

An abstract graphic at the top of the slide featuring a horizontal band of colorful splatters and dots. The colors transition from warm tones (yellow, orange, red) on the left to cool tones (purple, blue) on the right, with some green and cyan accents. The splatters vary in size and density, creating a dynamic, artistic effect.

CH-110 Advanced General Chemistry I

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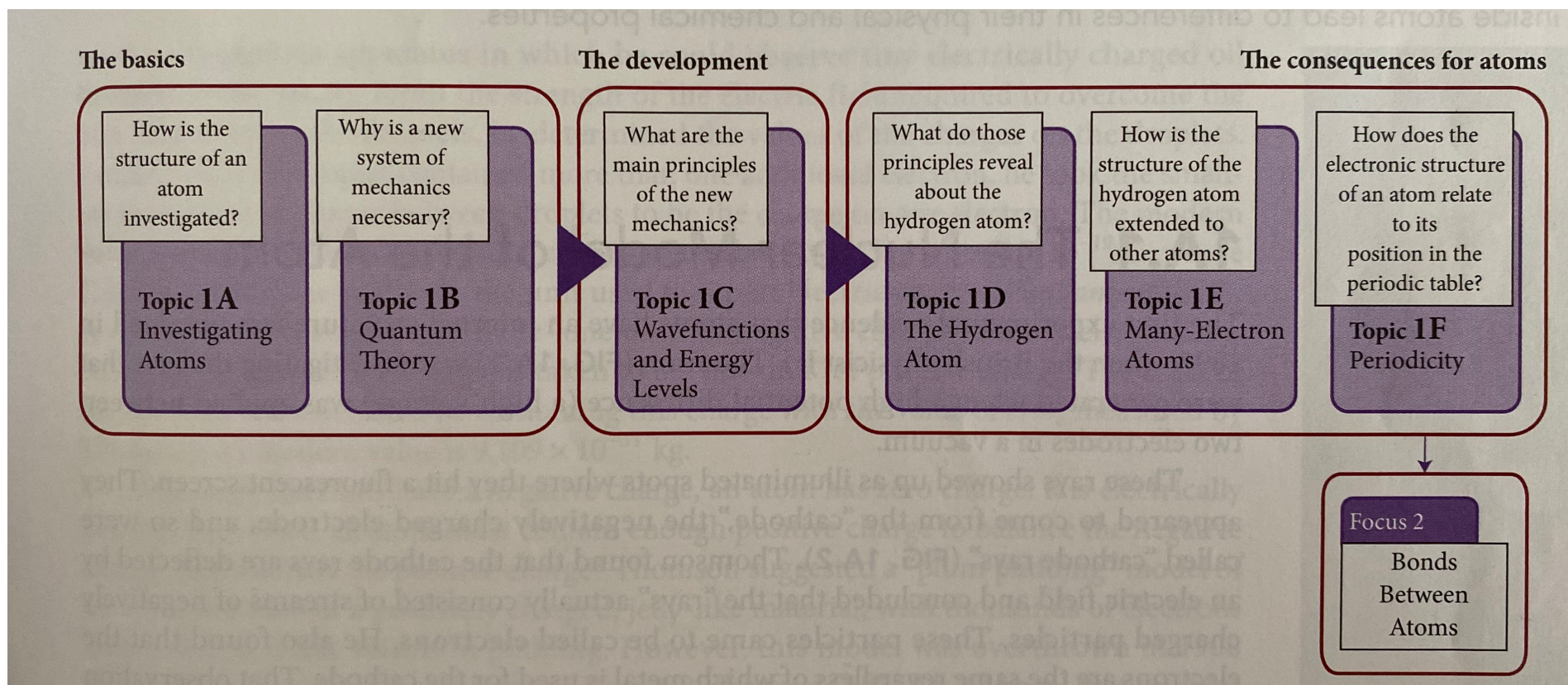
Housekeeping notes

- Sharing slides in advance
- Sharing PDF of book
- Feedback on Moodle: Thank you!
- What I can implement now:
 1. *Give you the solutions to the exercises earlier (as soon as available).*
 2. *There were supposed to be subtitles in French on Mediaspace, I will doublecheck what is going on with that.*
 3. *Develop more material on the board.*

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?

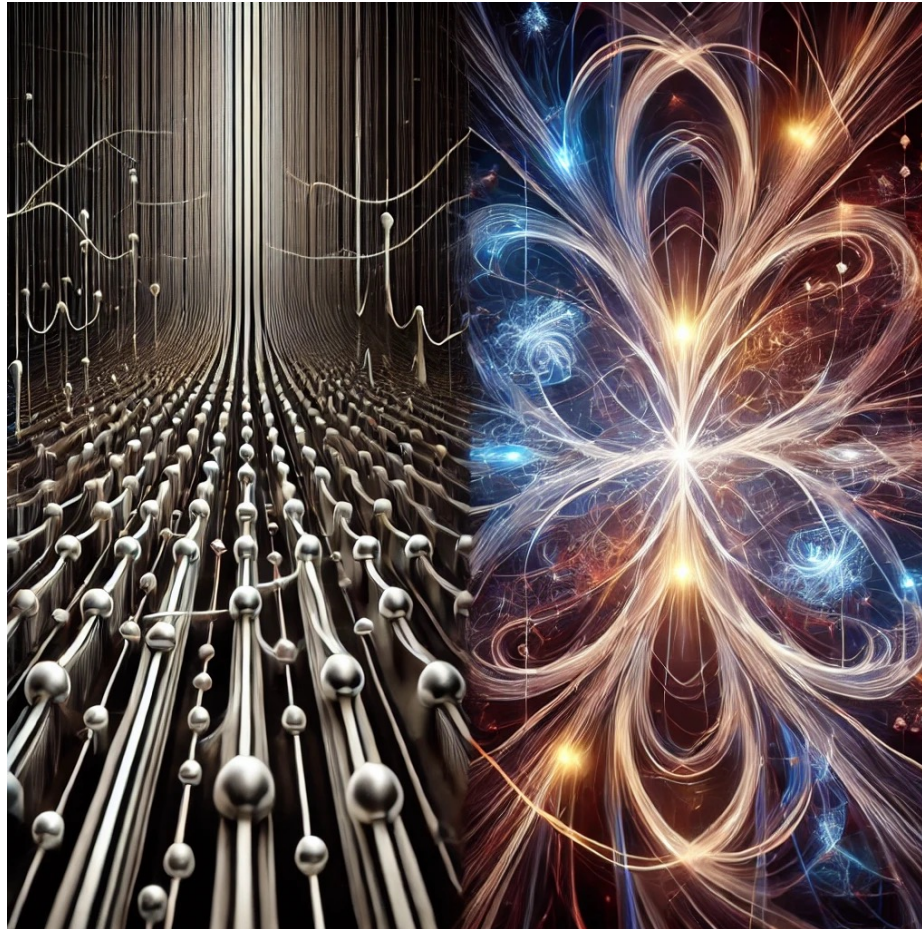
- Properties of sine functions ($\sin x$)
- Concept of duality
- De Broglie relation between momentum and wavelength
- Heisenberg uncertainty principle

The Wavefunction and Its Interpretation

Topic 1C.1

Classical
mechanics:

Fixed predictable
path

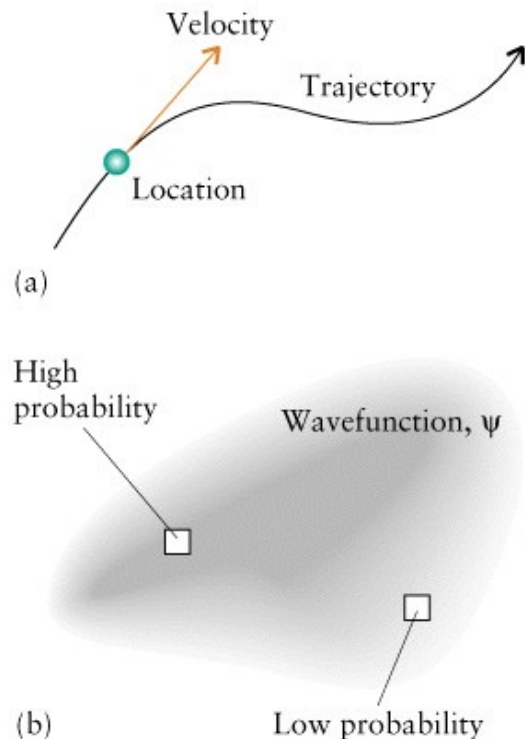


Quantum
mechanics:

Probability
distribution

1C.1 The wavefunction and its interpretation

Last time: Classical vs. quantum mechanics



- **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**.
- **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

Last time: The Schrödinger equation

- The Schrödinger equation is used to calculate the **wavefunction** for any **particle confined** to any region of space, including **electrons confined** within atoms and molecules.

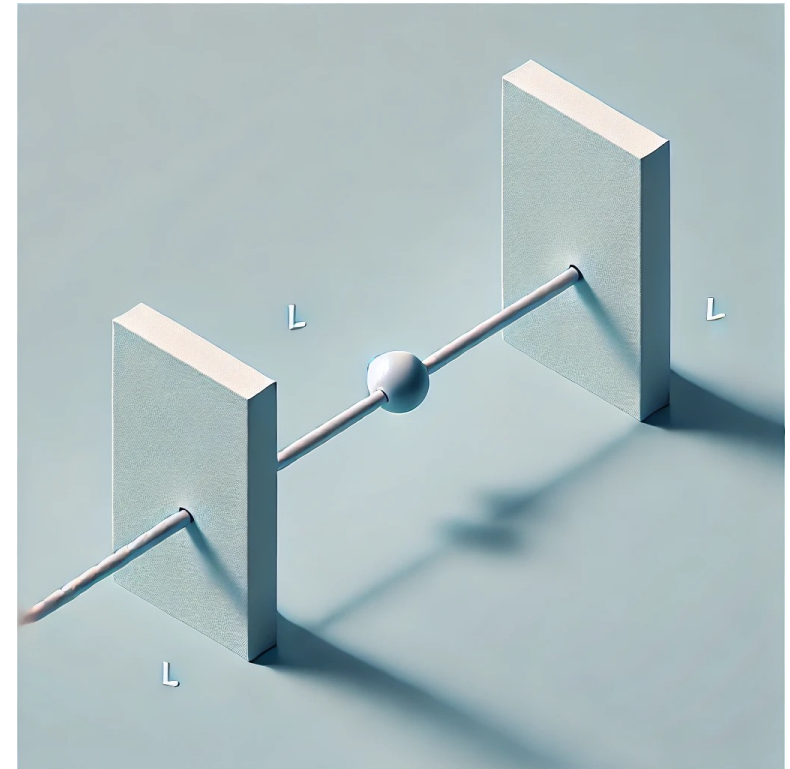
$$H\psi = E\psi$$

- Equation not used directly in this class.
- You will need to **recognize** (not know by heart, they would be on the formula sheet) the form of some of its solutions, but not how these solutions are found.

1C.1 The wavefunction and its interpretation

Last time: The particle-in-a-box model

- The Schrödinger equation is used to calculate both the **wavefunction ψ** and the corresponding **energy E** .
- The particle-in-a-box model is used to show **how the Schrödinger equation can be applied to describe quantum systems**.
- Simple **model system**: a **single particle of mass m** confined in a **one-dimensional** «box» between two impenetrable walls a distance L apart.



