CH-110 Advanced General Chemistry I

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Housekeeping notes

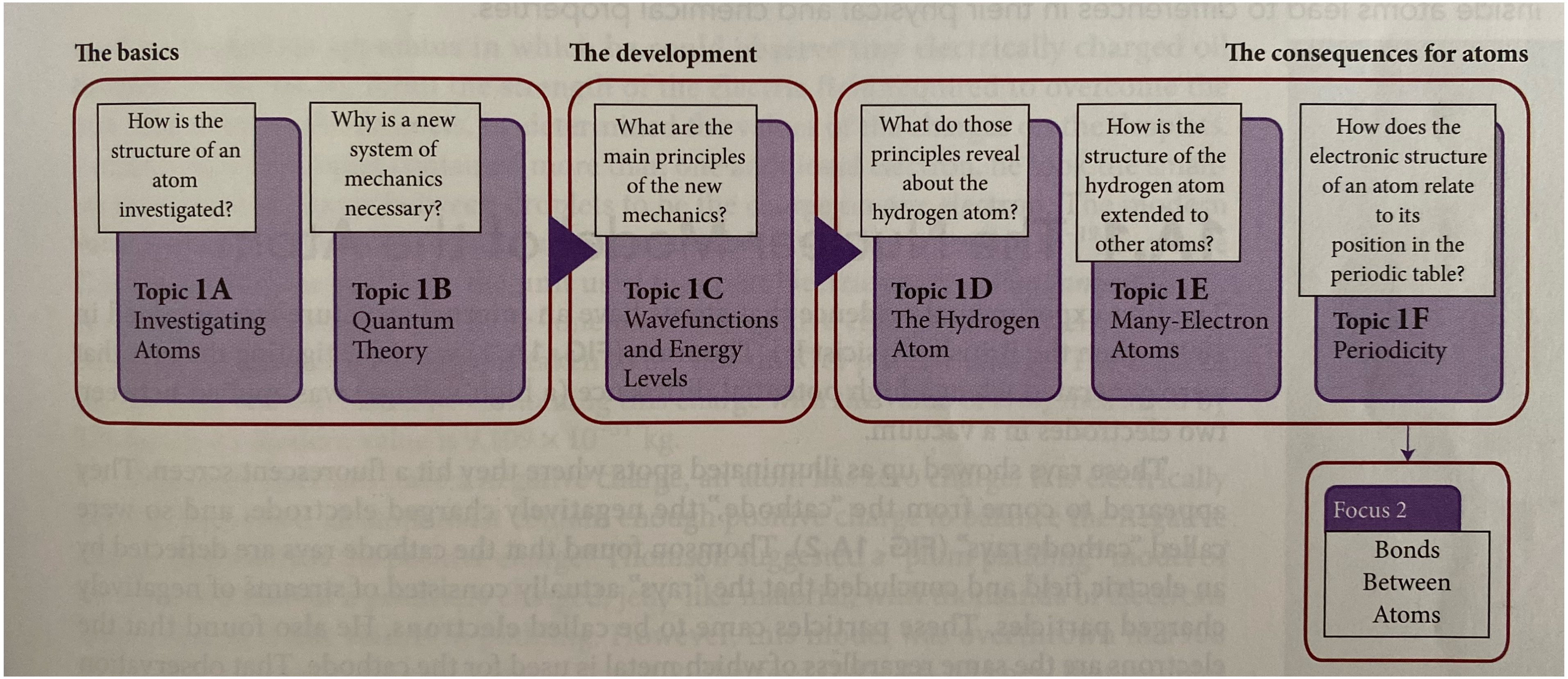
Calculator at exam: non-programmable. Examination mode is okay.

French: the subtitles on the Mediaspace recordings take at least one week to be generated by CeDE (week 1 now has French subtitles). My TAs translate the slides as we go.

Wavefunctions and Energy Levels

Topic 1C

Overview Chapter 1 (Focus 1: Atoms)



Topic 1C.1 The wavefunction and its interpretation
Topic 1C.2 The quantization of energy

WHY DO YOU NEED TO KNOW THIS MATERIAL?

