CH-110 Advanced General Chemistry I

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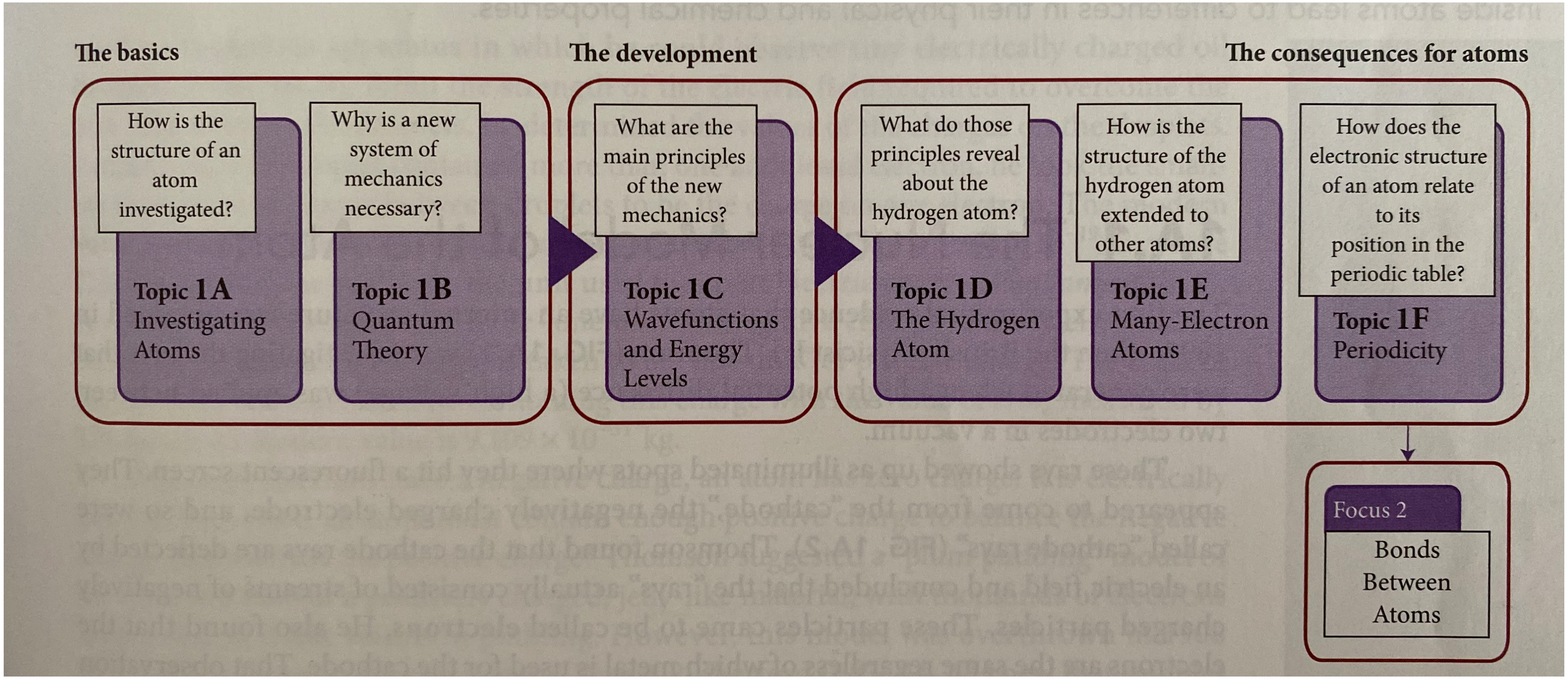
Housekeeping notes

Calculator at exam: non-programmable. If you have any doubts, you can post a photo of your calculator in the Ed discussion forum and we will let you know if this calculator is okay.