1C.1 The wavefunction and its interpretation

Last time: The time-independent Schrödinger equation

- For a particle of mass m moving in one dimension in a region where the potential energy is $V(x)$, the equation is

$$\underbrace{-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}}_{\text{Kinetic energy}} + \underbrace{V(x)\psi}_{\text{Potential energy}} = \underbrace{E\psi}_{\text{Total energy}}$$

$H\psi$

- Can also be written as:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$

Both notations are acceptable. Using ψ without explicitly stating the variable is common in theoretical discussions, while $\psi(x)$ is often used when emphasizing the dependence on position.

1C.1 The wavefunction and its interpretation

Last time: The mathematical form of the particle in the box

Due to boundary conditions, only wavefunctions with **certain wavelengths** can exist in the box. The wavefunction is derived as a **solution** to the **time-independent Schrödinger equation** for the particle in a box, which is given by:

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

- For $\psi_n(x)$ to satisfy the boundary $\psi_n(L) = 0$, $\frac{n\pi x}{L}$ must be **an integer multiple** of π when $x = L$, so that the sine function goes to zero. This only happens if n is a **positive integer** (1, 2, 3,...), because:
- $\sin(n\pi) = 0$ when $n=1, 2, 3, \dots$

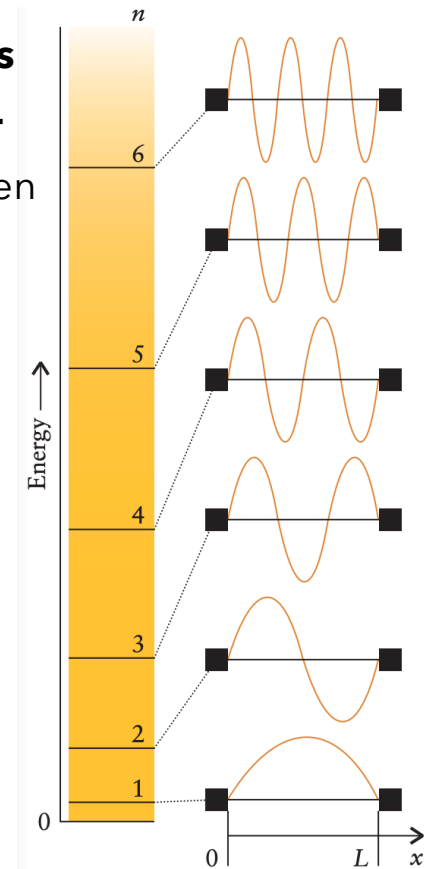


Figure 1C.3

1C.1 The wavefunction and its interpretation

Last time: The mathematical form of the particle in the box

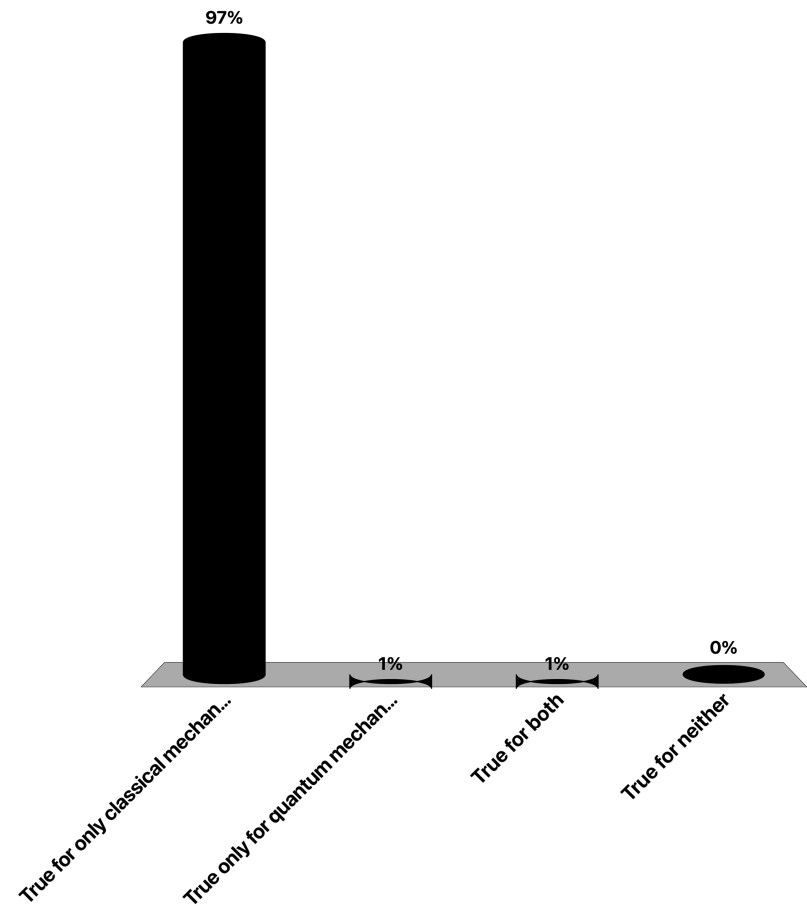
n , is a quantum number.

A **quantum number**:

- Is an integer (or sometimes a half-integer, such as $\frac{1}{2}$, see Topic 1D)
- Labels a wavefunction
- Specifies a state

Objects have well-defined positions and velocities.

- A. True for only classical mechanics
- B. True only for quantum mechanics
- C. True for both
- D. True for neither



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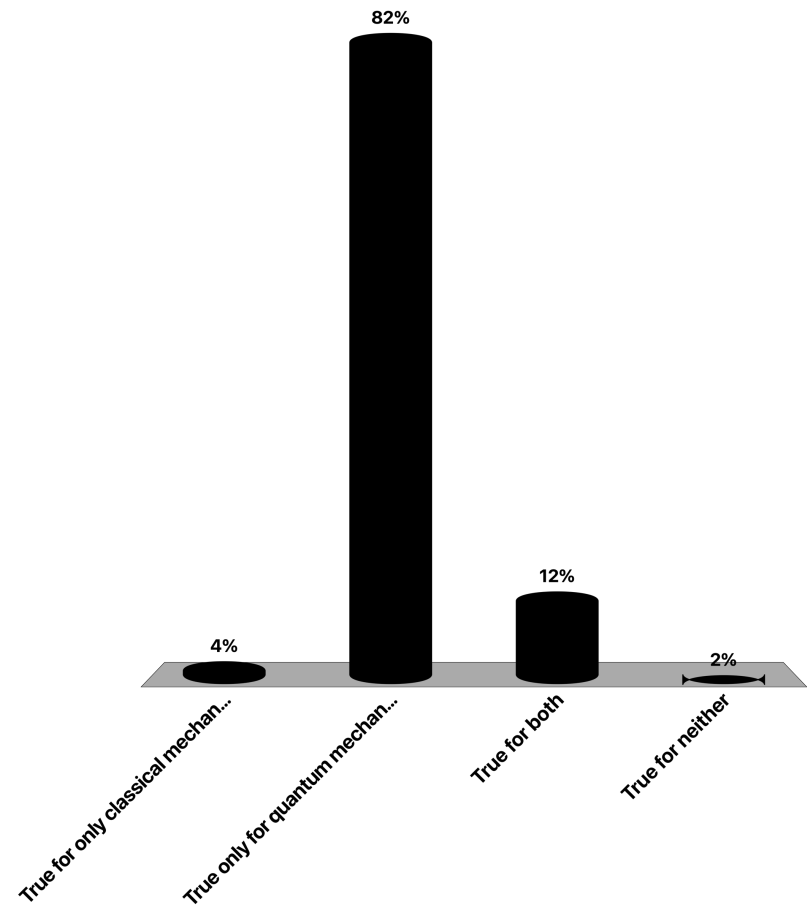
1C.2 The quantization of energy

Answer: True for only classical mechanics.

- In **classical mechanics**, objects are described as having **well-defined positions and velocities** at any given time. You can measure both quantities simultaneously with high precision.
- In **quantum mechanics**, particles do not have well-defined positions and velocities simultaneously due to the **Heisenberg Uncertainty Principle**. Instead, they are described by a wavefunction that gives probabilities for finding a particle in various positions and states, leading to inherent uncertainty.

Wave-like behaviors (such as interference patterns) can be observed for particles.

- A. True for only classical mechanics
- B. True only for quantum mechanics
- C. True for both
- D. True for neither



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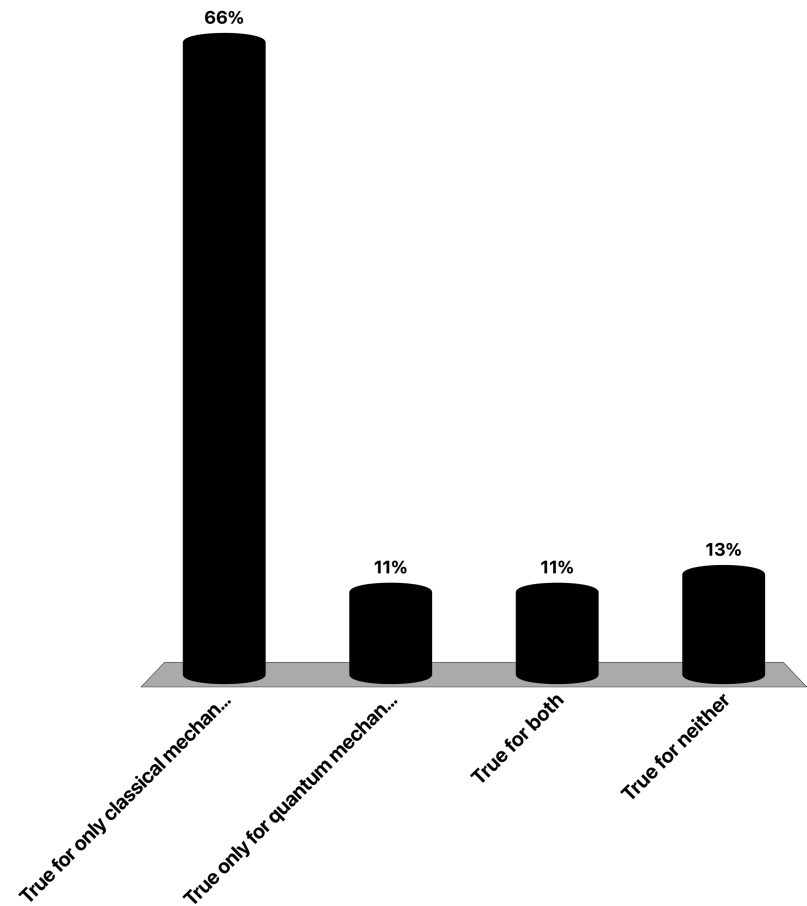
1C.2 The quantization of energy

Answer: True for both

- In **quantum mechanics**, particles such as electrons and photons exhibit **wave-like behaviors**, including **interference patterns**. This is famously demonstrated in the double-slit experiment, where individual particles can create an interference pattern when not observed, indicating their wave nature.
- In **classical mechanics**, wave-like behaviors can also be observed for macroscopic systems, such as water waves or sound waves, which also exhibit interference patterns.

Energy of systems is continuous and can have any value.

- A. True for only classical mechanics
- B. True only for quantum mechanics
- C. True for both
- D. True for neither



Session ID: 346047

1C.2 The quantization of energy

Answers: True for only classical mechanics.

