

1) Consider a particle of mass m confined by the following potential:

$$V(x) = \begin{cases} \infty & x \leq -\frac{L}{2} \\ 0 & -\frac{L}{2} < x < \frac{L}{2} \\ \infty & x \geq \frac{L}{2} \end{cases}$$

a) What is the wave function for $|x| > L/2$?

b) Consider the time independent Schrodinger equation:

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

What quantity from classical mechanics do the first and second quantity in the left side of the equation most closely represent?

c) First, independent of the boundary conditions, what is the most general solution that solves the Schrodinger equation above in the region where the potential vanishes.

d) State the boundary conditions that the wave function must satisfy.

e) Derive and normalize expressions for the allowed energies and energy eigenfunctions.

f) Sketch the first three eigenfunctions.

(a) For $x > \frac{L}{2}$, the potential $V(x)$ is infinite. This implies that the wave function $\psi(x)$ must be 0 in this region because the particle cannot exist where the potential is infinite.

Thus, $\psi(x) = 0$ for $|x| > \frac{L}{2}$

(b) The term $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2}$ represents the kinetic energy operator in quantum mechanics.

The term $V(x) \psi(x)$ represents the potential energy operator.

(c) In the region $-\frac{L}{2} < x < \frac{L}{2}$, the potential $V(x) = 0$, the equation simplifies to:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} = E \psi(x) \Leftrightarrow \frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi(x)$$

Let $k = \sqrt{\frac{2mE}{\hbar^2}}$, the general solution is $\psi(x) = A \sin(kx) + B \cos(kx)$

(d) The wave function must be 0 at the boundaries where the potential is infinite.

Therefore, $\psi(\pm \frac{L}{2}) = 0$

(e) Applying the boundary conditions: $\psi(\pm \frac{L}{2}) = A \sin(k \frac{L}{2}) + B \cos(k \frac{L}{2}) = 0$

The only non-trivial solution that satisfies these boundary conditions is $B = 0$ and $\sin(k \frac{L}{2}) = 0$

$$\Rightarrow k \frac{L}{2} = n\pi \quad \text{where } n \in \mathbb{N}^+ \Rightarrow k = \frac{2n\pi}{L}$$

$$\Rightarrow \text{The allowed energy levels are } E_n = \frac{\hbar^2 k^2}{2m} = \frac{2\hbar^2 \pi^2 n^2}{mL^2}$$

$$\Rightarrow \text{The normalized eigenfunctions are } \psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2n\pi x}{L}\right)$$

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import numpy as np
import matplotlib.pyplot as plt

# Define constants
L = 1.0 # Length of the box
x = np.linspace(-L/2, L/2, 1000) # Position array

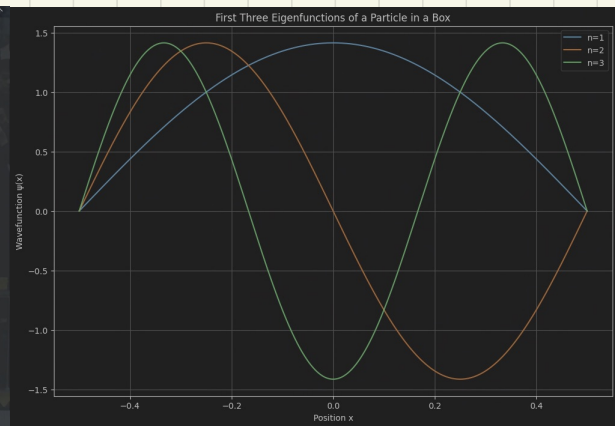
# Define the first three wavefunctions
def psi_n(n, x, L):
    return np.sqrt(2/L) * np.sin(n * np.pi * (x + L/2) / L)

# Plot the first three eigenfunctions
plt.figure(figsize=(12, 8))

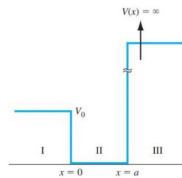
for n in range(1, 4):
    plt.plot(x, psi_n(n, x, L), label=f'n={n}')

# Add title and labels
plt.title('First Three Eigenfunctions of a Particle in a Box')
plt.xlabel('Position x')
plt.ylabel('Wavefunction ψ(x)')
plt.legend()
plt.grid(True)

# Show plot
plt.show()
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2) Consider the following one-dimensional potential function:



Assume the total energy of an electron is $E < V_0$.

