Atoms Lecture 2: Quantum Mechanics

Learning Objective	Openstax 2e Chapter
Wave-Particle Duality	6.3
The Heisenberg Uncertainty Principle	6.3
One-dimensional Particle in a Box	6.3

Suggested Practice Problems

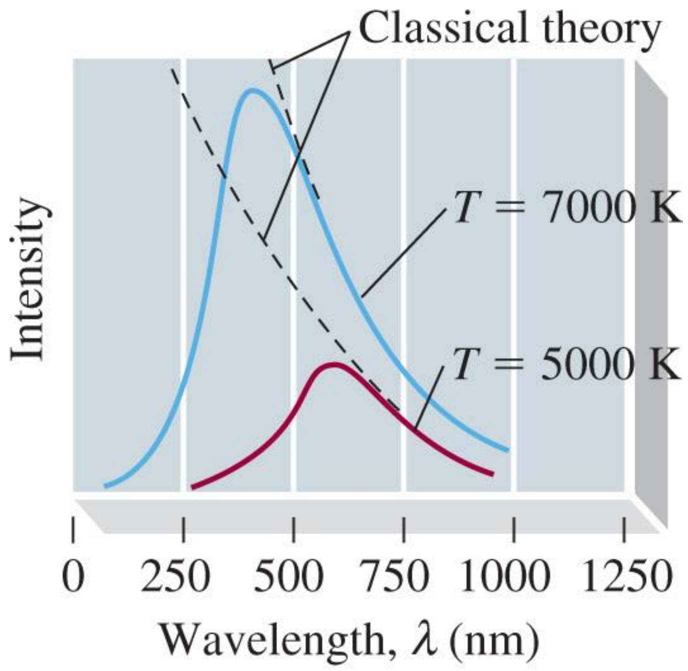
Chapter 6 Exercises – Questions: 35, 37

Answers can be found in the Chapter 6 Answer Key

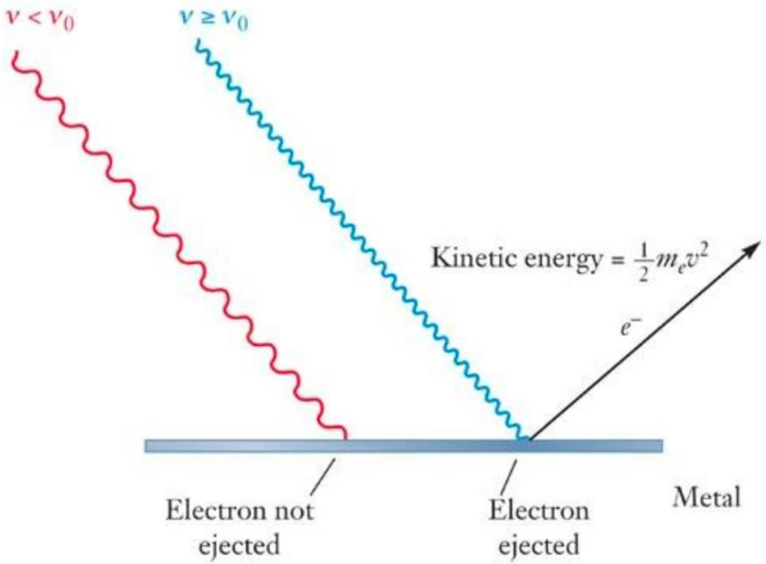
Wave-Particle Duality

We looked at phenomena that can only be explained if light is *quantized* and has *dual* nature.

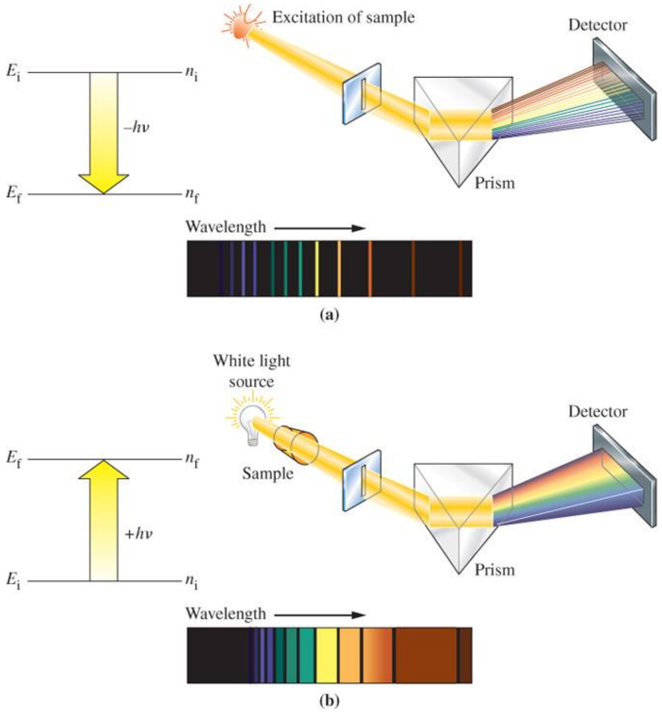
Black Body Radiation (Ultraviolet Catastrophe)