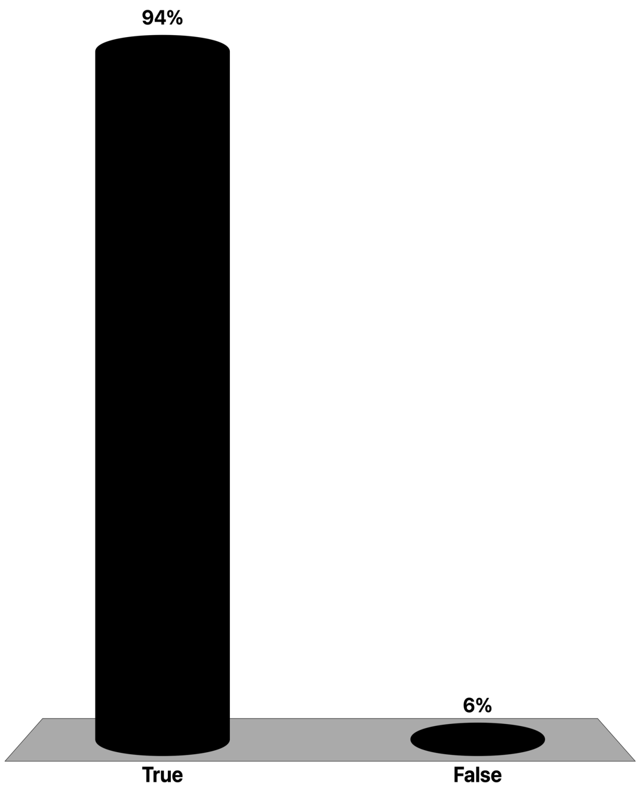
- Whenever you are dealing with quantum mechanics, you have to consider the **properties of wavefunctions and the information they contain**.

WHAT DO YOU NEED TO KNOW ALREADY?

- Properties of sine functions (sin x)
- Concept of duality
- De Broglie relation between momentum and wavelength
- Heisenberg uncertainty principle

Revision from Tuesday:
True/False: The concept of wave-particle duality asserts that particles, such as electrons, can exhibit both wave-like and particle-like properties.

A. True
B. False



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Revision from Tuesday:

True/False: Only light displays wave-particle duality; matter particles like electrons always behave as particles.

A. True

B. False

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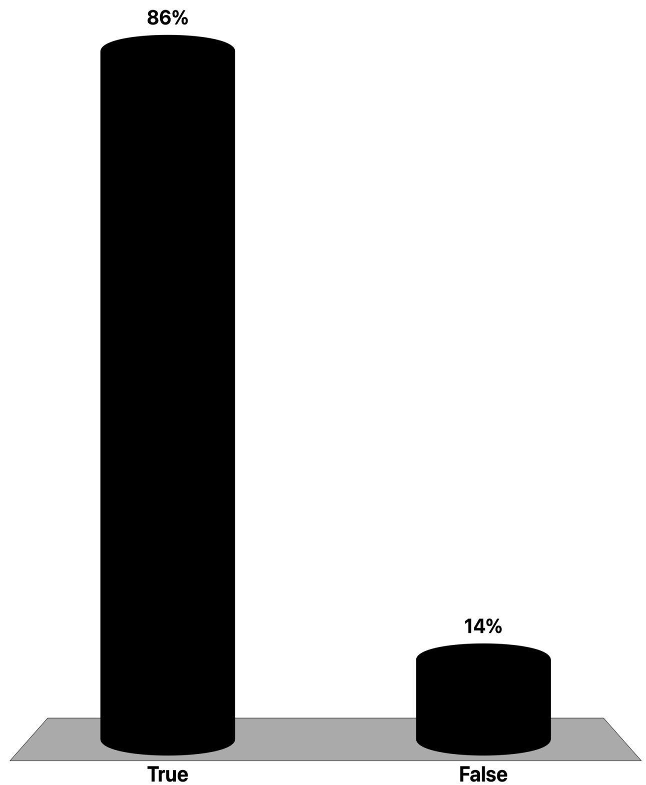
Revision from Tuesday:
True/False: The photoelectric effect, where electrons are emitted from a surface when it's illuminated by light of a particular frequency, provided evidence for the particle-like nature of light.