- Write the wave functions that apply in each region.
- State the boundary conditions that the wave function must satisfy.
- Show explicitly why, or why not, the energy levels of the electron are quantized.

a) Region I : $\frac{\partial^2 \psi_1(x)}{\partial x^2} - \frac{2m(V_0 - E)}{\hbar^2} \psi_1(x) = 0$

Region II : $\frac{\partial^2 \psi_2(x)}{\partial x^2} + \frac{2mE}{\hbar^2} \psi_2(x) = 0 \Rightarrow$ General $\psi_1(x) = B_1 e^{\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} x}$, $k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$
 Solution : $\psi_2(x) = A_2 \sin\left(\sqrt{\frac{2mE}{\hbar^2}} x\right) + B_2 \cos\left(\sqrt{\frac{2mE}{\hbar^2}} x\right)$, $k_2 = \sqrt{\frac{2mE}{\hbar^2}}$
 Region III : $\psi_3 = 0$
 $\psi_3(x) = 0$

b)

At $x = 0$, $\psi_1(x) = \psi_2(x)$ since continuity $\Rightarrow B_1 = B_2$ and $\frac{\partial \psi_1(x)}{\partial x} = \frac{\partial \psi_2(x)}{\partial x} \Rightarrow k_1 B_1 = k_2 A_2$

At $x = a$, $\psi_2(a) = \psi_3(a) = 0 \Rightarrow A_2 \sin(k_2 a) + B_2 \cos(k_2 a) = 0$

c) Given ① ② ③:

$$B_2 = -A_2 \tan(k_2 a) = -\left(\frac{k_1}{k_2}\right) B_2 \tan(k_2 a) \Rightarrow 1 = -\left(\frac{k_1}{k_2}\right) \tan(k_2 a)$$

Then we can write as: $1 = -\sqrt{\frac{V_0 - E}{E}} \tan\left(\sqrt{\frac{2mE}{\hbar^2}} \cdot a\right)$

This equation only establishes for specific E values $\Rightarrow E$ is quantized

3) List and explain at least three phenomena that can't be explained by classical physics but can be explained by quantum physics. You can answer in this form: "classical physics predicts that...., but the contradiction is...., quantum physics solves this problem by...."

Blackbody Radiation

Classical Physics Prediction: The energy density of blackbody radiation would increase indefinitely with frequency (ultraviolet catastrophe).

Contradiction: Actual observations show that the energy density peaks and then decreases at higher frequencies.

Quantum Physics Solution: Planck's quantum hypothesis states that energy is quantized and can be emitted or absorbed in discrete amounts $E=h\nu$, explaining the observed blackbody spectrum.

Photoelectric Effect

Classical Physics Prediction: Light of any frequency, if intense enough, should eject electrons from a metal.

Contradiction: Experiments show that only light above a certain frequency can eject electrons, regardless of intensity.

Quantum Physics Solution: Einstein proposed that light consists of photons with energy $E=h\nu$; only photons with sufficient energy (frequency) can eject electrons, explaining the observed threshold frequency.

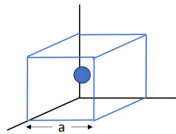
Stability of Atoms

Classical Physics Prediction: Electrons orbiting the nucleus should continuously emit radiation and spiral into the nucleus.

Contradiction: Atoms are observed to be stable.

Quantum Physics Solution: Bohr's model introduced quantized orbits where electrons do not radiate energy, explaining atomic stability and the discrete energy levels of electrons.

4) A lattice with a cubic unit cell as shown below has a single atom positioned at its center.