Photoelectric Effect

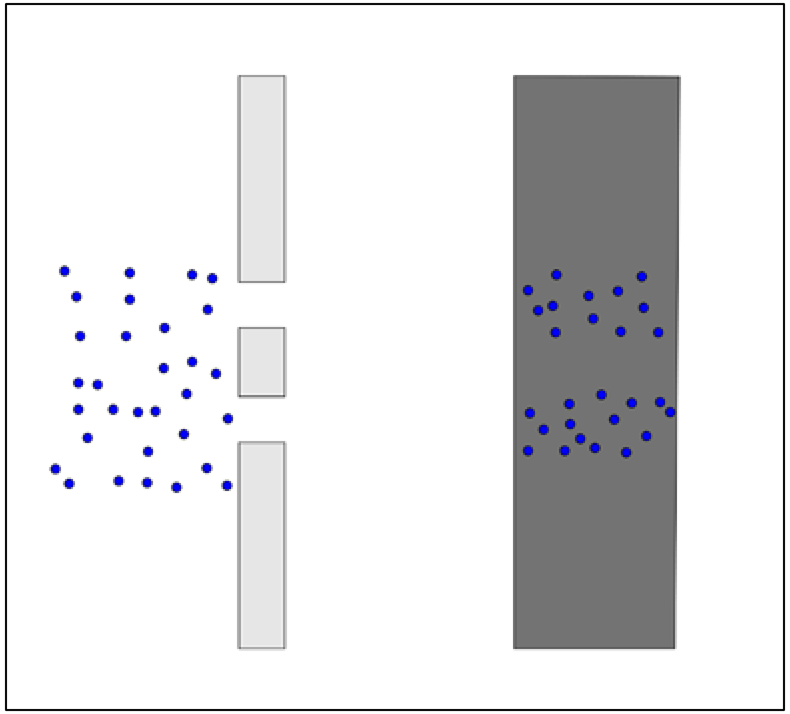


Atomic Spectra

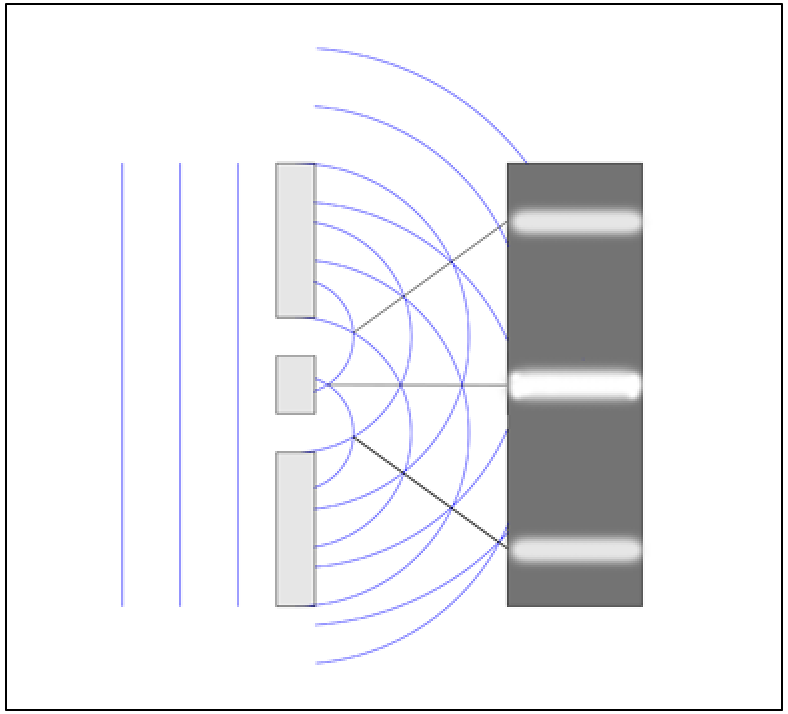


Wave-Particle Duality

Can matter have dual nature? In other words, does matter exhibit wave-like behaviour?