A. True
B. False



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Revision from Tuesday:
True/False: According to wave-particle duality, an electron in an atom is described by an orbit, much like planets orbiting the sun.

A. True
B. False

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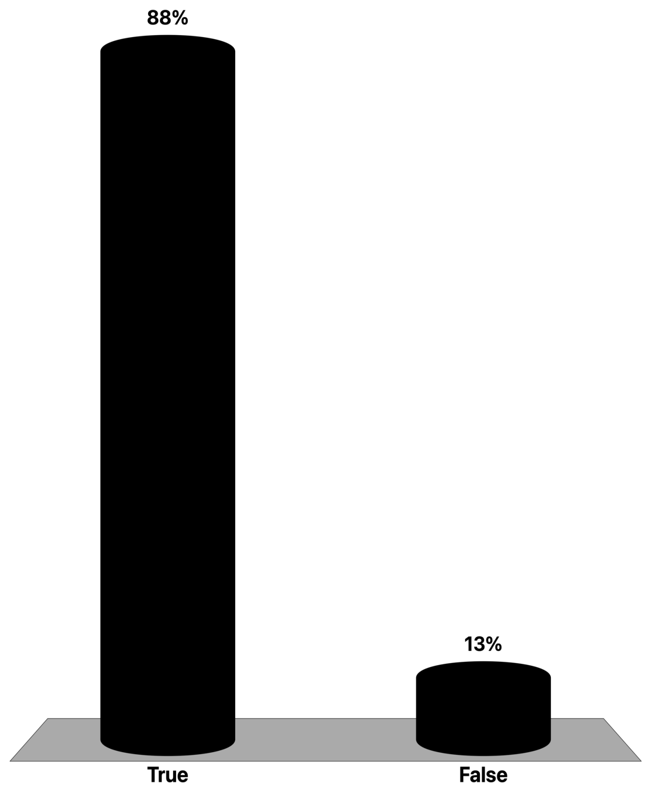
Revision from Tuesday:
True/False: The wavelength associated with a particle is inversely proportional to its momentum, as given by the de Broglie equation.

A. True
B. False



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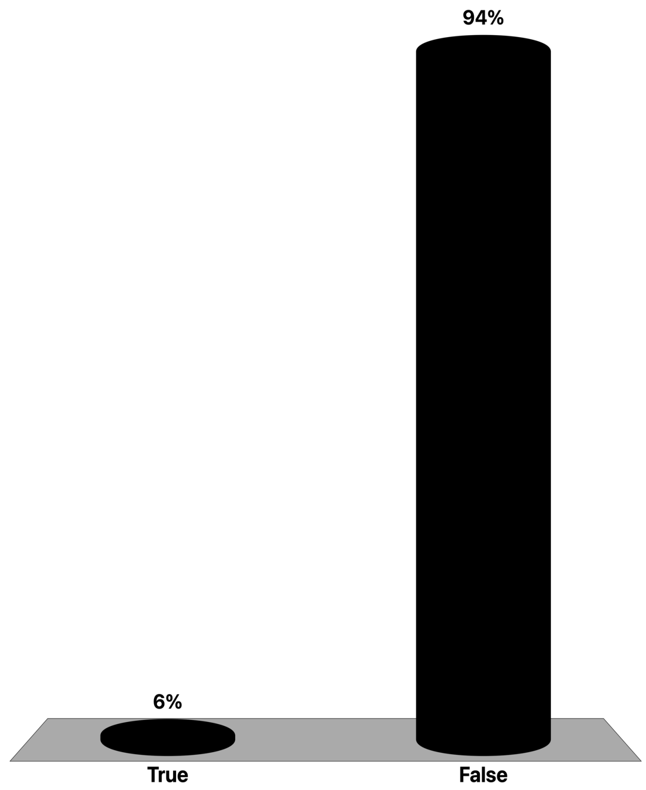
Revision from Tuesday:
True/False: The wave nature of particles is only observable at everyday, macroscopic scales and has no significance at the quantum level.

