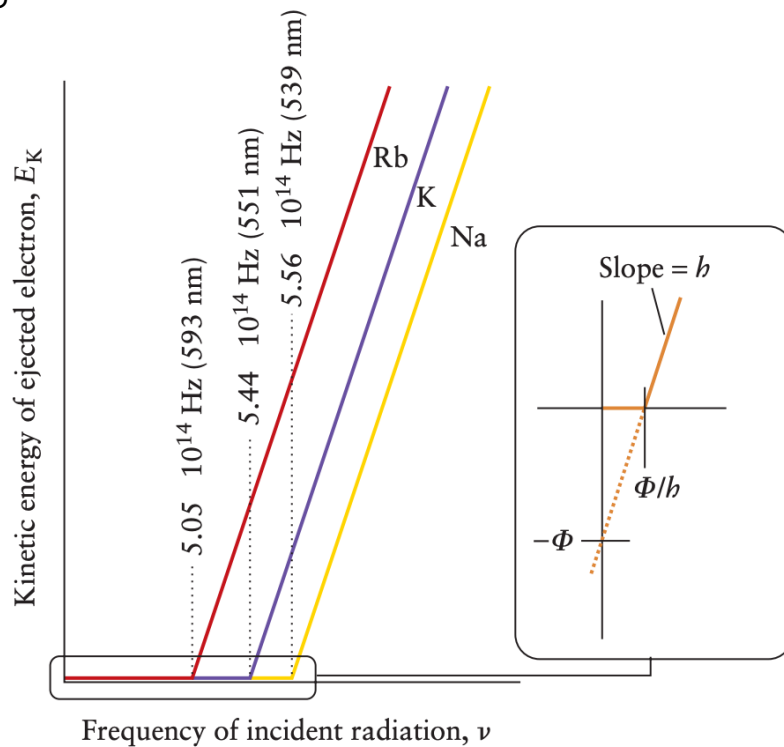


Figure 1.B4

# 1B.1 Radiation, quanta, and photons

## What does this equation tell you?

Figure 1.B5



- $E_k$  increases linearly with frequency.
- Slope =  $h$  (same for all metals).
- x-intercept = threshold frequency  $\nu_0 = \Phi/h$ .
- y-intercept =  $-\Phi$  (metal dependent).

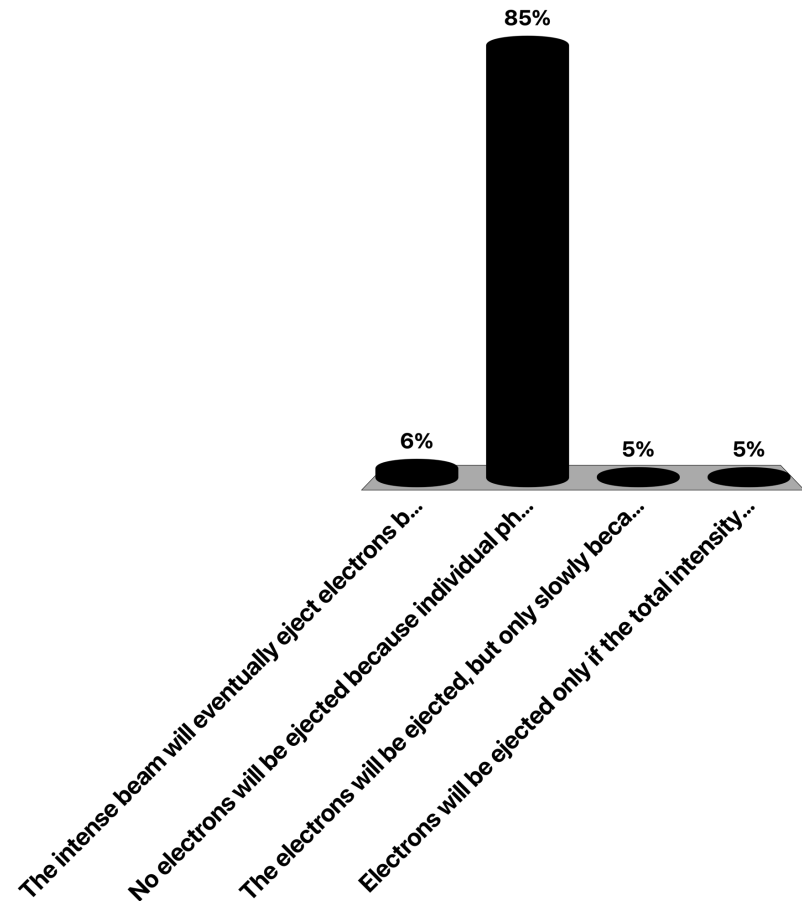
## 1B.1 Radiation, quanta, and photons

### Einstein's theory provides the following interpretation

1. Photon must have  $h\nu \geq \Phi$  to eject an electron.
2. Extra energy  $\rightarrow$  electron kinetic energy:  $E_k = h\nu - \Phi$ .
3.  $E_k$  increases linearly with frequency.