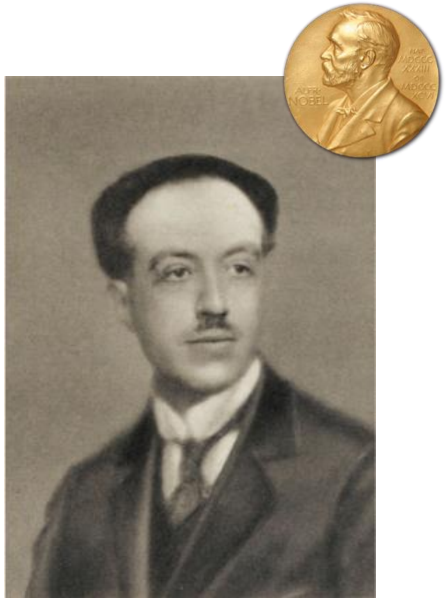


What we expect for particles



What we expect for waves

Figure 1: Schematic Representation of Particle vs. Wave Diffraction

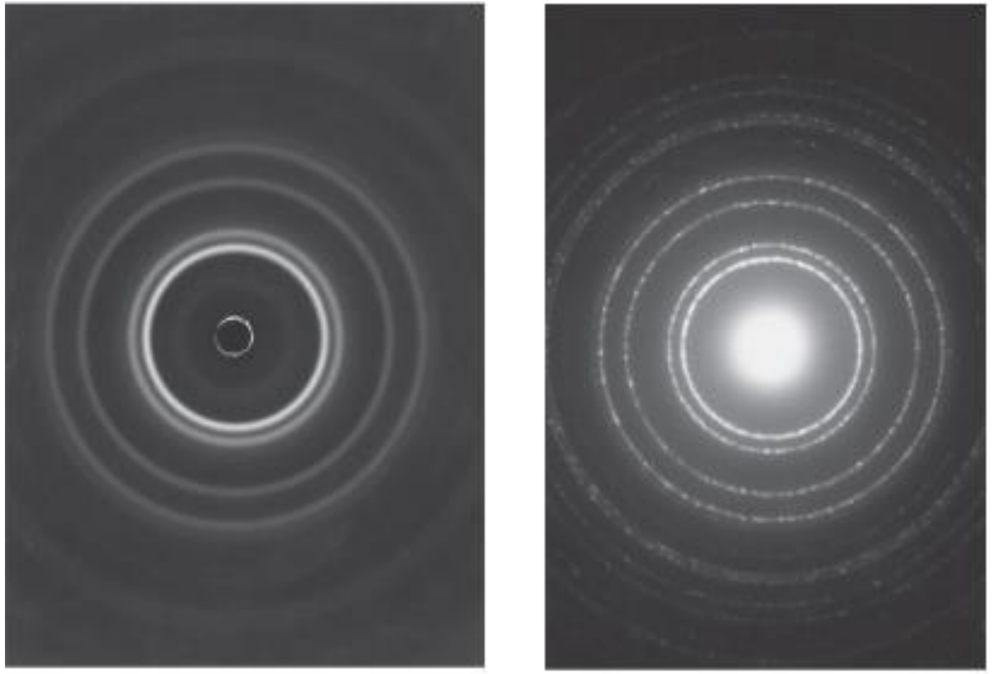


Louis de Broglie, 1924

Small particles of matter may at times display wavelike properties.

Wave-Particle Duality

Can matter have dual nature? In other words, does matter exhibit wave-like behaviour?



(a) (b)

Planck's Constant (6.626×10^{-34} J·s)

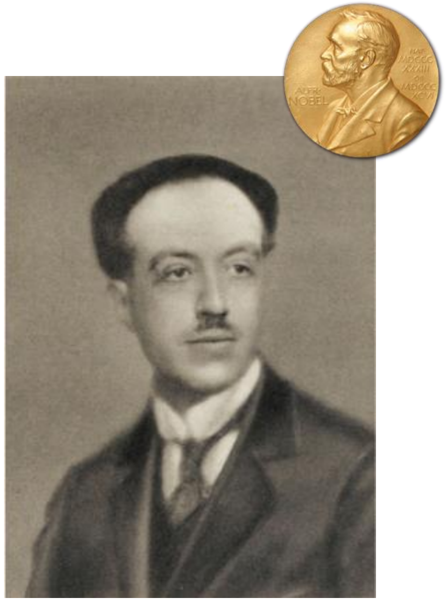
$$\lambda = \frac{h}{p} = \frac{h}{mu}$$