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

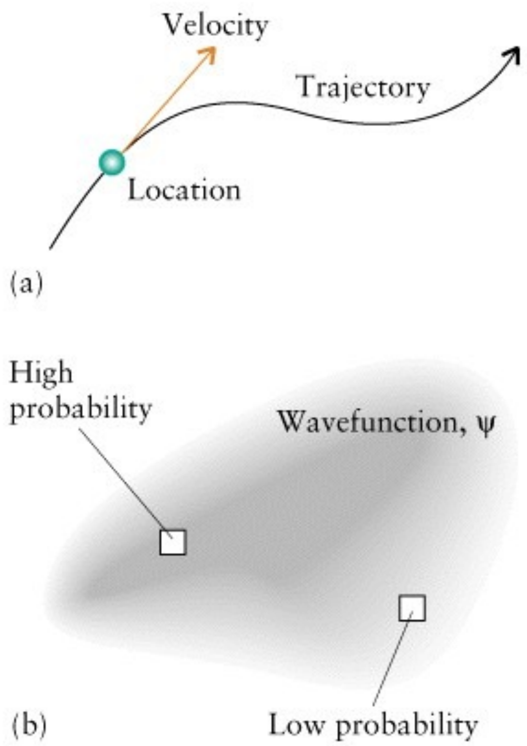
Summary of last Tuesday

The Wavefunction and Its Interpretation

Topic 1C.1

1C.1 The wavefunction and its interpretation

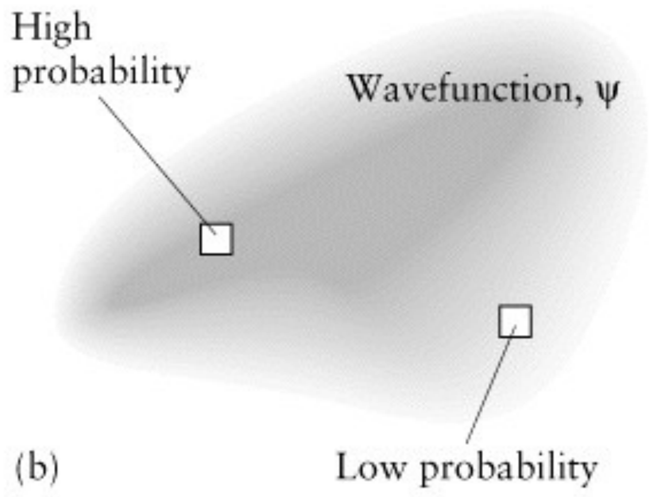
The wavefunction and probability density



- **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.

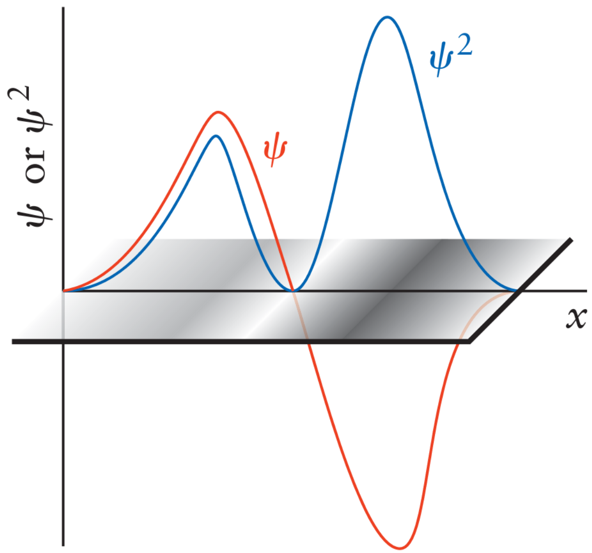
1C.1 The wavefunction and its interpretation

The wavefunction and probability density



1C.1 The wavefunction and its interpretation

ψ is a wave



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

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

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

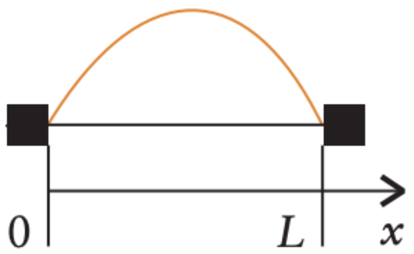
1C.1 The wavefunction and its interpretation

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

The particle-in-a-box model

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

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

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

$\Rightarrow$ $\psi^2_{max}(x)$ 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 more with the particle-in-a-box model more in exercises 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.