Imagine you are shining light on a metal surface to eject electrons. The metal has a work function of 5 eV. Your light source produces photons of 4 eV. What happens if you shine a very intense beam from Source A (with a large number of photons) on the metal surface?

- A. The intense beam will eventually eject electrons because the **total energy of the many photons adds up** to more than 5 eV.
- B. **No electrons will be ejected** because individual photons from Source A do not have enough energy to overcome the work function.
- C. The electrons will be ejected, but only **slowly** because the individual photon energy is slightly less than the work function.
- D. Electrons will be ejected only if the **total intensity of the light is increased** enough, regardless of the photon energy.



## 1B.1 Radiation, quanta, and photons

### Example 1B.3: Analyzing the photoelectric effect

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You are developing a **radiation detector for a spacecraft**.

You use a thin layer of metallic potassium to detect certain ranges of electromagnetic radiation. You need to make some estimates of the physical properties involved. In one test, the speed of an electron emitted from the surface of a sample of potassium by a photon is  $668 \text{ km s}^{-1}$ .

- (a) What is the kinetic energy of the ejected electron?
- (b) The work function of potassium is  $2.29 \text{ eV}$ , corresponding to  $3.67 \times 10^{-19} \text{ J}$ . What is the wavelength of the radiation that caused the photoejection of the electron?
- (c) What is the longest wavelength of electromagnetic radiation that could eject electrons from potassium?

## 1B.1 Radiation, quanta, and photons

### Example 1B.3: Analyzing the photoelectric effect

---

(a) What is the kinetic energy of the ejected electron?

(a) From  $E_k = \frac{1}{2}mv^2$ ,

$$\begin{aligned} E_k &= \frac{1}{2} \times (9.109 \times 10^{-31} \text{ kg}) \times (6.68 \times 10^5 \text{ m}\cdot\text{s}^{-1})^2 \\ &= 2.03 \times 10^{-19} \text{ J} \end{aligned}$$

## 1B.1 Radiation, quanta, and photons

### Example 1B.3: Analyzing the photoelectric effect

(b) The work function of potassium is 2.29 eV, corresponding to  $3.67 \times 10^{-19}$  J. What is the wavelength of the radiation that caused the photoejection of the electron?

(b) Convert the work function from electronvolts to joules.

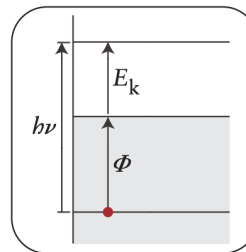
$$2.29 \text{ eV} \times \frac{1.602 \times 10^{-19} \text{ J}}{1 \text{ eV}} = 3.67 \times 10^{-19} \text{ J}$$

From  $\frac{1}{2}m_e v^2 = h\nu - \Phi$ ,  $h\nu = \Phi + \frac{1}{2}m_e v^2 = \Phi + E_k$ ,

$$h\nu = 3.67 \times 10^{-19} \text{ J} + 2.03 \times 10^{-19} \text{ J} = 5.70 \times 10^{-19} \text{ J}$$

so

$$\nu = \frac{5.70 \times 10^{-19} \text{ J}}{h}$$



Now use  $\lambda = c/\nu$ :

$$\begin{aligned} \lambda &= \frac{(3.00 \times 10^8 \text{ m}\cdot\text{s}^{-1}) \times (6.626 \times 10^{-34} \text{ J}\cdot\text{s})}{5.70 \times 10^{-19} \text{ J}} \\ &= 3.49 \times 10^{-7} \text{ m} \quad \text{or} \quad 349 \text{ nm} \end{aligned}$$

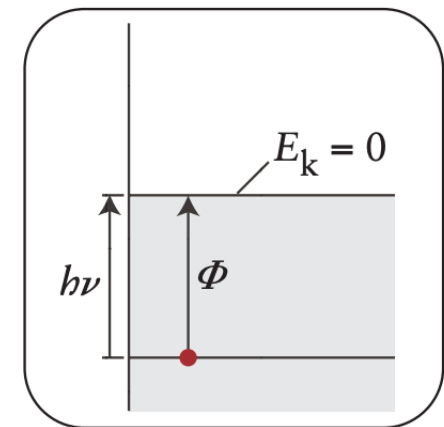
## 1B.1 Radiation, quanta, and photons

### Example 1B.3: Analyzing the photoelectric effect

(c) What is the longest wavelength of electromagnetic radiation that could eject electrons from potassium?