Wavelength (m)

Momentum $\left(\mathrm{kg}\frac{\mathrm{m}}{\mathrm{s}}\right)$

Mass (kg)

Speed (m/s)



Louis de Broglie, 1924

Figure 2: Wave properties of electrons:

(a) Diffraction of X-ray by metal foil

(b) Diffraction of electrons by metal foil.

Thomson & Davisson Nobel Prize (1937)

Small particles of matter may at times display wavelike properties.

Example

a) What is the wavelength of an electron traveling one tenth the speed of light?
b) What is the wavelength of car of mass 1000 kg traveling at 3 m/s?

de Broglie Equation: $$\lambda = \frac{h}{p} = \frac{h}{mu}$$

Physical constants:
h = 6.626 × 10^{-34} J s (J = kg m^2 s^{-2})
m_e = 9.109 × 10^{-31} kg
c = 2.9979 × 10^8 m s^{-1}

$$\mathbf{a)}\ u = \left(\frac{1}{10}\right) \times 2.9979 \times 10^8\ m\ s^{-1} = 2.9979 \times 10^7\ m\ s^{-1}$$

$$\lambda = \frac{6.626 \times 10^{-34} J\ s}{9.109 \times 10^{-31}\ kg\ \times 2.9979 \times 10^7\ m\ s^{-1}} = 2.426 \times 10^{-11}\ m$$