- Determine the number of atoms per unit volume in the crystal (state your answer in units of a).
- Determine the number of atoms per unit area on the (110) plane.
- A direction vector is drawn through the center of the atom in the unit cell. What is the direction vector?

a) # of atoms per unit volume : $\frac{1 \text{ atom}}{a^3}$ c) direction : $[1, 1, 1]$

b) area : $\sqrt{2} a \cdot a = \sqrt{2} a^2 \Rightarrow$ # of atoms per unit area : $\frac{1 \text{ atom}}{\sqrt{2} a^2}$

5) From the perspective of energy bands, explain the difference between conductors, semiconductors and insulators. Also explain the reason why metals are conductive while semiconductors are non-conductive at 0K.

Conductors (Metals)

Energy Bands: Conductors have overlapping valence and conduction bands, or a partially filled conduction band.

Conductivity at 0K: Metals are conductive at 0K because there are always free electrons available for conduction.

Semiconductors

Energy Bands: Semiconductors have a small energy gap (band gap) between the valence band and the conduction band.

Conductivity at 0K: At 0K, semiconductors are non-conductive because the electrons are in the valence band, and the thermal energy is insufficient to excite them across the band gap to the conduction band.

Insulators

Energy Bands: Insulators have a large energy gap between the valence band and the conduction band.

Conductivity: The large band gap prevents electrons in the valence band from being excited to the conduction band, making insulators non-conductive under normal conditions.

Why metals are conductive while semiconductors are non-conductive at 0K:

Metals: Always have free electrons in the conduction band, allowing for conductivity even at 0K.

Semiconductors: Lack free electrons in the conduction band at 0K due to the energy gap, resulting in no conductivity at this temperature.

6) Briefly explain what is doping and why doping is important in the field of semiconductor.
 What's the difference between p-type dopant and n-type dopant? List two potential p-type dopants and n-type dopants for silicon.

Doping:

Definition: Doping is the process of intentionally introducing impurities into a semiconductor to modify its electrical properties.

Importance: Doping is crucial because it allows control over the conductivity of semiconductors, enabling the creation of p-n junctions essential for semiconductor devices like diodes, transistors, and integrated circuits.

Types of Dopants:

p-type Dopant:

Definition: p-type dopants add holes (positive charge carriers) to the semiconductor.

Mechanism: Elements with one less valence electron than the semiconductor (e.g., boron in silicon) create holes in the valence band.

Examples for Silicon: Boron (B), Gallium (Ga).

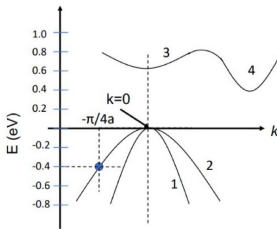
n-type Dopant:

Definition: n-type dopants add electrons (negative charge carriers) to the semiconductor.

Mechanism: Elements with one more valence electron than the semiconductor (e.g., phosphorus in silicon) add extra electrons to the conduction band.

Examples for Silicon: Phosphorus (P), Arsenic (As).

7) The band structure of a semiconductor is shown below:



- Is this a direct or indirect band gap semiconductor?
- Label the conduction band, the valence band and the energy gap on this diagram. What is the value of the energy gap approximately?
- Compare the magnitude of the effective masses between points 1-2 and points 3-4. Which are electron and which are hole masses?
- The E-K relationship of a hole is located at the point of the circle on band 2. State the momentum and the kinetic energy of the hole at the point of the circle.
- Calculate the velocity and effective mass of the hole.

2 has a smaller effective mass compared to 1, and 3 has a smaller effective mass compared to 4

d) $k = -\frac{\pi}{4a} \Rightarrow p = -\hbar \frac{\pi}{4a}$, kinetic energy -0.4 eV

c) $v = \frac{1}{\hbar} \frac{dE}{dk}$, $m^* = \frac{\hbar^2}{d^2E/dk^2}$

Since the exact functional form of the energy vs momentum relation is not provided in the diagram, the exact calculations would require more detailed information.

a) This is an indirect band gap semiconductor.

Since the minimum of the conduction band (1) and the maximum of the valence band (3) do not occur at the same k value

b) Conduction Band: 1 and 2

Valence Band: 3 and 4

Energy Gap: 0.4 eV

c) 1-2: conduction band \Rightarrow electron masses

3-4: valence band \Rightarrow hole masses