1C.1 The wavefunction and its interpretation

The particle-in-a-box model

- **Physical analog**: a bead free to slide along a rigid rod lying between two walls a distance *L* apart.
- **Classical mechanics**: the bead has the same probability of being found on the rod at any point inside the box, any speed, any kinetic energy

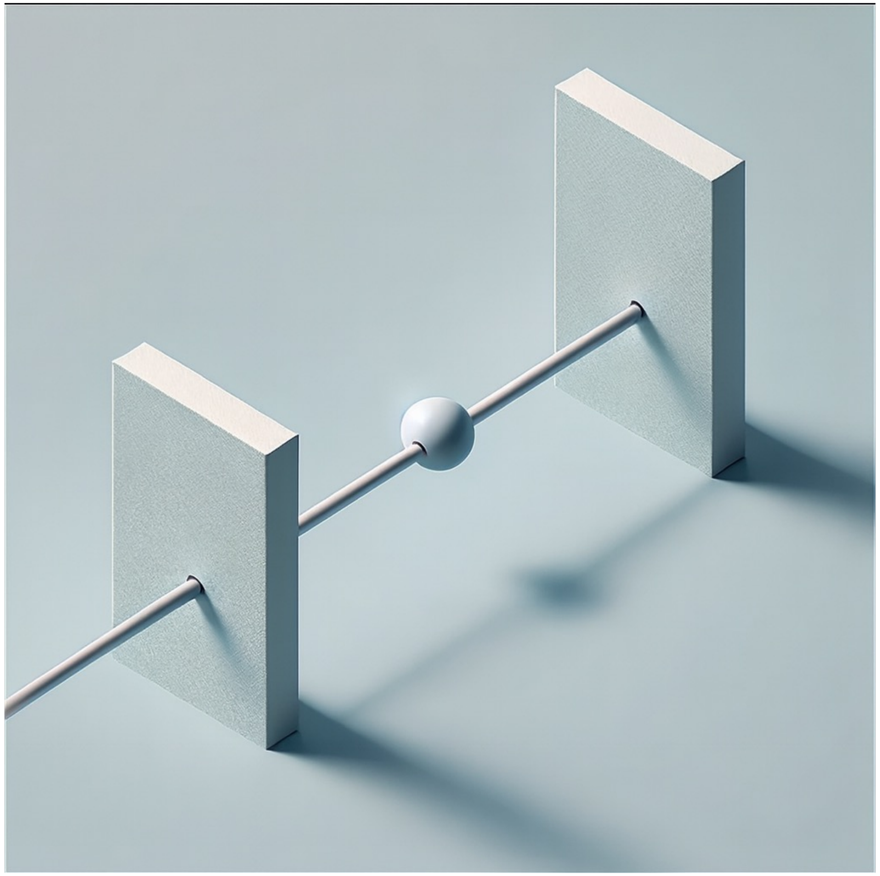


Image source: ChatGPT.
Bead on a rigid rod..

1C.1 The wavefunction and its interpretation

The particle-in-a-box model: n<1

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

- The integer n labels the wavefunctions and is called a "quantum number".