(c) To find the longest wavelength of radiation able to eject an electron, set  $E_k = 0$  in Eq. 5, so  $h\nu = \Phi$ , and therefore  $\lambda = ch/\Phi$ .

$$\begin{aligned}\lambda &= \frac{(3.00 \times 10^8 \text{ m}\cdot\text{s}^{-1}) \times (6.626 \times 10^{-34} \text{ J}\cdot\text{s})}{3.67 \times 10^{-19} \text{ J}} \\ &= 5.42 \times 10^{-7} \text{ m} \quad \text{or} \quad 542 \text{ nm}\end{aligned}$$



## 1B.1 Radiation, quanta, and photons

### Summary

Planck's postulates the quantization of energy.

The photoelectric effect provides evidence for the particulate nature of electromagnetic radiation and the existence of photons.

# Wave-particle duality

Topic 1B.2

## 1B.2 Wave-particle duality

### The double-slit experiment

- Photoelectric effect → photons behave like particles
- Before: wave-like nature of electromagnetic radiation was well supported (Newton, Young, Maxwell)
- Most compelling evidence for wave-like nature: **diffraction, the pattern of high and low intensities generated by an object in the path of a ray of light.**

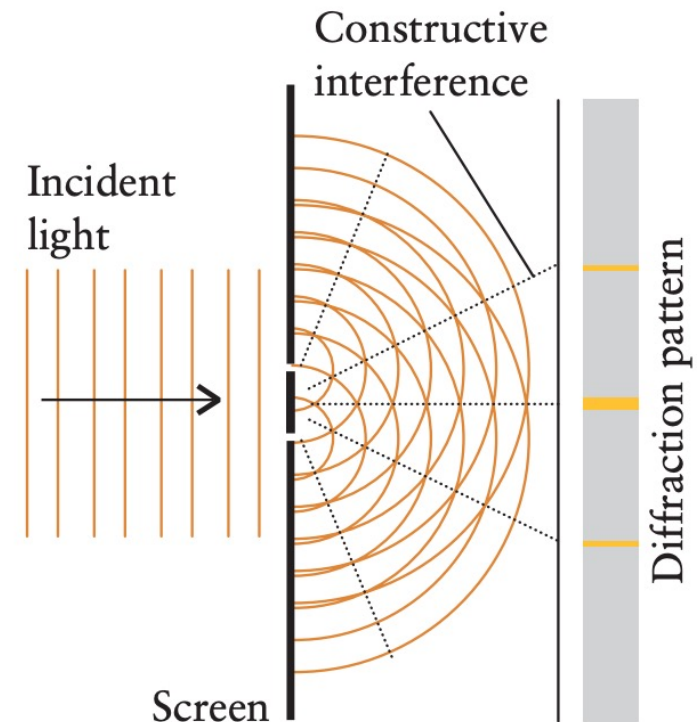
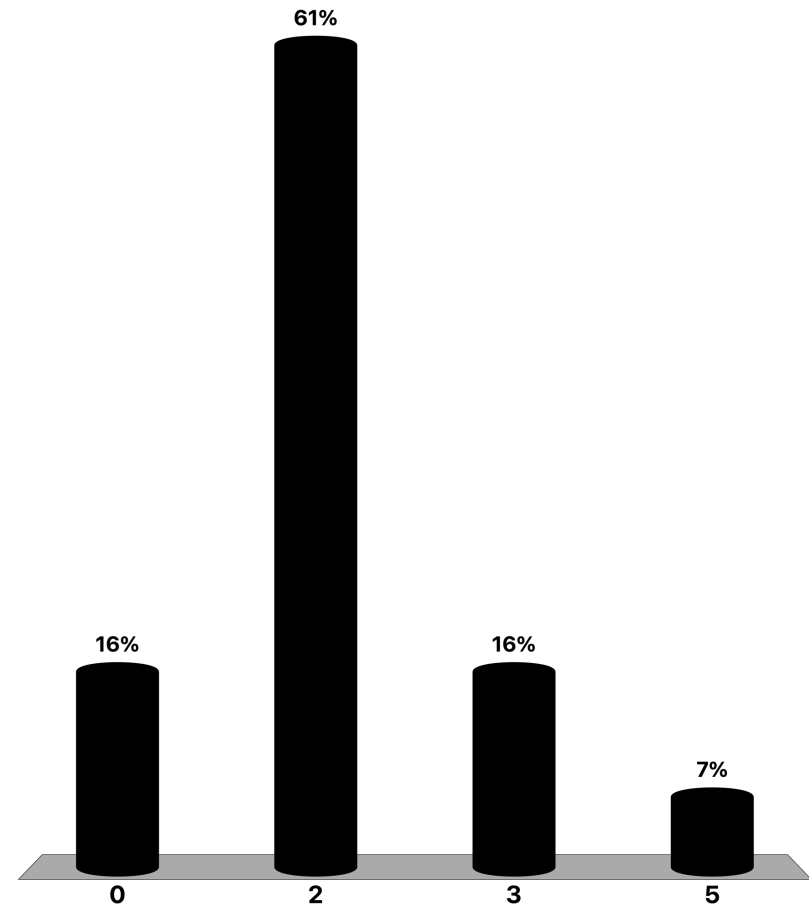