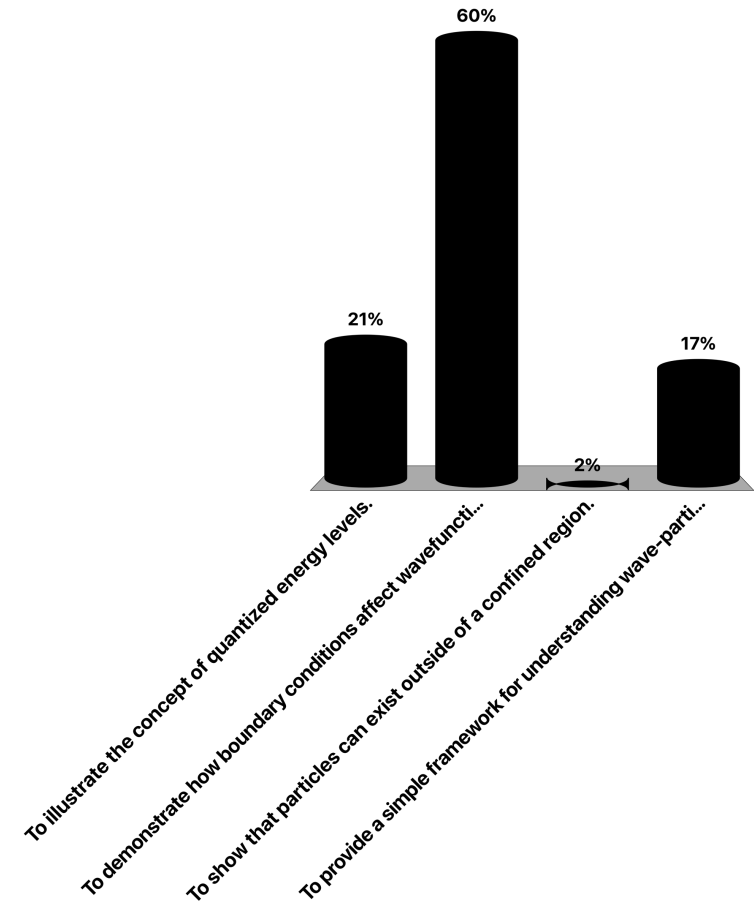
- In **classical mechanics**, energy is considered to be **continuous** and can take any value. For example, a classical particle can have any amount of kinetic or potential energy depending on its position and motion. In **quantum mechanics**, energy levels are **quantized**, meaning that particles (like electrons in an atom) can only occupy specific energy levels. They cannot have arbitrary values; instead, they can only exist at discrete energy states.

The Quantization of Energy

Topic 1C.2

What is the purpose of the particle in a box model in quantum mechanics? Multiple answers can apply.

- A. To illustrate the concept of quantized energy levels.
- B. To demonstrate how boundary conditions affect wavefunctions.
- C. To show that particles can exist outside of a confined region.
- D. To provide a simple framework for understanding wave-particle duality.



Session ID: 346047

1C.2 The quantization of energy

Energies of a particle in a box

The wavefunctions associated with different quantum numbers also have different energies associated with them. How do we calculate these energies?

If the particle stays in the box, the potential energy is zero:

$$E_k = E_{total}$$

Use de Broglie relation ($\lambda = \frac{h}{p}$):

$$E_k = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{(p)^2}{2m} = \frac{\left(\frac{h}{\lambda}\right)^2}{2m} = \frac{h^2}{2m\lambda^2}$$

1C.2 The quantization of energy

Energies of a particle in a box

$$E_k = \frac{1}{2}mv^2 = \frac{(mv)^2}{2m} = \frac{(p)^2}{2m} = \frac{\left(\frac{h}{\lambda}\right)^2}{2m} = \frac{h^2}{2m\lambda^2}$$

Recognize, only **whole-number multiples of half-wavelengths** can fit into the box:

The wavelengths possible for a particle in a box of length L must meet the condition that $\lambda = 2L, \frac{2}{3}L, \dots$

In other words, the allowed wavelengths are

$$\lambda = \frac{2L}{n}, \text{ with } n = 1, 2, \dots$$

Insert this expression for λ into the expression for energy:

$$E_n = \frac{h^2}{2m\lambda^2} = \frac{h^2}{2m\left(\frac{2L}{n}\right)^2} = \frac{n^2 h^2}{8mL^2}$$

1C.2 The quantization of energy

What does this equation tell you?

$$E_n = \frac{h^2}{2m\lambda^2} = \frac{h^2}{2m\left(\frac{2L}{n}\right)^2} = \frac{n^2 h^2}{8mL^2}$$

Mass in denominator: energy levels are lower and closer together for heavy particles than for light ones.

Length in denominator: as the walls become more confining (L smaller), the energy levels rise and become more widely spaced. In contrast, as the walls become less confining (L larger), the levels fall and get closer together.

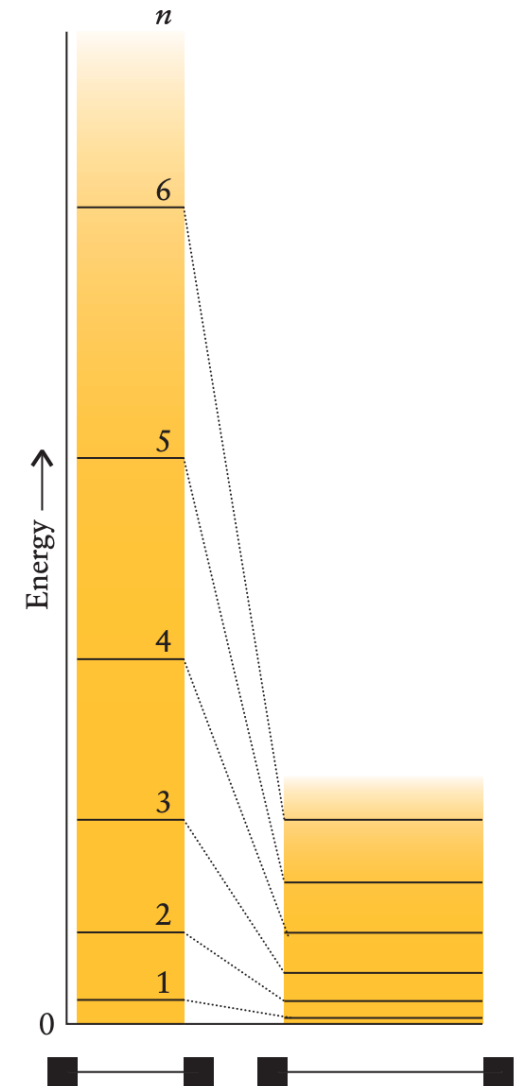


Figure 1C.4

1C.2 The quantization of energy

What does this equation tell you?

$$E_n = \frac{n^2 h^2}{8mL^2}$$

- n can only be integer values → **energy is quantized!**
- Energy quantization stems from the boundary conditions on the wavefunction.
- **Particle in a box translates to atoms:**
- Electrons must also satisfy certain boundary conditions, but now in three dimensions.
- We will revisit spectral lines in hydrogen absorption spectrum! (TOPIC 1D)

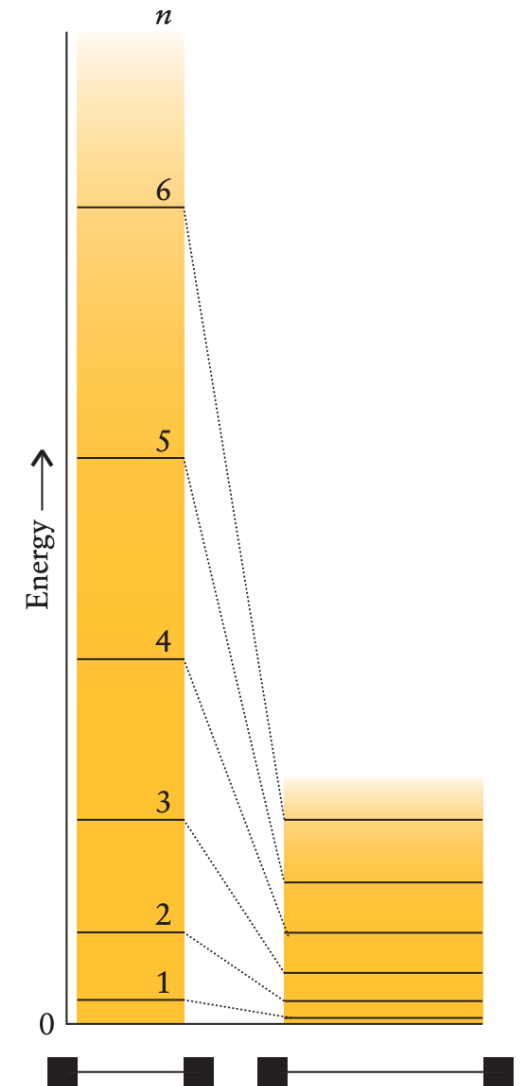


Figure 1C.4

1C.2 The quantization of energy

Energy separation between neighboring levels

$$\begin{aligned} E_{n+1} - E_n &= \frac{(n+1)^2 h^2}{8mL^2} - \frac{n^2 h^2}{8mL^2} \\ &= \{(n+1)^2 - n^2\} \frac{h^2}{8mL^2} = \frac{(2n+1)h^2}{8mL^2} \end{aligned}$$

As L or m increases, the separation between neighboring energy levels decreases.

Macroscopic objects in ordinary-sized containers have energy levels that are extremely close together:
undetectable quantization.