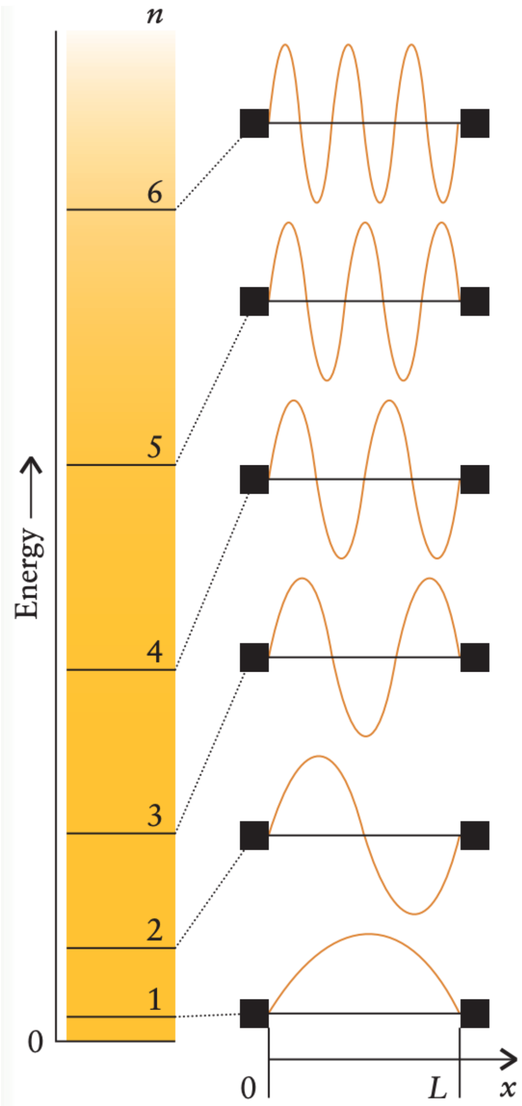


Figure 1C.3

1C.1 The wavefunction and its interpretation

Wavefunctions vs. guitar strings

Because the particle acts like a wave with zero amplitude at each end of the box

- → Only wavefunctions with **certain wavelengths** can exist in the box
- → Think of a **guitar string**: because it is tied down at each end, it can support only shapes like the ones shown.
- → The shapes of the wavefunctions for the particle in the box are the same as the displacements of a vibrating string.

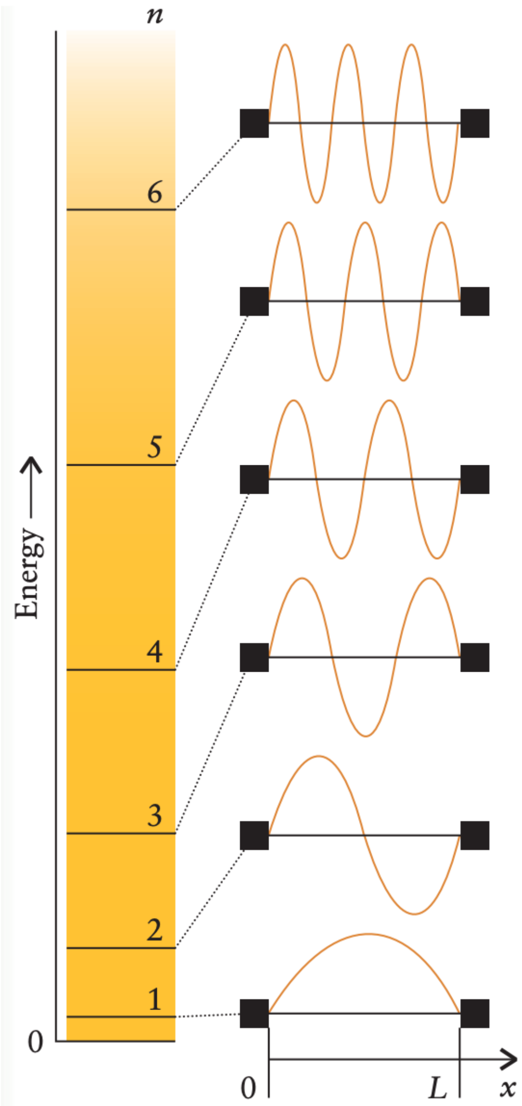
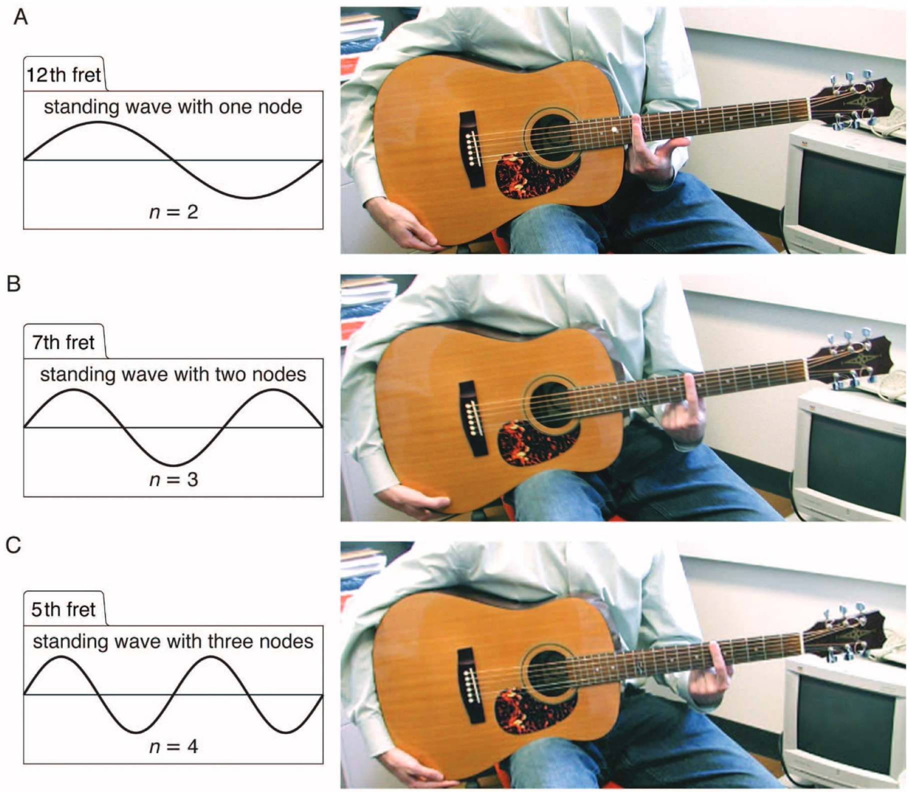