Figure 1.B6

How many bands would you expect to see on the screen if light behaved like particles in this experiment?

- A. 0
- B. 2
- C. 3
- D. 5



## 1B.2 Wave-particle duality

### The double-slit experiment

- Homework: watch Dr. Quantum (link on Moodle)



Dr. Quantum - Double slit experiment

## 1B.2 Wave-particle duality

### Constructive and destructive interference

(a) **Constructive interference:** if peaks coincide, the amplitude of the wave (its height) is enhanced.

(b) **Destructive interference:** if the peaks of one wave coincide with the valleys of another wave, the amplitude of the wave is diminished.

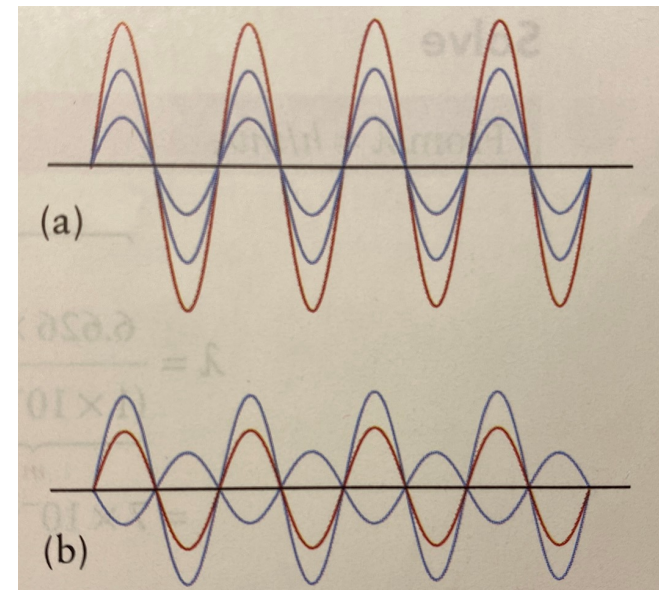
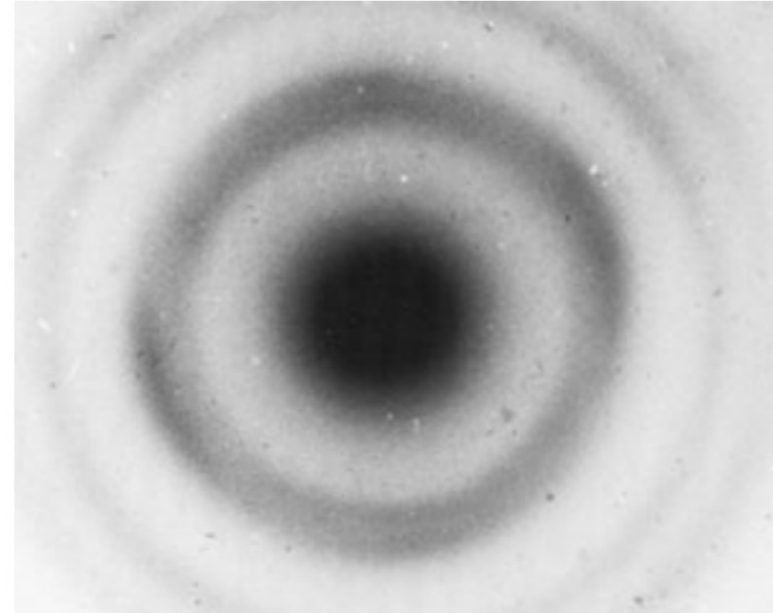


Figure 1.B7

## 1B.2 Wave-particle duality

### Wave or particle?

- Photoelectric effect → particle behavior.
- Diffraction → wave behavior.
- Light shows **wave-particle duality**.
- Intensity = wave amplitude<sup>2</sup> = number of photons.