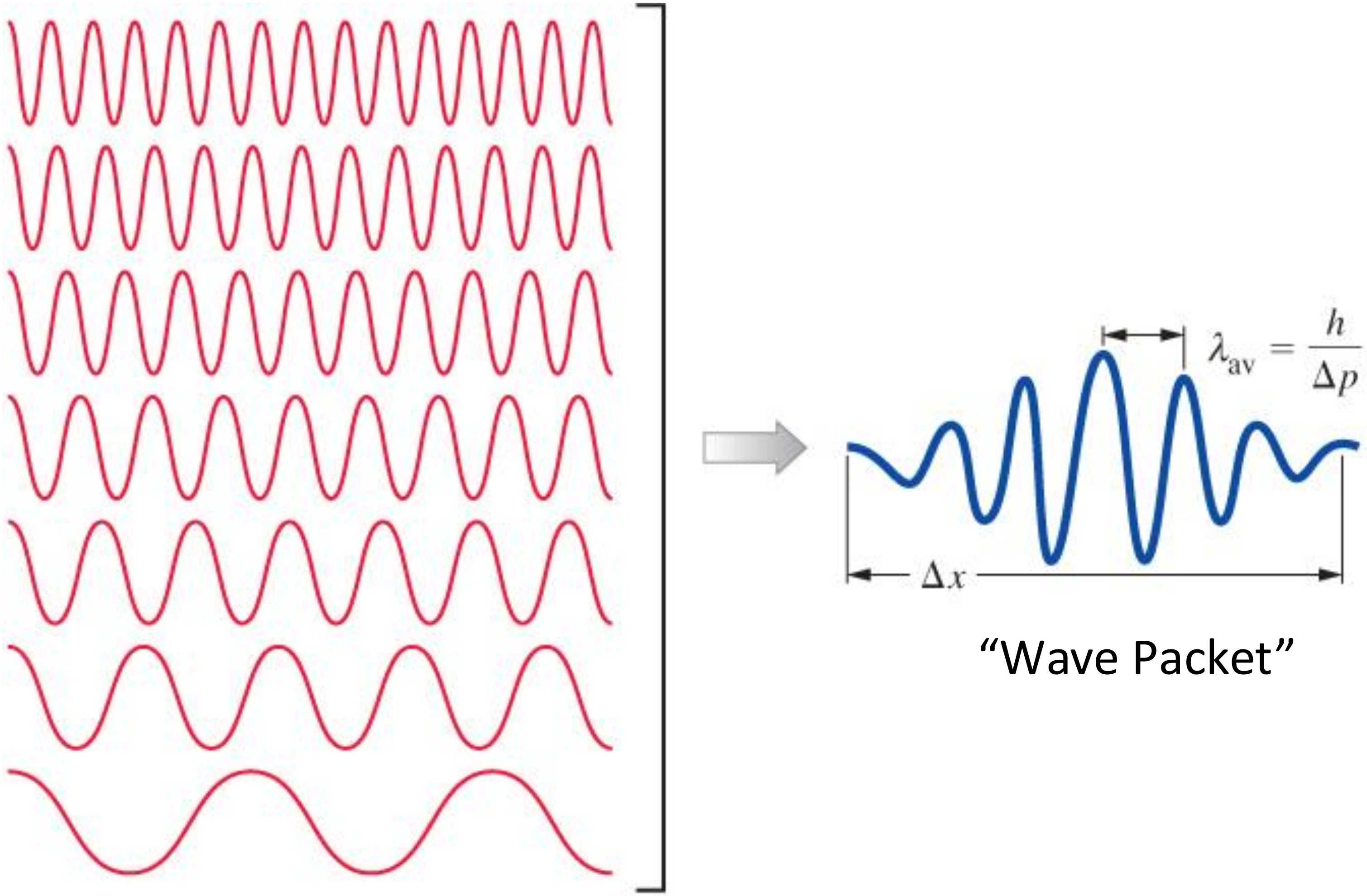
Wavelength in x-ray range

$$\mathbf{b)}\ \lambda = \frac{6.626 \times 10^{-34} J\ s}{1000\ kg \times 3.0\ m\ s^{-1}} = 2.21 \times 10^{-37} m$$

Note: diameter of a proton is ~1.6x10^{-15} m. A wavelength of ~10^{-37} m is too small to exist/interact with matter, and the intensity of this wave character will be vanishingly small

The (Heisenberg's) Uncertainly Principle

Are there any consequences to having a dual nature?



"Wave Packet"

Figure 3: The uncertainty principle interpreted graphically

Werner Heisenberg

$$\Delta x \, \Delta p \geq \frac{h}{4\pi}$$

Δx: uncertainty in position
Δp: uncertainty in momentum

Example

An electron can be shown to have a speed of 2.05×10^6 m/s. Assuming that the precision (uncertainty) of this value is 1.5%, with what maximum precision can we measure the position of the electron?

$$\Delta x\, \Delta p \;\geq\; \frac{h}{4\pi}$$

Physical constants:

$h = 6.626 \times 10^{-34}$ J s (J = kg m^2 s^{-2})

$m_e = 9.109 \times 10^{-31}$ kg

Compute the uncertainty in momentum by first computing the uncertainty in speed:

$$\Delta u = 0.015 \;\times\; \left(2.05 \;\times\; 10^6 \frac{m}{s}\right) = 3.1 \times\; 10^4 \frac{m}{s}$$

$$\Delta p = m\, \Delta u = (9.109 \times\; 10^{-31} kg) \times \left(3.1 \times\; 10^4 \frac{m}{s}\right) = 2.8 \times\; 10^{-26} \frac{kg\, m}{s}$$

Then, compute the uncertainty in position:

$$\Delta x \;\geq \frac{h}{4\pi\Delta p} \to \Delta x \;\geq \frac{6.626 \times 10^{-34} J\, s}{4 \times 3.14 \times \left(2.8 \times\; 10^{-26} \frac{kg\, m}{s}\right)} \;\to \Delta x \;\geq 1.9 \times\; 10^{-9} m$$