Figure 1C.3

1C.1 The wavefunction and its interpretation

Wavefunctions vs. guitar strings



Michael Davis, Journal of Chemical Education **2007**, 1287.

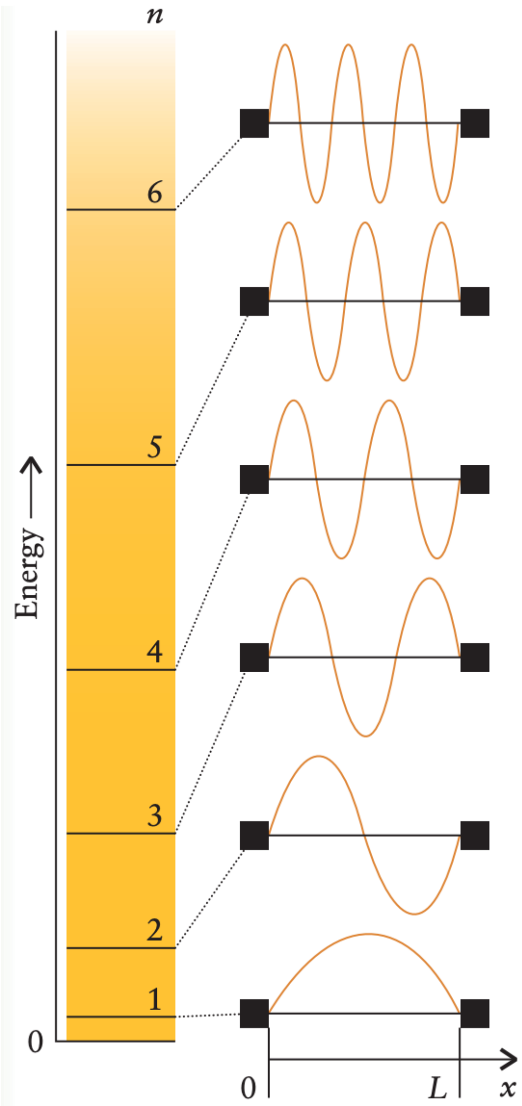


Figure 1C.3

1C.1 The wavefunction and its interpretation

Connecting concepts across Topics 1B and 1C

1C.1 The wavefunction and its interpretation

Summary

The **probability density** for a particle at a location is proportional to the square of the wavefunction at that point; places where the wavefunction passes through zero are called **nodes**, and the particle will not be found there. A wavefunction is found by **solving the Schrödinger equation** for the particle and recognizing the existence of certain **boundary conditions**.

URL
Quantum mechanics and guitars