A. True
B. False



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Solutions

True: The concept of wave-particle duality asserts that particles, such as electrons, can exhibit both wave-like and particle-like properties. Explanation: This foundational idea of quantum mechanics arose from experiments showing that certain phenomena (e.g., interference and diffraction) can only be explained if particles also have wave-like properties.

False: Only light displays wave-particle duality; matter particles like electrons always behave as particles. Explanation: Both light (traditionally considered a wave) and matter particles (like electrons) exhibit wave-particle duality. This was famously demonstrated with the electron double-slit experiment.

True: The photoelectric effect, where electrons are emitted from a surface when it's illuminated by light of a particular frequency, provided evidence for the particle-like nature of light. Explanation: Albert Einstein explained the photoelectric effect by proposing that light can be thought of as discrete packets or quanta of energy, later termed photons. This quantized view of light demonstrated its particle-like nature.

False: According to wave-particle duality, an electron in an atom is described by an orbit, much like planets orbiting the sun. Explanation: In quantum mechanics, electrons in atoms are described by wavefunctions, not classical orbits. These wavefunctions represent the probability density of finding an electron in a particular location.

True: The wavelength associated with a particle is inversely proportional to its momentum, as given by the de Broglie equation. Explanation: Louis de Broglie proposed that particles could have wavelengths given by $\lambda = h/p$, where h is Planck's constant and p is the momentum of the particle.

False: The wave nature of particles is only observable at everyday, macroscopic scales and has no significance at the quantum level. Explanation: It's the opposite. The wave-like properties of particles are most significant and observable at the quantum (microscopic) scale and become negligible at macroscopic scales due to the very small wavelengths involved.

Summary of last Tuesday

- Particle-like nature of electromagnetic radiation
- Exchange of energy between matter and light is not continuous, but happens in the form of equal packets of energy, called quanta → flow of photons
- Photon: particle without mass that travels at the speed of light, *c*
- Analogy: jet of water (flow of water molecules)

The Wavefunction and Its Interpretation

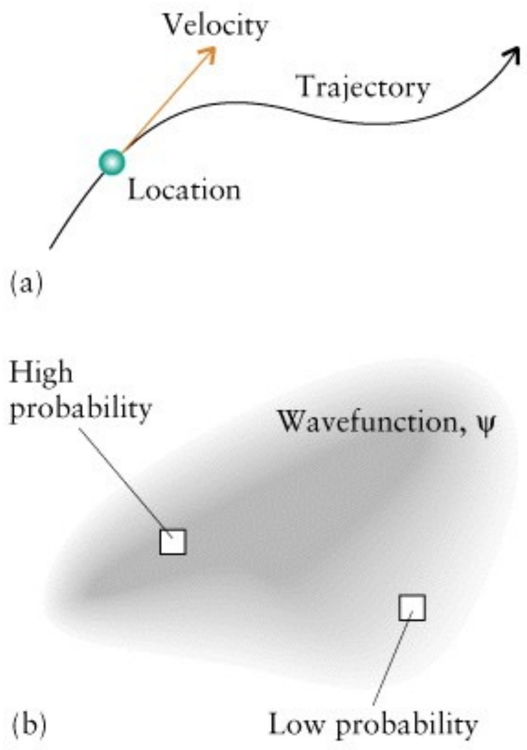
Topic 1C.1

The skills you have mastered are the ability to

- **Describe** the origin and shapes of the wavefunctions of a particle in a box. (TODAY)
- **Calculate** the allowed energies of a particle in a box and **explain** how they depend on the length of the box and the mass of the particle. (Next week)
- **Explain** what is meant by zero-point energy and accounts for its origin. (Next week).