Maximum precision of position measurement

= $1.9 \times\; 10^{-9} m$

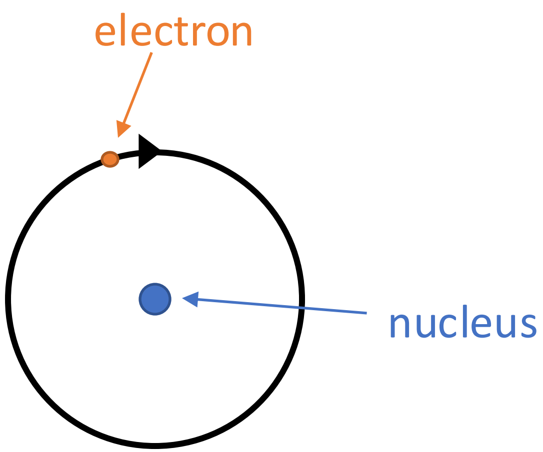
= $1.9\, nm$

Toward Quantum Mechanics

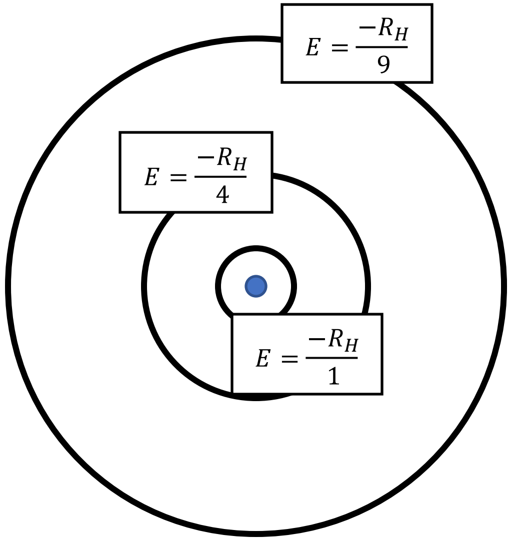
How should we view electrons in an atom?

Bohr's Atomic Model

1. Electrons move in circular orbits around the nucleus
2. Orbitals have fixed radius and energy levels
3. An electron can move between orbits by accepting or emitting discrete amounts of energy



Bohr's Hydrogen Model



<u>Successes:</u>

- Reproduces absorption/emission spectra of hydrogen
- Reproduces ionization potential of H atom

<u>Failures:</u>

- Only works for systems with 1 electron (H, He^+, Li^{2+}, …)
- Classical mechanics predicts that a circling electron will continually lose energy and spiral into the nucleus.

Wave Mechanics

Considering that the dual nature of electrons and the uncertainty principle, how are we to view them?

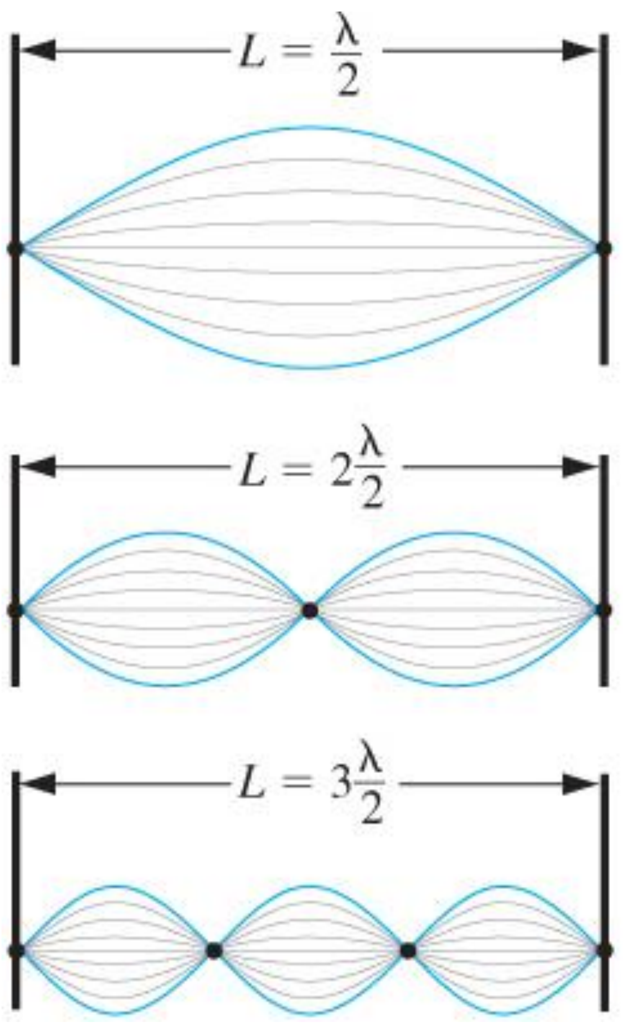
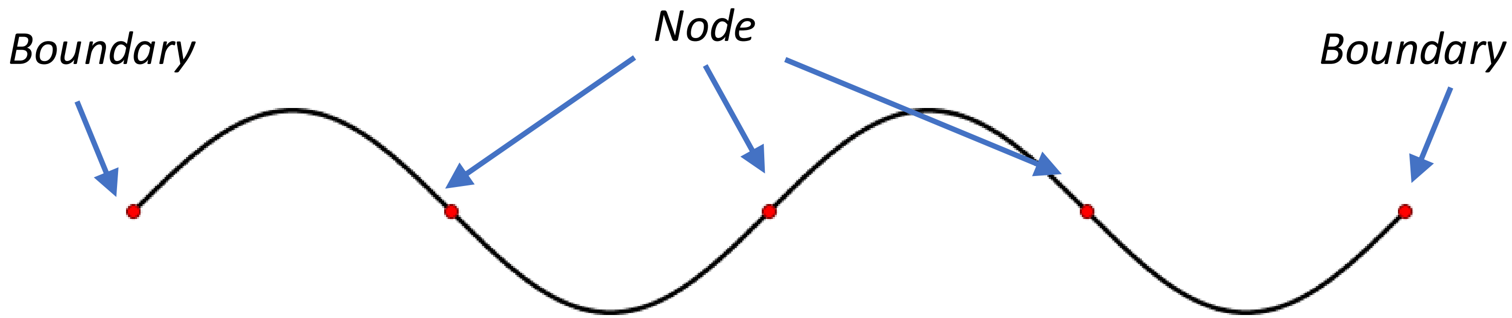