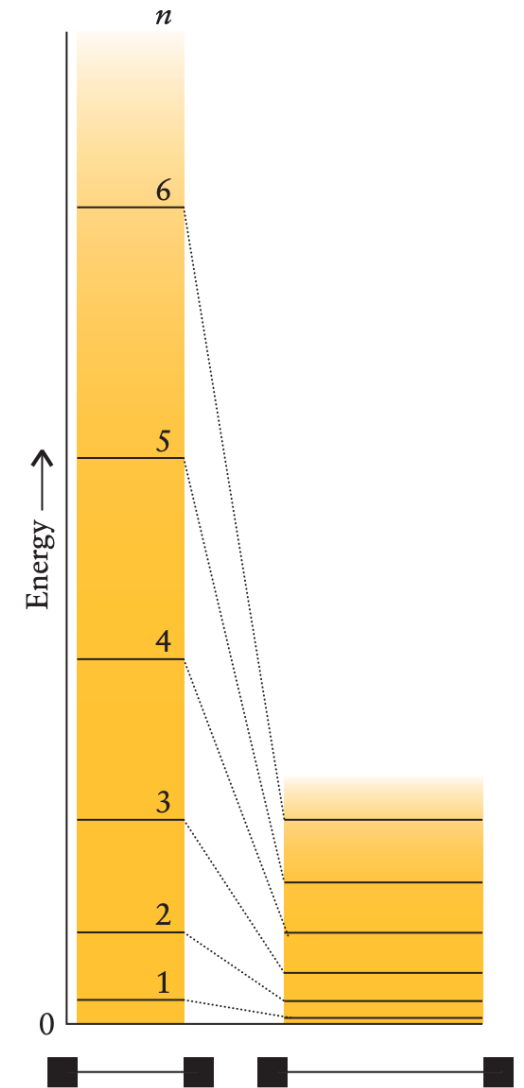


Figure 1C.4

1C.2 The quantization of energy

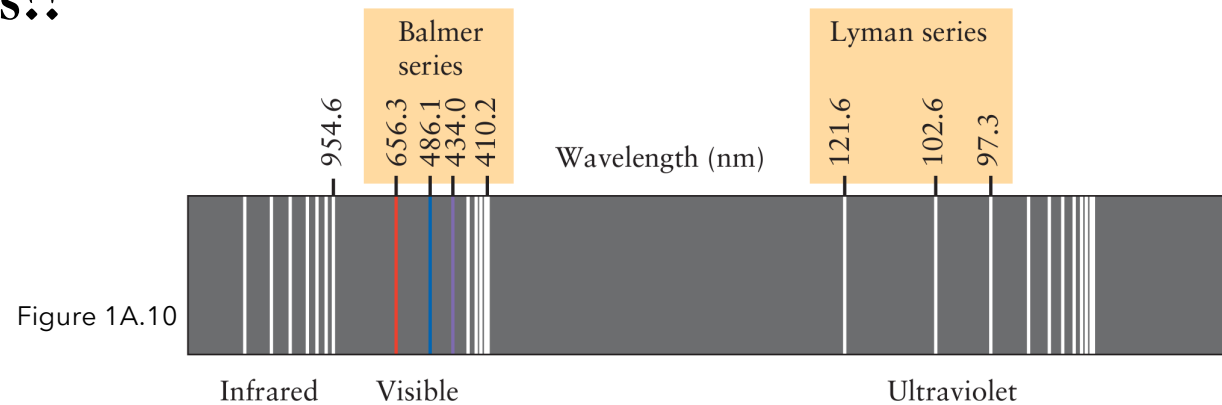
Quantization of energy and the atomic spectrum of hydrogen

Energy is quantized → this realization is key to understanding the **atomic spectrum of hydrogen** (Topic 1A).

Particle in a box	Hydrogen atom
1D	3D
Physical walls	No physical walls, and electrons are confined by pull of the nucleus
Energy quantized	

1C.2 The quantization of energy

What are these lines?!



A spectral line arises from a **transition of an electron between allowed energy levels**.

The difference in energy is carried away as a photon.

$$h\nu = E_{upper} - E_{lower} = \Delta E$$

This equation is known as the **Bohr frequency condition**.

1C.2 The quantization of energy

Example 1C.1: Calculating the energies of a particle in a box

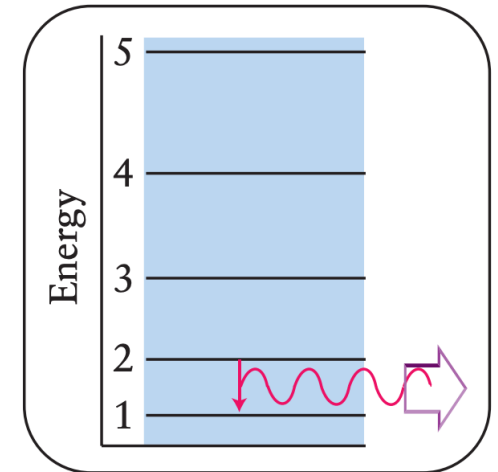
We will estimate the energies of the hydrogen atom.

Estimate: «back of the envelope» calculation

Treat hydrogen atom as a **one-dimensional box of length 150. pm** (the approximate diameter of the atom) with one electron.

Predict energy level separation **between the lowest and next higher** energy levels.

If the electron falls from the **upper level to the lower level**, what would be the wavelength of the radiation emitted as a photon?



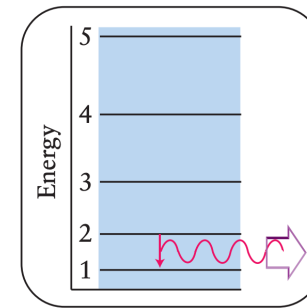
1C.2 The quantization of energy

Example 1C.1: Calculating the energies of a particle in a box

SOLVE The mass of the electron is found inside the back cover.

From Eq. 12 with $n = 1$, $2n + 1 = 3$,

$$E_2 - E_1 = \frac{3h^2}{8m_e L^2}$$



From $E_2 - E_1 = h\nu$,

$$h\nu = \frac{3h^2}{8m_e L^2}, \text{ so } \nu = \frac{3h}{8m_e L^2}$$

From $\lambda = c/\nu$,

$$\lambda = \frac{c}{(3h/8m_e L^2)} = \frac{8m_e c L^2}{3h}$$

1C.2 The quantization of energy

Example 1C.1: Calculating the energies of a particle in a box

Now substitute the data:

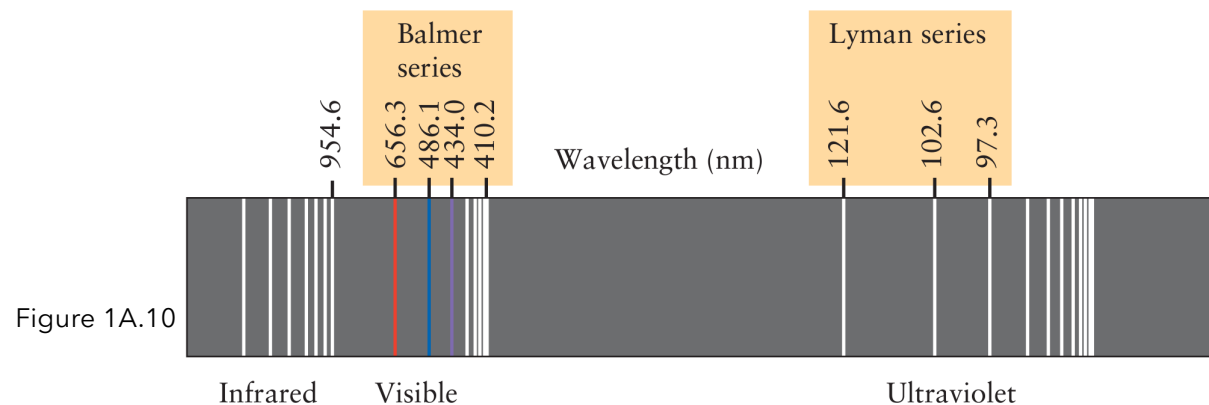
$$\begin{aligned}\lambda &= \frac{8 \times \overbrace{(9.109\,39 \times 10^{-31} \text{ kg})}^{m_e} \times \overbrace{(2.998 \times 10^8 \text{ m}\cdot\text{s}^{-1})}^c \times \overbrace{(1.50 \times 10^{-10} \text{ m})^2}^{L=150 \text{ pm}}}{3 \times \underbrace{(6.626 \times 10^{-34} \text{ J}\cdot\text{s})}_h} \\&= \frac{8 \times 9.109\,39 \times 10^{-31} \times 2.998 \times 10^8 \times (1.50 \times 10^{-10})^2 \text{ kg}\cdot\text{m}\cdot\text{s}^{-1}\cdot\text{m}^2}{3 \times 6.626 \times 10^{-34} \underbrace{\text{kg}\cdot\text{m}^2\cdot\text{s}^{-2}\cdot\text{s}}_{\text{J}}} \\&= 2.47 \times 10^{-8} \text{ m}\end{aligned}$$

A note on good practice: Note once again how the complicated collection of units is treated: arriving at the correct units for the answer is a sign that you have set up the equation correctly. As usual, it is good practice to go as far as possible symbolically and then to insert numerical values at the last possible stage.

1C.2 The quantization of energy

Example 1C.1: Calculating the energies of a particle in a box

Evaluate This wavelength corresponds to 24.7 nm. The experimental value for the actual transition in a hydrogen atom is 122 nm. Although there is a big discrepancy, an atom does not have the hard boundaries that confine a particle in a box, and is three-dimensional. The fact that the predicted wavelength has nearly the same order of magnitude as the actual value suggests that a quantum theory of the atom, based on a more realistic three-dimensional model, should give good agreement.



1C.2 The quantization of energy

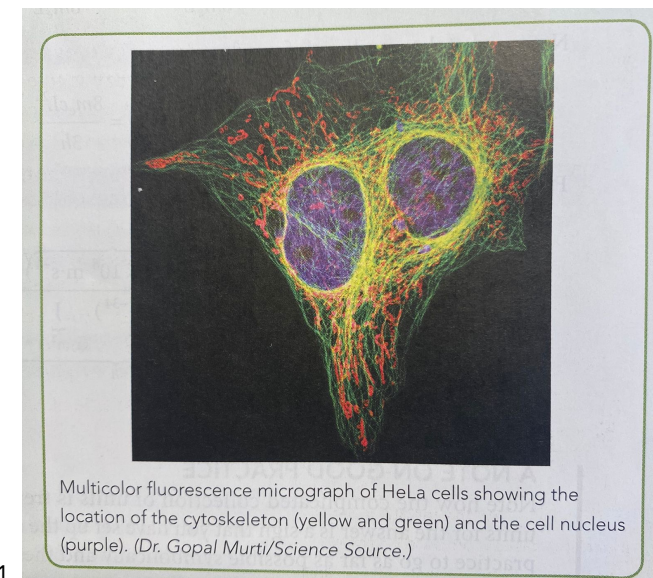
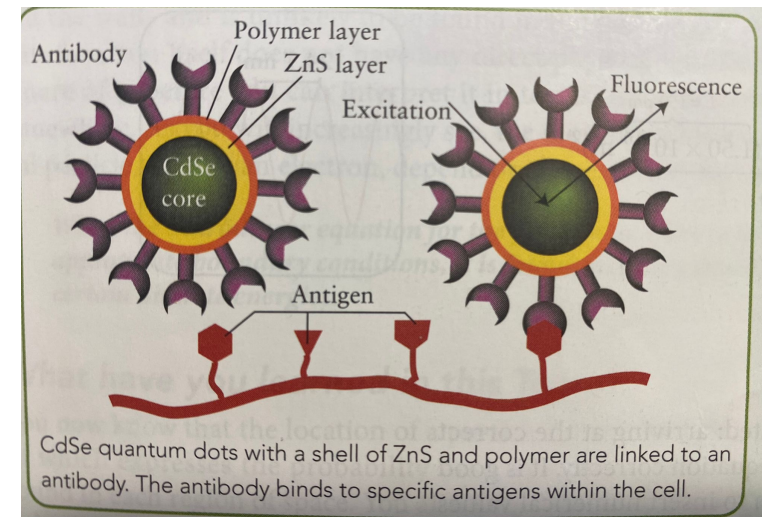
Nanocrystals

Electrons in nanoscale particles (1-100 nm diameter) made of semiconductor materials are **quantum confined** and behave like a particle in a box: Quantum dots or nanocrystals.

CdSe (cadmium selenide) nanoparticles coated with shell of ZnS plus polymer, modified with antibodies.

Antigen-specific binding on cells.

Size of quantum dot will change emitted light wavelength: imaging at multiple wavelengths possible.



1C.2 The quantization of energy

Particle in a box: zero-point energy

- Surprising implication of equation: $E_n = \frac{n^2 h^2}{8mL^2}$
- A particle in a container **cannot have zero energy**.
- The lowest value of n is 1.
- Lowest energy is $E_1 = \frac{h^2}{8mL^2}$ (**Zero-point energy**)
- What this means: A particle can never be perfectly still when it is confined between two walls, it must always possess an energy, in this case, at least the kinetic energy $\frac{h^2}{8mL^2}$.