**Figure 1.B8:** *Instead of behaving like little billiard balls, the electrons created a wave-like interference pattern, very similar to light diffraction. The bright and dark rings come from constructive and destructive interference of electron waves scattered by the crystal lattice.*

## 1B.2 Wave-particle duality

### Matter has wave-like properties: The de Broglie relation

- **If light (wave) can act like particles, matter (particles) can act like waves.**
- Wavelength of a particle:

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

Important formula.  
Need to know how to apply.

- The product of mass,  $m$ , and speed,  $v$ , is called the linear momentum,  $p$ , of a particle.
- Small mass / high speed  $\rightarrow$  shorter wavelength.

## 1B.2 Wave-particle duality

### Example 1B.4: Calculating the wavelength of a particle

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Now suppose you were de Broglie and you had just devised your formula. A friend points out that the world obviously isn't wave-like. Maybe you should check whether your formula has worrying consequences for everyday objects.

Calculate the wavelength of a particle of mass 1 g traveling at 1 m s<sup>-1</sup>.

## 1B.2 Wave-particle duality

### Example 1B.4: Calculating the wavelength of a particle

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#### SOLVE

From  $\lambda = h/mv$ ,

$$\begin{aligned}\lambda &= \frac{6.626 \times 10^{-34} \text{ J}\cdot\text{s}}{(1 \times 10^{-3} \text{ kg}) \times (1 \text{ m}\cdot\text{s}^{-1})} = \frac{6.626 \times 10^{-34} \text{ kg}\cdot\text{m}^2\cdot\text{s}^{-2}\cdot\text{s}}{1 \times 10^{-3} \text{ kg}\cdot\text{m}\cdot\text{s}^{-1}} \\ &= 7 \times 10^{-31} \text{ m}\end{aligned}$$

*Evaluate* As expected, this wavelength is very—in fact, undetectably—small; the same is true for any macroscopic (visible) object traveling at normal speeds.

## 1B.2 Wave-particle duality

### Summary

Electrons (and matter in general) and radiation have both wave-like and particle-like properties.

# The Uncertainty Principle

Topic 1B.3

## 1B.3 The uncertainty principle

Electrons do **NOT** have a definite trajectory

### Limits of Classical Trajectories

- Classical particle: position + momentum known  $\rightarrow$  definite path.
- Electrons: wave-particle duality means position & momentum cannot both be known exactly.
- For heavy objects, uncertainty negligible; for subatomic particles, it's significant.



Image source: ChatGPT. Artsy rendition:  
*From Classical Paths to Quantum Uncertainty*

## 1B.3 The uncertainty principle

### The Heisenberg uncertainty principle (1927)

- **Position and momentum cannot both be known exactly.**
- If position is known within  $\Delta x$ , momentum is uncertain by  $\Delta p$ :

$$\Delta p \times \Delta x \geq \frac{1}{2} \hbar$$

Important formula.  
Need to know how to apply.

- The symbol  $\hbar$ , reads «h bar», stands for  $\frac{h}{2\pi}$ . Its value is  $1.054 \times 10^{-34}$  J s.

## 1B.3 The uncertainty principle

### A note of interest

What do we mean by the “uncertainty”  $\Delta X$  in a property  $X$ ?

Formally, it is the «standard deviation» of  $X$ , which is defined as  $\Delta X = \sqrt{\langle X^2 \rangle - \langle X \rangle^2}$ , where the angle brackets denote mean values.

## 1B.3 The uncertainty principle

### Example 1B.5: Using the uncertainty principle

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To what extent does the Heisenberg uncertainty principle affect your ability to specify the properties of objects you can see? Can you be confident about their location?

Estimate the minimum uncertainty.

- (a) in the position of a marble of mass 1.0 g given that its speed is known to within  $\pm 1.0$  mm/s and
- (b) the speed of an electron confined to an atom within the diameter 200.0 pm.