Figure 4: Standing waves in a string



Standing waves:

Nodes do not undergo displacement (#nodes = $n - 1$)

$$\lambda = \frac{2L}{n} \quad n = 1, 2, 3, \cdots$$

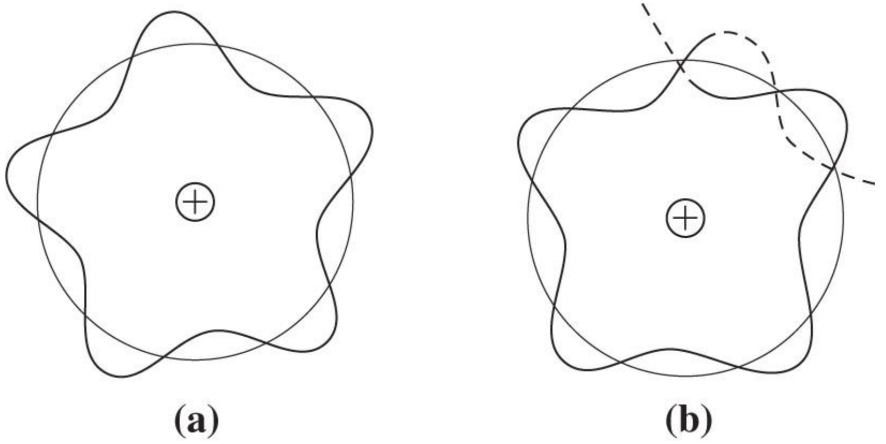


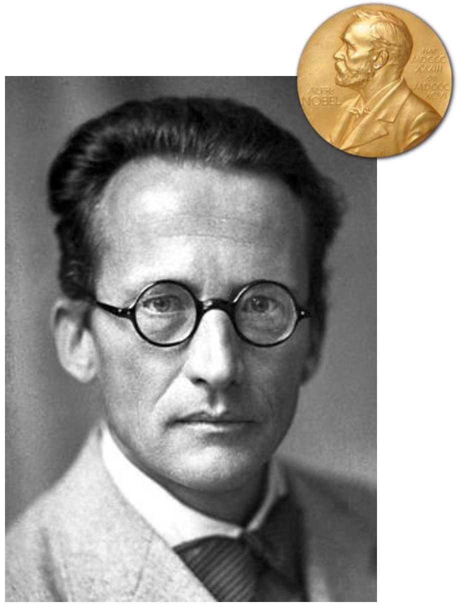
Figure 5: Electron as a **<u>matter wave</u>**

Wave Mechanics

Considering that the dual nature of electrons and the uncertainty principle, how are we to view them?

Schrödinger suggested that electrons (or any other particle) exhibiting wavelike properties should be described by a mathematical function called the **wave function**.