1C.2 The quantization of energy

Zero-point energy is consistent with uncertainty principle

The **Heisenberg uncertainty principle** states that there is a fundamental limit to how precisely we can simultaneously know a particle's **position** and **momentum**:

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

- The particle is confined within a box, so its **position uncertainty** Δx is on the order of the size of the box, L .

$$\Delta x \approx L$$

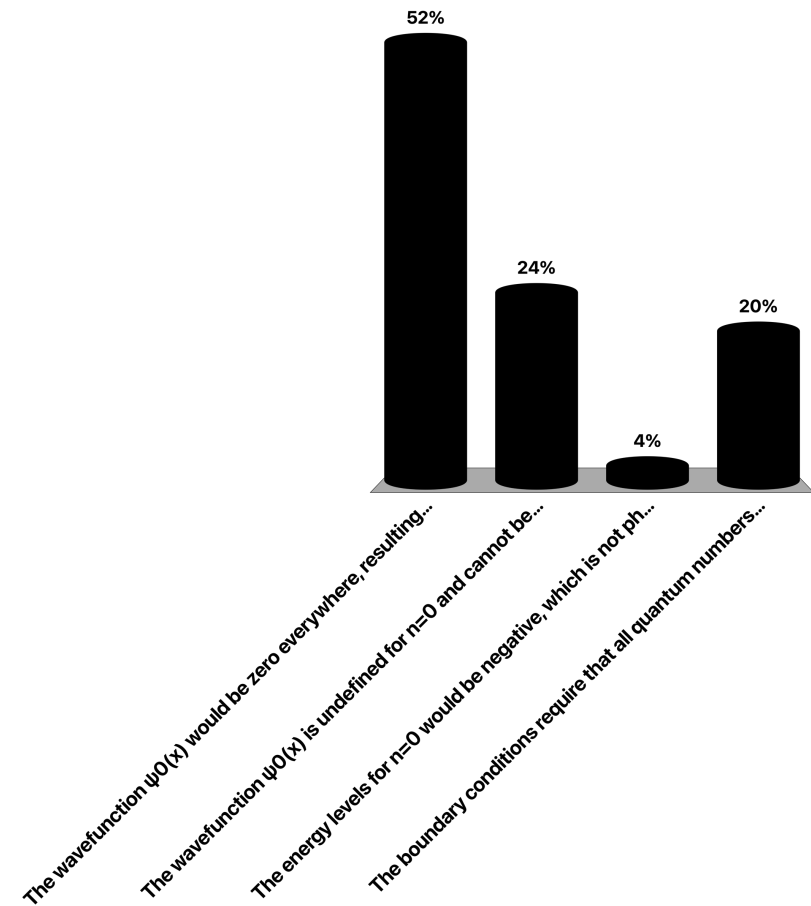
- Due to the **Uncertainty Principle**, if the particle's position is confined, the **momentum** p (and hence its velocity) cannot be zero. There must be some uncertainty in momentum Δp , meaning the particle has a **nonzero minimum momentum**.

$$\Delta p \geq \hbar/2L$$

- This nonzero momentum means the particle always has some **kinetic energy**, even in the ground state, and cannot be perfectly still. This nonzero energy is the **zero-point energy**.

Why is $n = 0$ not a valid solution for the particle in a box? Hint: think of the Born interpretation of the wavefunction.

- A. The wavefunction $\psi_0(x)$ would be zero everywhere, resulting in no probability of finding the particle in the box.
- B. The wavefunction $\psi_0(x)$ is undefined for $n=0$ and cannot be calculated.
- C. The energy levels for $n=0$ would be negative, which is not physically possible.
- D. The boundary conditions require that all quantum numbers must be non-negative.



1C.2 The quantization of energy

Answer: Why is $n = 0$ not a valid solution for the particle in a box?

- If $n = 0$, the wavefunction $\psi_0(x)$ would be:

$$\psi_0(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{0\pi x}{L}\right) = \sqrt{\frac{2}{L}} \sin(0) = 0$$

- the wavefunction $\psi_0(x)$ would be **zero everywhere** inside the box, meaning that there is **no probability** of finding the particle anywhere inside the box. This contradicts the Born interpretation of the wave function.
- According to the **Born interpretation**, the square of the wavefunction's absolute value, $|\psi_0(x)|^2$ represents the **probability density** of finding the particle at a given position x within the box.
- If $n = 0$, then $\psi_0(x) = 0$ everywhere, which implies that $|\psi_0(x)|^2 = 0$ everywhere.
- This would mean the **probability density** is zero at all positions, indicating there is **zero probability** of finding the particle **anywhere** inside the box. Physically, this is nonsensical because the particle **must** be somewhere in the box.

1C.2 The quantization of energy

The shapes of the wavefunctions

- The shapes reveal interesting information.
- The two lowest-energy wavefunctions are displayed on the right, $n = 1$ and $n = 2$.
- **Density of shading:** likelihood of finding a particle (formally: probability density)
- For ψ_1 with energy $h^2/8mL^2$: the particle is most likely found at the **center** of the box.
- For ψ_2 with energy $h^2/2mL^2$: the particle is least likely found at the center of the box, most likely to be found in regions between the center and the walls.
- **The most likely locations of a quantum mechanical particle, such as an electron, depend on the quantum state it is in.**

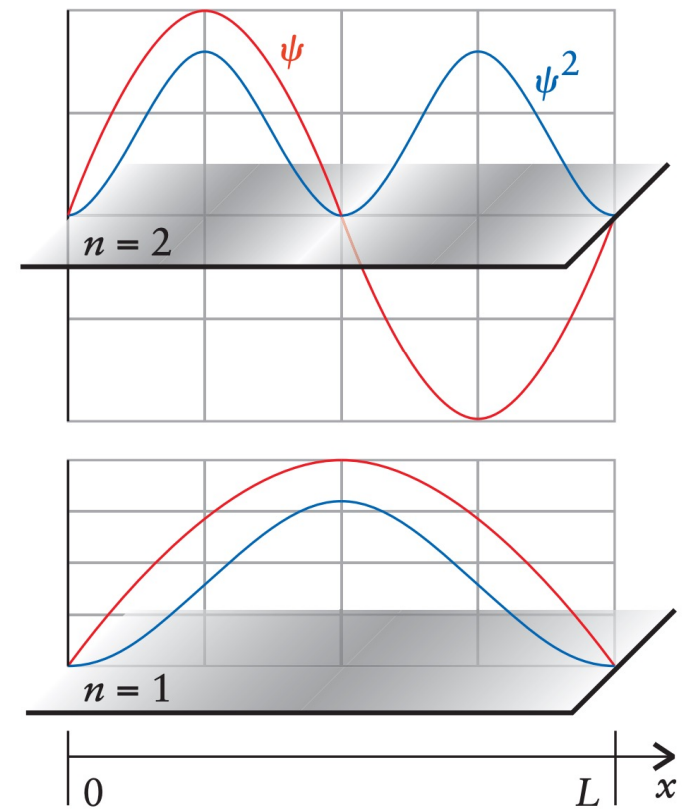


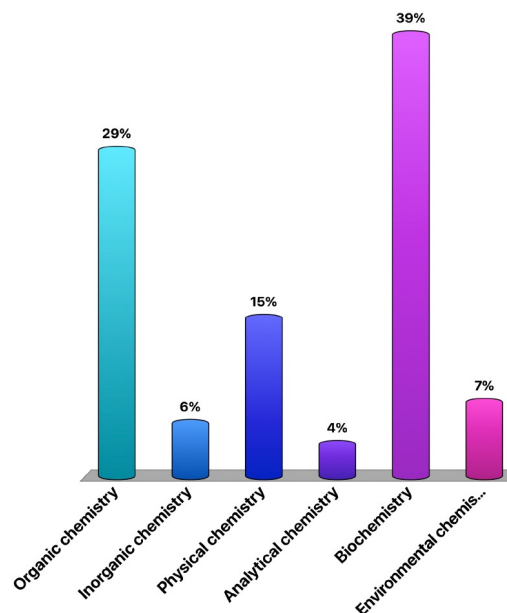
Figure 1C.5

1C.2 The quantization of energy

Why is this statement relevant for you even if you don't plan on studying quantum chemistry again?

The most likely locations of a quantum mechanical particle, such as an electron, depend on the quantum state it is in.

- A. Organic chemistry
- B. Inorganic chemistry
- C. Physical chemistry
- D. Analytical chemistry
- E. Biochemistry
- F. Environmental chemistry



1C.2 The quantization of energy

Why is this relevant for you even if you don't plan on studying quantum chemistry again?

- **Organic Chemistry:** Quantum mechanical electron locations dictate **bonding, molecular structure**, and **reactivity** in chemical reactions.
- **Biochemistry:** Electron distributions in quantum states help explain **enzyme catalysis, electron transport** in metabolic pathways, and **drug interactions**.
- **Physical Chemistry:** Quantum state electron positions are crucial for **spectroscopy, reaction kinetics**, and **thermodynamic properties** through quantum models and calculations.
- etc.

Student quotes

"BECAUSE I WANT TO WORK IN PERFUMES."

"BECAUSE I WANT TO MAKE PERFUMES."

Your interest in creating perfumes connects to the quantum mechanics concept that the **most likely locations of electrons** in fragrance molecules depend on their quantum states. This understanding is crucial for predicting and manipulating the chemical properties that define different scents, thus bridging their passion for perfumery with the principles of quantum chemistry.