1C.1 The wavefunction and its interpretation

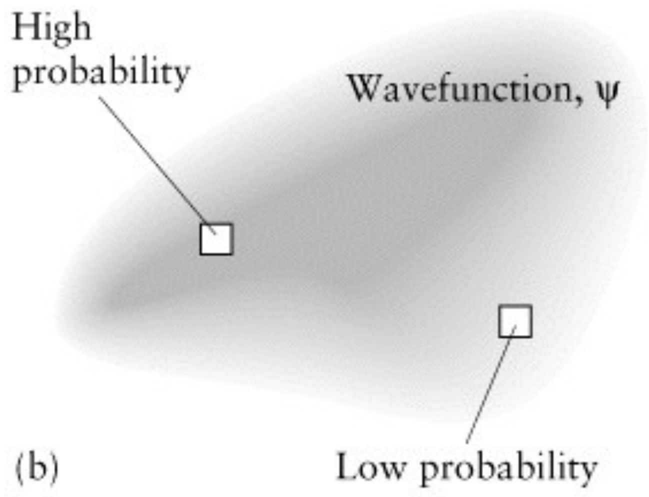
The wavefunction and probability density



- **Classical mechanics:** the location and velocity of a particle are known precisely at each point in time (**trajectory**), described by a **path or position function *x(t)*.**
- **Quantum mechanics**: the particle is better described by its wave-like character with a **wavefunction** ψ (position not defined) and a **probability density** ψ^2.

1C.1 The wavefunction and its interpretation

The wavefunction and probability density



$|\psi|^2$: The **square of the wavefunction** is a measure of the **probability density** of finding the particle at a given point.

P(r) is the probability of finding the particle in an infinitesimally small volume element *dV* around *r*.

$$P(r) = \psi^2(r)dV$$

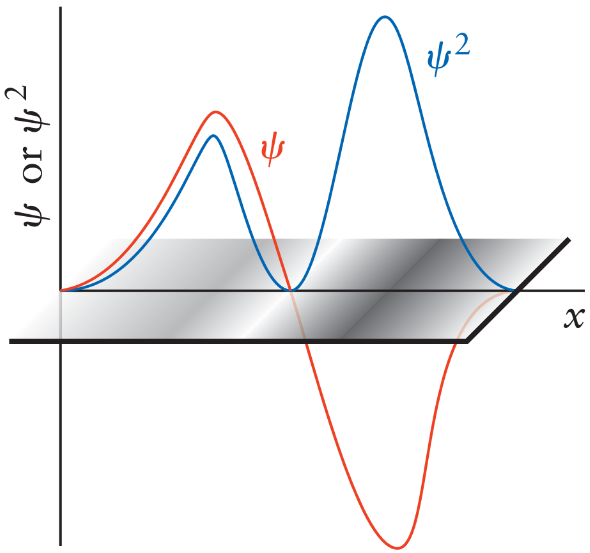
The **total probability** of finding the particle anywhere in space **is equal to 1** (i.e. the particle is certain to be located somewhere within this volume).

$$\int \psi^2(r)dV = 1$$

1C.1 The wavefunction and its interpretation

ψ is a wave

- ψ = wave, can be + or - → interference.
- ψ^2 = probability density, always ≥ 0.
- Large |ψ| → high probability of finding particle.
- ψ = 0 → particle not found.
- Nodes = points where ψ crosses 0 → zero probability.



1C.1 The wavefunction and its interpretation

Analogy: density vs. probability density

- **Mass density**: tells you how much mass is in each unit of volume.

  Mass in a region = density × volume.

- **Probability density**: tells you how likely it is to find the particle in each unit of volume (always positive).

  Probability in a region = probability density × volume.

Key takeaway: Multiply density by volume → get total mass (classical) or total probability (quantum).

1C.1 The wavefunction and its interpretation

Example: Physical density analogy

Numerical Example

- **Mass density**: A metal has a density of 10 g/cm^3.

  In a volume of 2 cm^3: Mass $= 10 \times 2 = 20$ g

- **Probability density**: A particle has a probability density of 0.2 per cm^3.