Chernoff Hall
Main Entrance



Erwin Schrödinger, 1927

$$\hat{H}\psi = E\psi$$

E: Energy
ψ: wave function
$\hat{H}$: Hamiltonian Operator

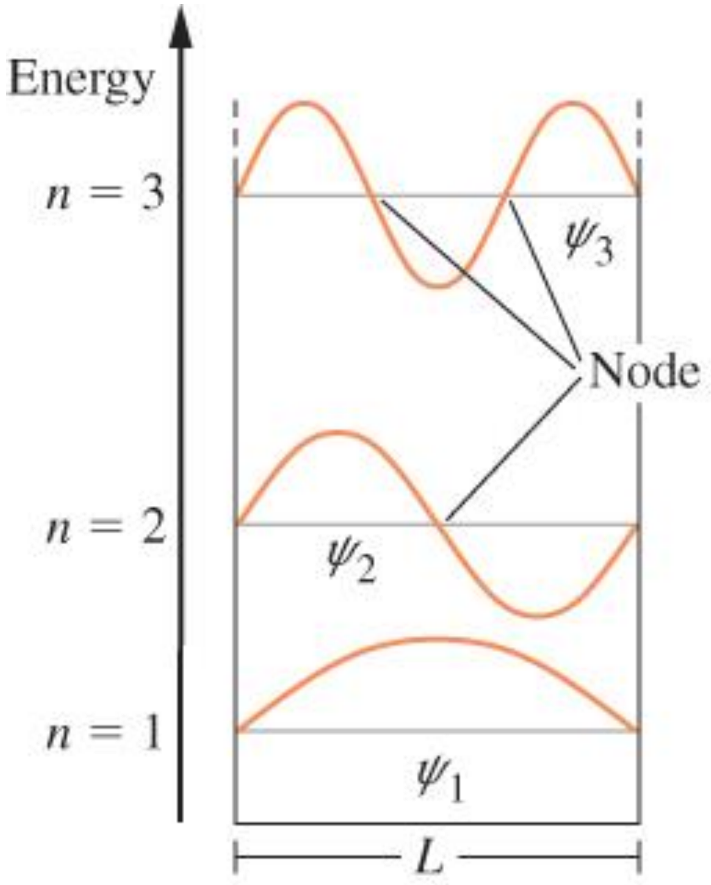
1-Dimensional Particle in a Box

Matter waves for a particle are all standing waves.

- Schrödinger postulated that for a 1-dimensional box, wave function must correspond to a standing wave within the box.

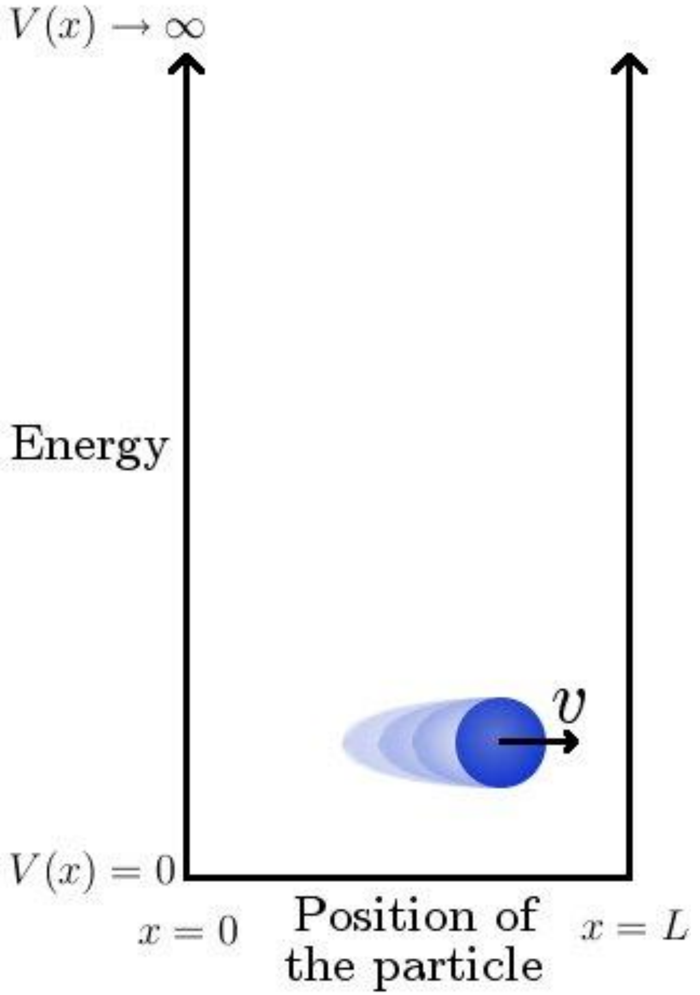
$$E_n = \frac{n^2\, h^2}{8\, m\, L^2} \qquad n = 1, 2, 3, \cdots$$

Quantum Number



$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

The wave functions



1-Dimensional Particle in a Box

Matter waves for a particle are all standing waves.

- The total probability of finding a particle in a small volume of space is the product of the square of the wave function, and the volume of interest.