The skills you have mastered are the ability to

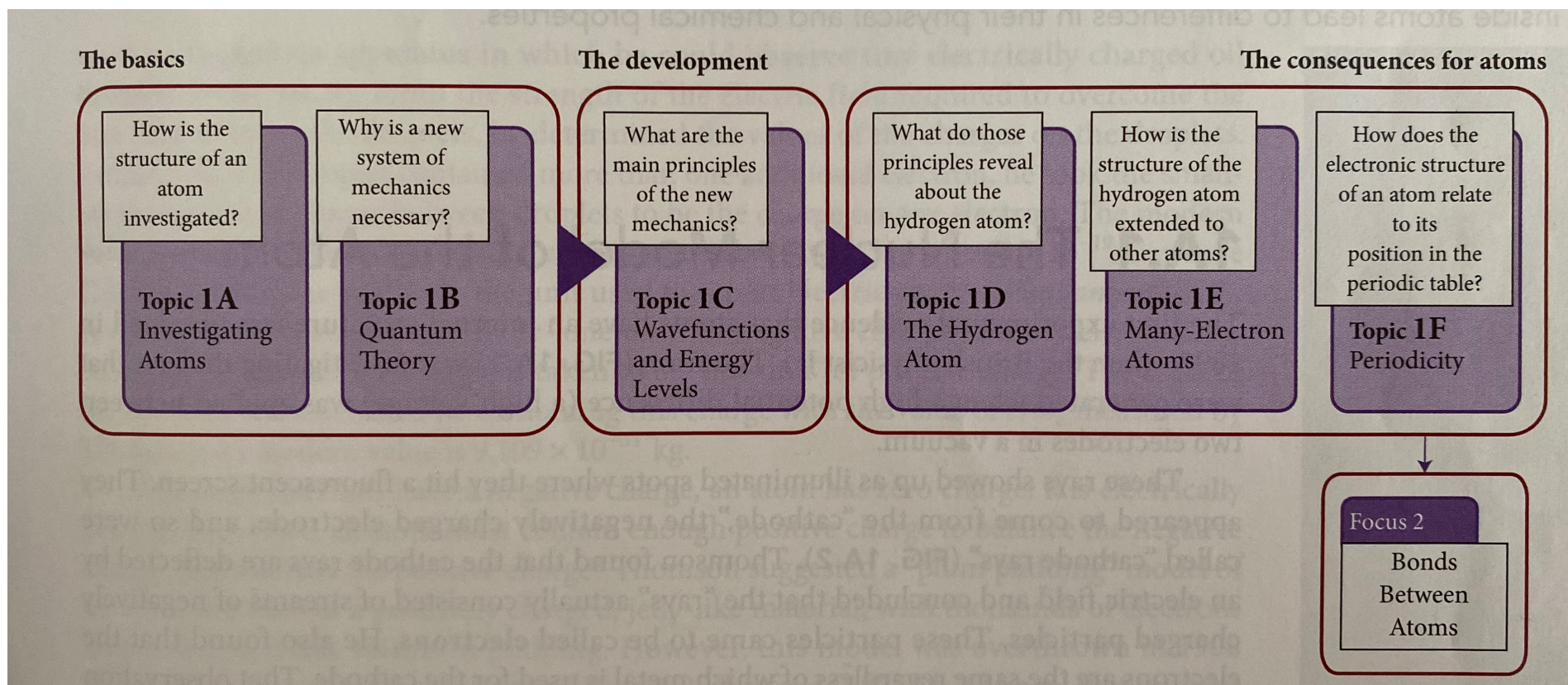
- ❑ Describe the origin and shapes of the wavefunctions of a particle in a box.
- ❑ Calculate the allowed energies of a particle in a box and explain how they depend on the length of the box and the mass of the particle.
- ❑ Explain what is meant by zero-point energy and accounts for its origin

Summary: You now know that the location of a particle is expressed by a wavefunction, the square of which expresses the probability (as a probability density) that the particle will be found in each region of space. You also know that a wavefunction is found by solving the Schrödinger equation and that one consequence of the wavefunction having to fit into a region of space is that a particle confined to a region can have only certain discrete energies known as energy levels.

The Hydrogen Atom

Topic 1D

Overview Chapter 1 (Focus 1: Atoms)



Topic 1D.1 Energy levels

Topic 1D.2 Atomic orbitals

Topic 1D.3 Quantum numbers, shells, and subshells

Topic 1D.4 The shapes of orbitals

Topic 1D.5 Electron spin

Topic 1D.6 The electronic structure of hydrogen: a summary

WHY DO YOU NEED TO KNOW THIS MATERIAL?

- The hydrogen atom is the **simplest atom of all** and is used to discuss the **structures of all atoms**.
- It is therefore **central** to many explanations in chemistry.

WHAT DO YOU NEED TO KNOW ALREADY?

- Features of spectrum of atomic hydrogen (Topic 1A)
- Concepts of wavefunction and energy level in quantum mechanics (Topic 1C)

1D The hydrogen atom

Setting the stage

In Topic 1A, we have seen this puzzle

$$\nu = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad n_1 = 1, 2, \dots, n_2 = n_1 + 1, n_1 + 2, \dots$$

Value of Rydberg constant, $R = 3.29 \times 10^{15} \text{Hz}$

- Why such a **pattern** and why does R have that **value**?
- Example 1C.1 gave clues: lines in spectrum are due to transitions between allowed energy levels of the atom, the difference in energy is carried away by a photon of energy $h\nu$
- **Aim of this topic:** construct a quantum mechanical model of the hydrogen atom using the fact that an electron has wave-like properties and is described by a wavefunction, and has quantized energy levels.

Energy Levels

Topic 1D.1

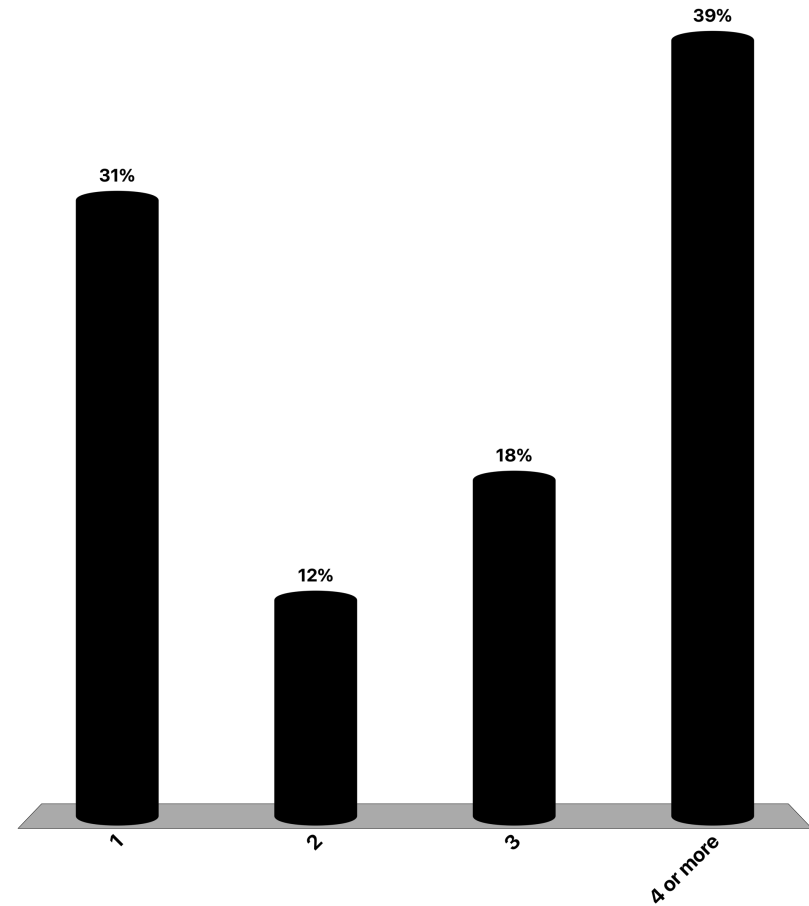
1D.1 Energy levels

Setting the stage

- **Again:** an **electron** in an atom is like a **particle** in a box in the sense that it is confined within the atom, not by the **walls**, but by the **electrostatic pull of the nucleus**.
- It follows **boundary conditions** are also applicable for atom.
- Solving Schrödinger equation for the hydrogen atom will result in existence of **discrete energy levels**.

The state of a particle in a 1D box is defined by one quantum number.
How many quantum numbers do you think will be needed to specify the
wavefunction of an electron in a hydrogen atom?

- A. 1
- B. 2
- C. 3
- D. 4 or more



1D.1 Energy levels

Allowed energy levels for electron in hydrogen atom

To find allowed energy levels of an electron in a hydrogen atom, you need to solve appropriate Schrödinger equation. Consider:

1. Motion in three dimensions.
2. Instead of simple walls, the electron experiences a **Coulomb potential** due to the nucleus. The Coulomb potential energy of an electron of charge $-e$ at a distance r from the nucleus of charge $+e$:

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

ϵ_0 : electric constant

1D.1 Energy levels

Allowed energy levels for electron in hydrogen atom

Schrödinger managed to solve his equation with this potential energy:

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

ϵ_0 : electric constant

He found that the allowed energy levels of an electron in a hydrogen atom are:

$$E_n = -\frac{hR}{n^2}$$

$$R = \frac{m_e e^4}{8h^3 \epsilon_0^2} \text{ with } n = 1, 2, \dots$$

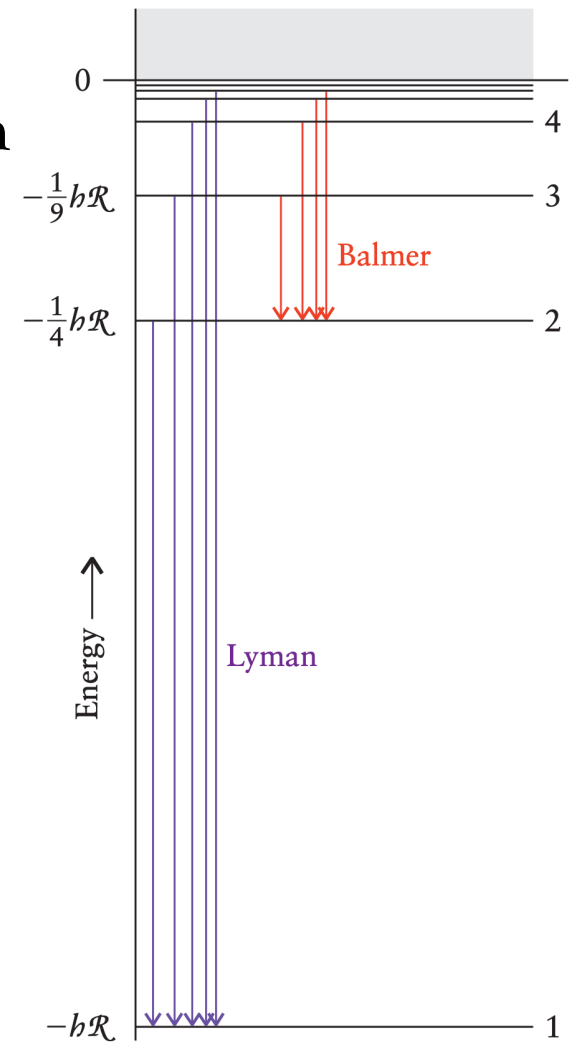


Figure 1D.1

1D.1 Energy levels

What does this equation tell you?

$$E_n = -\frac{hR}{n^2}$$

$$R = \frac{m_e e^4}{8h^3 \epsilon_0^2} \text{ with } n = 1, 2, \dots$$

- All energies are **negative**: electron has a lower energy far from the nucleus, it takes energy to remove an electron from an atom.
- There is a **quantum number**, n , like for the particle in a box. Energy is quantized, can only have discrete values.
- n appears in the **denominator**: as n increases, the energies of successive levels increase (become less negative).
- As the energies approach zero, the electron is on the point of **escaping** from the atom.