## 1B.3 The uncertainty principle

### Example 1B.5: Using the uncertainty principle

---

**SOLVE** (a) First we convert mass and speed into SI base units. The mass,  $m$ , is  $1.0 \times 10^{-3}$  kg, and the uncertainty in the speed,  $\Delta v$ , is  $2 \times (1.0 \times 10^{-3} \text{ m}\cdot\text{s}^{-1})$ . The minimum uncertainty in position,  $\Delta x$ , is then:

---

From  $\Delta p \Delta x = \frac{1}{2} \hbar$  and  $\Delta p = m \Delta v$ ,

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$$m \Delta v \Delta x = \frac{\hbar}{2} \quad \text{or} \quad \Delta x = \frac{\hbar}{2m \Delta v}$$

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From  $\Delta x = \hbar / 2m \Delta v$ ,

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$$\begin{aligned} \Delta x &= \frac{1.054\,57 \times 10^{-34} \text{ J}\cdot\text{s}}{2 \times \underbrace{(1.0 \times 10^{-3} \text{ kg})}_{1.0 \text{ g}} \times \underbrace{(2.0 \times 10^{-3} \text{ m}\cdot\text{s}^{-1})}_{2.0 \text{ mm}\cdot\text{s}^{-1}}} \\ &= \frac{1.054\,57 \times 10^{-34} \text{ J}\cdot\text{s}}{2 \times 1.0 \times 10^{-3} \times 2.0 \times 10^{-3} \text{ kg}\cdot\text{m}\cdot\text{s}^{-1}} \\ &= 2.6 \times 10^{-29} \frac{\text{kg}\cdot\text{m}^2\cdot\text{s}^{-2}\cdot\text{s}}{\text{kg}\cdot\text{m}\cdot\text{s}^{-1}} = 2.6 \times 10^{-29} \text{ m} \end{aligned}$$

**Evaluate** As expected, this uncertainty is very small.

## 1B.3 The uncertainty principle

### Example 1B.5: Using the uncertainty principle

(b) The mass of the electron is given inside the back cover; the diameter of the atom is  $200. \times 10^{-12}$  m, or  $2.00 \times 10^{-10}$  m. The uncertainty in the speed,  $\Delta v$ , is equal to  $\Delta p/m$ :

From  $\Delta p \Delta x = \frac{1}{2} \hbar$  and  $\Delta p = m \Delta v$ ,

$$\Delta v = \frac{\Delta p}{m} \stackrel{\Delta p = \hbar/2\Delta x}{=} \frac{\hbar}{2m\Delta x}$$

From  $\Delta x = \hbar/2m\Delta v$ ,

$$\begin{aligned} \Delta v &= \frac{1.054\,57 \times 10^{-34} \text{ J}\cdot\text{s}}{2 \times \underbrace{(9.109\,39 \times 10^{-31} \text{ kg})}_{m_e} \times \underbrace{(2.00 \times 10^{-10} \text{ m})}_{200. \text{ pm}}} \\ &= \frac{1.054\,57 \times 10^{-34} \text{ J}\cdot\text{s}}{2 \times 9.109\,39 \times 10^{-31} \times 2.0 \times 10^{-10} \text{ kg}\cdot\text{m}} \\ &= 2.89 \times 10^5 \frac{\overbrace{\text{kg}\cdot\text{m}^2\cdot\text{s}^{-2}\cdot\text{s}}^{\text{J}}}{\text{kg}\cdot\text{m}} = 2.89 \times 10^5 \text{ m}\cdot\text{s}^{-1} \end{aligned}$$

**Evaluate** As predicted, the uncertainty in the speed of the electron is very large, nearly  $\pm 150 \text{ km}\cdot\text{s}^{-1}$ .

## 1B.3 The uncertainty principle

### Summary

The location and momentum of a particle are complementary; that is, the location and the momentum cannot both be known simultaneously with arbitrary precision. The quantitative relation between the uncertainty of each measurement is described by the Heisenberg uncertainty principle.

## The skills you have mastered are the ability to

- ❑ Use the relation  $E = h\nu$  to calculate the energy, frequency, or number of photons emitted from a light source.
- ❑ Analyze the photoelectric effect in terms of a metal's work function.
- ❑ Estimate the wavelength of a particle of known linear momentum.
- ❑ Use the uncertainty principle to estimate the uncertainty in the location or speed of a particle.

**Summary: You have seen that not all classical concepts are applicable to subatomic particles, and you now know that the concepts of waves and particles blend together. You have learned that one consequence of this blending is that it is impossible to specify the trajectory of a particle with arbitrary precision.**