  In a region of 2 cm^3: $Probability = 0.2{\times}2 = 0.4$

  → 40% chance to find the particle there.

Image source: ChatGPT.
A golden cube.

1C.1 The wavefunction and its interpretation

Probability vs. probability density

- Probability: **unitless**, can have values between 0 (certainly *not* there) and 1 (certainly there)
- Probability density: units are **1/volume**

1C.1 The wavefunction and its interpretation

What information about position can we obtain from the wavefunction?

- The **probability density** of finding the particle at different positions (where it is most/least likely).
- The **probability** of finding the particle inside a given volume.

To make predictions, however, we still need to know the actual form of the wavefunction, ψ.

This function is not arbitrary: it is determined **by the Schrödinger equation**, which plays the same role in quantum mechanics that Newton's laws ($F = ma$) play in classical mechanics.

1C.1 The wavefunction and its interpretation

The Schrödinger equation

$$H\psi = E\psi$$

ψ = the wavefunction, tells us where the particle is likely to be.

E = the energy of the particle.

$\hat{H}$ = the "Hamiltonian," an operator that represents the *total energy* of the system (kinetic + potential).

The equation says: *only certain wavefunctions ψ are allowed, and each corresponds to a specific energy E.*

Image source: ChatGPT.
Erwin Schrödinger, featuring his signature round glasses, along with the wavefunction background in the Vienna Secessionist style.

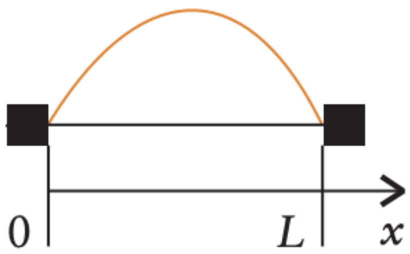
1C.1 The wavefunction and its interpretation

The Schrödinger equation

- The Schrödinger equation is used to calculate the **wavefunction (ψ)** and the **corresponding energy (E)** for a particle confined to a region of space, such as electrons in atoms or molecules.
- In this class, **we will not solve the equation directly**, but you should recognize the form of some of its solutions.
- The Schrödinger equation is a **differential equation**. You will study this topic in more depth later.

1C.1 The wavefunction and its interpretation

The particle-in-a-box model



The wavefunction of the particle in its lowest-energy state (ground state, *n* = 1):

$$\psi_1(x) = \left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{\pi x}{L}\right)$$

And therefore:

$$\psi_1^2(x) = \left(\left(\frac{2}{L}\right)^{\frac{1}{2}} \sin\left(\frac{\pi x}{L}\right)\right)^2 = \frac{2}{L}\, sin^2\left(\frac{\pi x}{L}\right)$$

And P(x=0) = P(x=L) = 0

1C.1 The wavefunction and its interpretation

PREVIEW: The particle-in-a-box model

Where is the probability maximum? (Where is the electron most likely to be?)

$$\frac{d\psi^2(x)}{dx} = \frac{2}{L}\left(\frac{d}{dx}\right)\left[sin^2(\frac{\pi x}{L})\right] = 0 \Rightarrow \frac{4}{L}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\left(\frac{\pi}{L}\right) = 0$$

$$\frac{4\pi}{L^2}\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right) = 0 \Rightarrow \cos\left(\frac{\pi x}{L}\right) = 0 \Rightarrow \left(\frac{\pi x}{L}\right) = \frac{\pi}{2}$$

$\Rightarrow$ $\psi^2_{max}(x)$ is at $x = L/2$

The probability density is highest in the middle of the box.

Note: in the classical case, the probability density is the same for all x! P(x) is constant.

1C.1 The wavefunction and its interpretation

Exercise 3 (Next week)

- You'll get a chance to familiarize yourselves with the particle-in-a-box model more during the exercise session on Friday, 26.9.25.
- Yannick will demonstrate the first exercise on the board.
- However: On the final exam, we will *NOT* ask you to do derivatives or integrals.