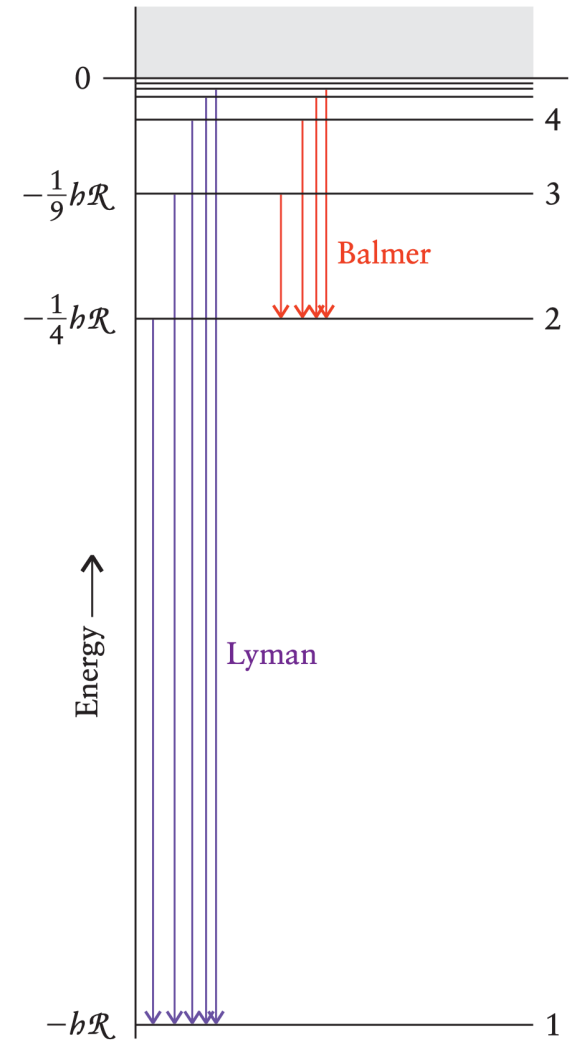


Figure 1D.1

1D.1 Energy levels

Relationship to Bohr frequency condition

Bohr frequency condition:

$$h\nu = \Delta E$$

Insert into previous equation. In the case of the hydrogen atom, if the electron falls from a level with quantum number n_2 to one with quantum number n_1 , then:

$$h\nu = \Delta E = \left(-\frac{hR}{n_2^2}\right) - \left(-\frac{hR}{n_1^2}\right) = hR \left\{\frac{1}{n_1^2} - \frac{1}{n_2^2}\right\} \text{ with } n_1 = 1, 2, \dots, n_2 = n_1 + 1, n_1 + 2, \dots$$

Compare to previous Rydberg equation:

$$\nu = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \text{ with } n_1 = 1, 2, \dots, n_2 = n_1 + 1, n_1 + 2, \dots$$

1D.1 Energy levels

Finally, it makes sense

You can now see:

- Balmer series, for example, arises from transitions starting at $n_2 = 3, 4, 5 \dots$ and all ending at $n_1 = 2$
- Lyman series: $n_2 = 2, 3, 4, 5 \dots$ to $n_1 = 1$

Rydberg constant

$$R = \frac{m_e e^4}{8h^3 \epsilon_0^2} = 3.29 \times 10^{15} \text{ Hz}$$

- Imagine Schrödinger calculating this constant!

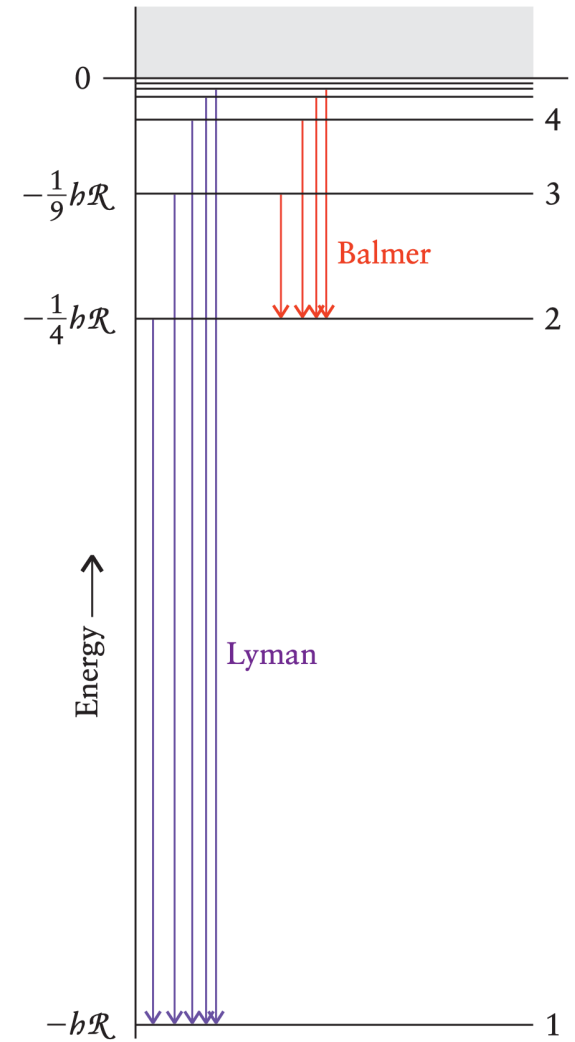


Figure 1D.1

1D.1 Energy levels

Finally, it makes sense

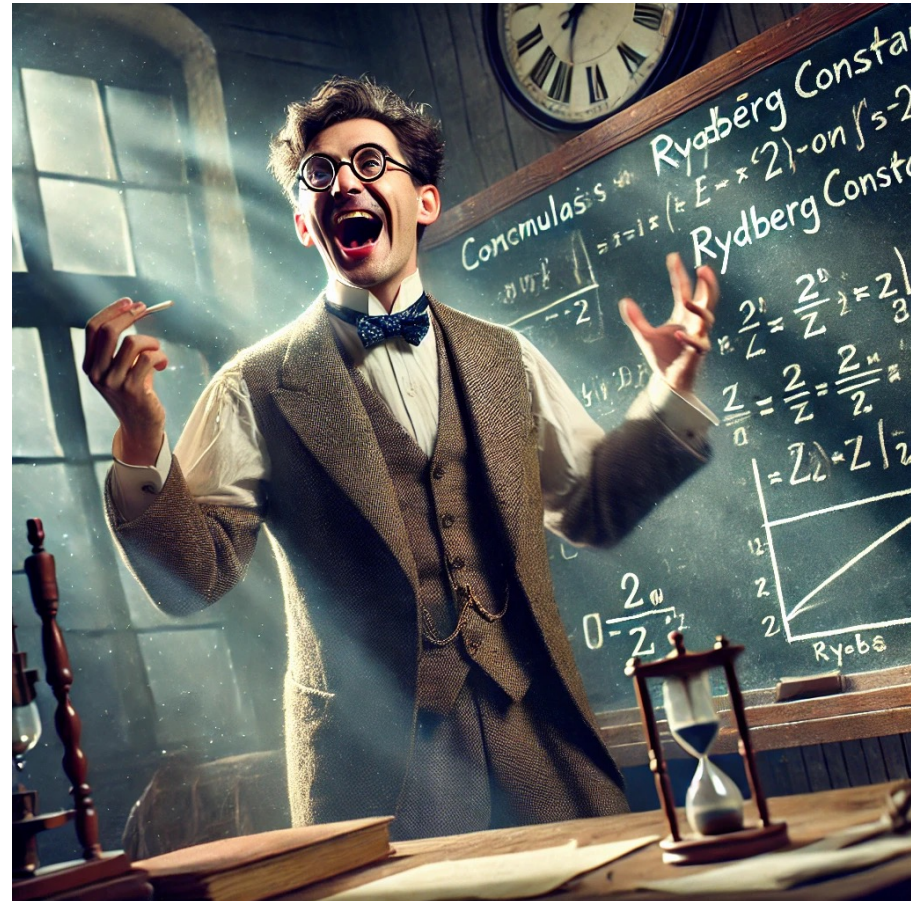
generate an image of erwin schrödinger when he found was able to calculate the rydberg constant using fundamental constants.



1D.1 Energy levels

Finally, it makes sense

give me more excitement



Student quotes

"IT'S FUN AND SATISFYING AND VERY INTERESTING."

"NEW DISCOVERIES, RESEARCH, CURIOSITY."

Your enthusiasm for discovery and satisfaction in learning resonates with the spirit of **innovation and exploration** embodied by Schrödinger's work. His ability to connect theoretical principles with fundamental constants like the Rydberg constant reflects the excitement of scientific inquiry, aligning perfectly with their passion for research and the joys of unraveling the mysteries of the universe.

1D.1 Energy levels

Generalization to other one-electron ions possible

Schrödinger was able to generalize this equation

$$E_n = -\frac{hR}{n^2}$$

$$R = \frac{m_e e^4}{8h^3 \epsilon_0^2} \text{ with } n = 1, 2, \dots$$

to other one-electron ions such as He^+ and even C^{5+} . For a nucleus with atomic number Z and charge Ze , the energy levels are:

$$E_n = -\frac{Z^2 hR}{n^2} \quad n = 1, 2, \dots$$

Note: because Z appears in the **numerator**, the greater the value of the nuclear charge, the lower the energy (more negative) of the electron and the more tightly it is bound to the nucleus.

This equation can be used for **one-electron ions**, for many-electron atoms, see Topic 1E.

1D.1 Energy levels

Key terms to remember

- The integer $n = 1, 2, \dots$ is called the **principal quantum number**.
- Coming soon: more quantum numbers.
- The lowest (most negative) energy possible for an electron in a hydrogen atom is obtained when $n = 1$ and E_n is equal to $-hR$: **ground state of the atom**.
- When the atom absorbs a **photon** or collides with other particles, it may be **excited from the ground state** to a level with a higher value of n .
- If collision are very energetic, n might reach infinity, a process called **ionization**. An electron is removed from the hydrogen atom.
- The minimum ionization energy starting from an electron in the ground state for a hydrogen atom is equal to hR . (numerical value: $2.18 \times 10^{-17}J$ or 13.6 eV).
- Any further energy beyond the ionization energy adds kinetic energy to the liberated electron.

1D.1 Energy levels

Summary

The energy levels of a hydrogen atom are defined by the principal quantum number, $n = 1, 2, \dots$, and form a converging ladder, as shown in Figure 1D.1. Spectroscopic lines arise from transitions between the levels.

Atomic Orbitals

Topic 1D.2

1D.2 Atomic orbitals

Wavefunction and atomic orbitals

The wavefunction of an electron in an atom is called an atomic orbital.

Less finite than «orbit» of an electron around the nucleus, to account for wave-like nature.

Again: the square of a wavefunction tells you the probability density of finding an electron at each point in space.

In context of hydrogen atom: imagine a cloud centered on the nucleus.

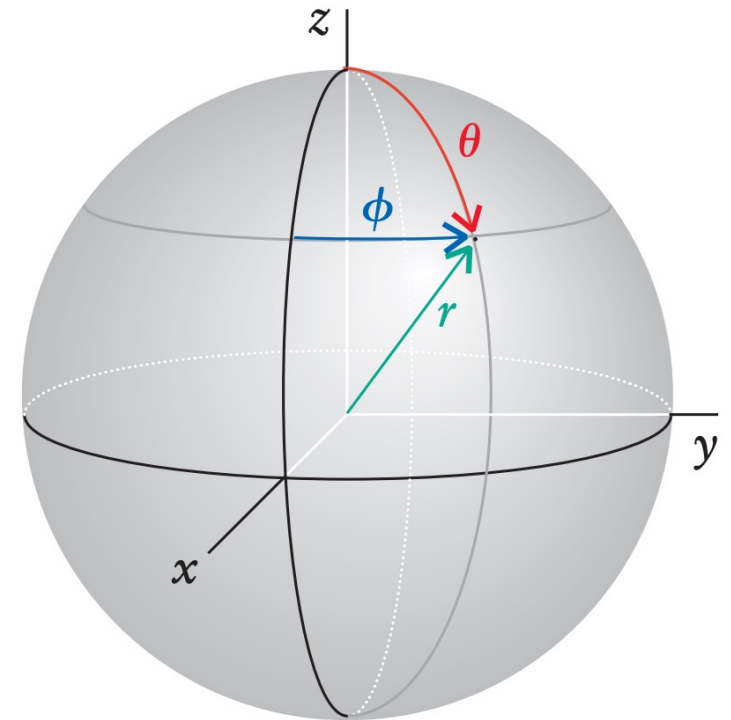
Dense regions: locations where the electron is most likely to be found.

1D.2 Atomic orbitals

Spherical polar coordinates

The atom is like a sphere (3D), spherical polar coordinates apply:

- r is the **radius**, the distance from the nucleus
- θ (theta) is the **colatitude**, the angle from the positive z -axis (the «north pole»), which can be thought of as playing the role of the geographical «latitude» (north or south)
- ϕ (phi) is the **azimuth**, the angle about the z -axis, the geographical «longitude» (east or west)

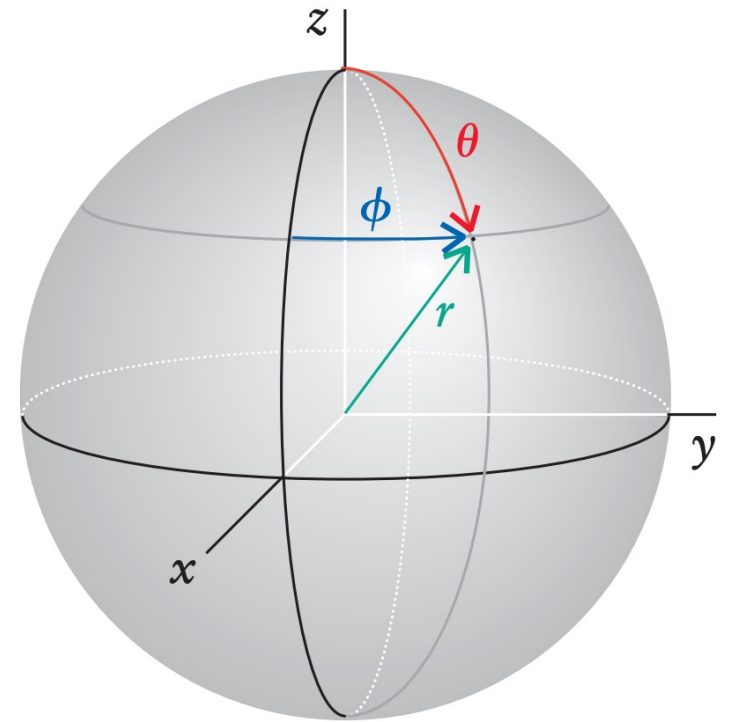


1D.2 Atomic orbitals

Spherical polar coordinates

The below applet allows you to see how the location of a point changes as you vary r , θ , and ϕ

https://mathinsight.org/spherical_coordinates



1D.2 Atomic orbitals

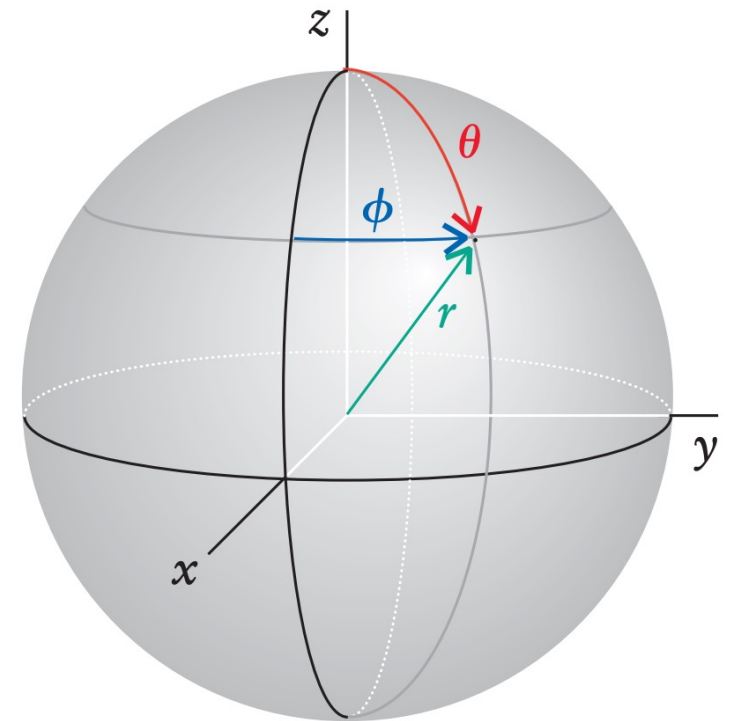
Wavefunction and atomic orbitals

Each **wavefunction** has a value that **depends on these three coordinates** and is therefore denoted as $\Psi(r, \theta, \phi)$. You can also express it as the product of a function that depends only on r and another function that depends on the angles θ and ϕ :

$$\Psi(r, \theta, \phi) = R(r) \times Y(\theta, \phi)$$

$R(r)$: **radial wavefunction**, expresses how the wavefunction varies with distance from the nucleus.

$Y(\theta, \phi)$: **angular wavefunction**, expresses how the wavefunction varies as the angles θ and ϕ change.



1D.2 Atomic orbitals

Expressions for atomic orbitals

- Expressions for some atomic orbitals are shown in table on next slide
- Looks complicated at first glance, do not worry about knowing these by heart.
- Some are not complicated, e.g. the wavefunction corresponding to the ground state of the hydrogen atom ($n = 1$) is:

$$\Psi(r, \theta, \phi) = \left(\frac{1}{\pi a_0^3} \right)^{\frac{1}{2}} e^{-\frac{r}{a_0}}$$

a_0 : Bohr radius (52.9 pm)

- Wavefunction is **spherically symmetric**: independent of θ and ϕ and for a given radius, its value is the same in all directions.
- Wavefunction **decays exponentially** toward zero as r increases. Probability density is highest close to the nucleus (at $r = 0$, $e^0 = 1$)
- In contrast to particle in a box: no physical, confining walls for electron in atom, but **the pull of nucleus** weakens with distance.

1D.2 Atomic orbitals

TABLE 1.2 Hydrogenlike Wavefunctions* (Atomic Orbitals), $\psi = RY$

(a) Radial wavefunctions			(b) Angular wavefunctions		
n	l	$R_{nl}(r)$	l	" m_l " [†]	$Y_{l,m_l}(\theta, \phi)$
1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$	0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
2	0	$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$	1	x	$\left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \cos \phi$
	1	$\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$		y	$\left(\frac{3}{4\pi}\right)^{1/2} \sin \theta \sin \phi$
3	0	$\frac{2}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2} \left(3 - \frac{2Zr}{a_0} + \frac{2Z^2r^2}{9a_0^2}\right) e^{-Zr/3a_0}$		z	$\left(\frac{3}{4\pi}\right)^{1/2} \cos \theta$
	1	$\frac{2}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{3a_0}\right) e^{-Zr/3a_0}$	2	xy	$\left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \sin 2\phi$
	2	$\frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$		yz	$\left(\frac{15}{4\pi}\right)^{1/2} \cos \theta \sin \theta \sin \phi$
				zx	$\left(\frac{15}{4\pi}\right)^{1/2} \cos \theta \sin \theta \cos \phi$
				$x^2 - y^2$	$\left(\frac{15}{16\pi}\right)^{1/2} \sin^2 \theta \cos 2\phi$
				z^2	$\left(\frac{5}{16\pi}\right)^{1/2} (3 \cos^2 \theta - 1)$

*Note: In each case, $a_0 = 4\pi\epsilon_0^2/m_e e^2$, or close to 52.9 pm; for hydrogen itself, $Z = 1$.

[†]In all cases except $m_l = 0$, the orbitals are sums and differences of orbitals with specific values of m_l .

1D.2 Atomic orbitals

Example from Table 1.2

- For example, a $2p_x$ -orbital ($n = 2, l = 1, \text{«}m_l\text{»} = x$) of hydrogen ($Z = 1$) is

$$\Psi(r, \theta, \phi) = R_{2,1}(r) \times Y_{1,x}(\theta, \phi) = \frac{1}{2\sqrt{6}} \left(\frac{1}{a_0}\right)^{\frac{3}{2}} \frac{r}{a_0} e^{-\frac{r}{2a_0}} \times \left(\frac{3}{4\pi}\right)^{\frac{1}{2}} \sin(\theta) \cos(\phi)$$

1D.2 Atomic orbitals

Summary

The distribution of an electron in an atom is described by a wavefunction known as an atomic orbital.

Student questions 1/2

For the zero-point energy in the particle in a box, what happens to the energy at $n=1$ when the sample is cooled to 0 Kelvin?

At absolute zero (0 K), a quantum system like a particle in a box cannot have zero energy due to the uncertainty principle, which dictates that particles cannot be at rest. Therefore, even when cooled to 0 K, the particle retains its zero-point energy, which corresponds to the energy level at $n=1$. This means that the particle will still possess a minimum kinetic energy, reflecting its quantum nature, and cannot fall to a lower state (like $n=0$) since that state is not physically valid in this model.

What does the notation $|\psi|^2$ (with vertical bars) signify in the context of probability density?

The wavefunction ψ can be a complex number, represented as $\psi = Re(\psi) + iIm(\psi)$, where $Re(\psi)$ is the real part and $Im(\psi)$ is the

imaginary part. The magnitude of the wavefunction, $|\psi| = \sqrt{(Re(\psi))^2 + (Im(\psi))^2}$, indicates the "size" of the wavefunction in the complex plane. To find the probability density of locating the particle, we use $|\psi|^2$, which provides the likelihood of finding the particle in a specific region of space. Reminder: complex numbers are outside the scope of this class. For our purposes $|\psi|^2$ could also be written as ψ^2 or $\psi(x)^2$ because in our examples, we do not deal with complex numbers.

Are there any energy levels at point zero for the hydrogen atom, given that all energies are negative and approach zero?

There are no energy levels at point zero; while the energy levels approach zero as the electron moves further from the nucleus, zero energy indicates a free electron would no longer be bound to the atom.

Student questions 2/2

What's the difference between the wavelength in the sine function of the wavefunction and the wavelength of emitted light from an electron transitioning to a lower energy level?

In quantum mechanics, the **wavelength in the wavefunction**, represented by the sine function $\psi_0(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{0\pi x}{L}\right)$, corresponds to the spatial distribution of the particle's probability density. This wavelength, λ_n , can be determined from the condition that only certain wavelengths fit into the "box" of length L. Specifically, for a particle in a box, the relationship is given by:

$$\lambda_n = \frac{2L}{n}$$

where n is the quantum number (an integer representing different energy levels).

On the other hand, the **wavelength of the emitted light** when an electron transitions from a higher energy state E_2 to a lower energy state E_1 is given by the energy difference between these states, according to Planck's equation:

$$E = h\nu = \frac{hc}{\lambda}$$

where E is the energy of the emitted photon, h is Planck's constant, ν is the frequency of the emitted light, c is the speed of light, and λ is the wavelength of the emitted photon.

Thus, the wavelength of the emitted light can be calculated using the energy difference:

$$\Delta E = E_2 - E_1 = \frac{hc}{\lambda}$$

In summary, the wavelength in the wavefunction relates to the spatial characteristics of the quantum state of the electron in the box, while the wavelength of the emitted light is directly related to the energy transitions of the electron as it moves between discrete energy levels, reflecting the quantized nature of its energy states.