INDIAN INSTITUTE OF TECHNOLOGY, PATNA

Department of Physics

Introduction to Nanomaterials

Report on

Predicting Density of States and Energy Levels in Nanomaterials

by

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Link to Code: https://github.com/anuragdasgroup97/nanomaterials_project/tree/main

1. Problem Statement

Write a program to predict the density of states and energy levels for different nanomaterials. Use any computer language to write the program.

AIM:

1. Calculate and visualize the density of states for a free electron model within a nanomaterial.

2. Predict and plot energy levels versus quantum number n for a particle confined in a one-dimensional box.

2. Overview

The study and analysis of nanomaterials involve understanding their electronic properties, particularly the density of states (DOS) and energy levels. We know at nanoscale the elctrons behave differently and their properties differ from the bulk materiuals due to qunatum cofinement and dimensional effects. The density of states (DOS) refers to the number of available states at a given energy level. It is a very crucial parameter for understanding electronic and optical behavior in materials. The energy levels of a confined electron system, modeled by quantum numbers, provide insight into the quantization effects in nanoscale systems.

In this project, we have-

- Calculated Density of States (DOS) for free elctrons using the free electron model.
- Employed a histogram-based approach to approximate DOS values for different energy levels.
- Visualized the results to observe how DOS evolves with energy in a nanomaterial.
- Computed the energy levels for a particle confined in a one-dimensional box using the particle-in-a-box formula.
- Plotted these levels against quantum numbers to visualize the impact of quantum confinement.

Both DOS and Energy Level analyses were implemented in Python and we find a foundational understanding of quantum behavior in nanomaterials.

3. Theoretical Background

The concepts of DOS and quantized energy levels are rooted in quantum mechanics and condensed matter physics and are pivotal in explaining the behavior of electrons in nanostructures.

3.1 Density of States(DOS)

Definition:
The density of states (DOS) describes the number of electronic states available within a material at a specific energy level per unit volume. Mathematically, it is expressed as:

$D(E)=dN(E)/dE$

where $N(E)$ is the total number of states with energy less than E.

Physical Significance:

- The DOS provides insight into how electrons populate energy levels.
- It governs the electrical, optical, and thermal properties of materials. For example, materials with a high DOS at the Fermi level tend to exhibit better conductivity.

Free Electron Model in 3D:

In a 3D material, electrons are treated as free particles confined in a box, leading to the dispersion relation:

$E = \hbar^2 \cdot k^2 / 2 \cdot m$

Here, $\hbar$ is the reduced Planck's constant, k is the wave vector, and mmm is the mass of the electron.

The DOS for 3D systems is derived as: D(E) $\propto \mathrm{sqrt(E)}$

This implies that the DOS increases with energy, which is typical of bulk materials like metals and semiconductors.

Variations in Lower Dimensions:

1. **2D Materials:**

   In two dimensions, such as graphene, the DOS becomes constant: D(E)=constant. This unique property influences the optical and electronic behavior of 2D materials.

2. **1D Systems:**
   In one dimension (e.g., nanowires), the DOS diverges at certain energy levels: D(E) $\propto 1/\mathrm{sqrt(E)}$. Such singularities, called Van Hove singularities, arise due to the reduced availability of energy states.
3. **3D Systems:**
   For a free electron model in 3D systems, the DOS generally **increases with energy** as D(E) $\propto \mathrm{sqrt(E)}$

3 .2 Energy Levels in Quantum Confinement

Definition:

When electrons are confined to dimensions comparable to their de Broglie wavelength, their energy levels become quantized. This phenomenon, known as quantum confinement, is observed in nanomaterials like quantum dots, nanowires, and thin films.

Particle-in-a-Box Model:

This model illustrates quantum confinement by considering a particle of mass m confined in a box of length L. The energy levels are given by:

$E_n = n^2\pi^2 \cdot \hbar^2 / 2 \cdot m \cdot L^2$, where n=1,2,3,…i.e the quantum number.

Key Features:

- Energy levels are discrete and depend on n^2, indicating that higher levels are spaced further apart.
- Smaller confinement dimensions (smaller L) lead to larger energy gaps, a signature of quantum confinement.

Physical Implications:

❖ **Electronic Properties:**

The quantization of energy levels directly affects electron transport and optical absorption. For example, smaller quantum dots absorb and emit light at higher energies (blue-shifted).

❖ **Applications:**

- **Quantum Dots:** Tunable emission wavelengths in displays and bioimaging.
- **Nanowires:** Enhanced carrier mobility in transistors.

4. Formulae Used

1. Energy of Free Electrons for DOS:

For a free electron model, the energy E for an electron with wave vector k is given by:

E = $\hbar^2 \cdot k^2 \,/\, 2 \cdot m$

where:

- $\hbar$: Reduced Planck constant (1.0545718×10^{34} J·s),

- k: Wave vector of the electron,

- m: Mass of the electron ($9.10938356 \times 10^{-31}$ kg).

2. Quantized Energy Levels for a Particle in a Box:

For an electron confined within a one-dimensional box (nanomaterial of size L, the energy levels are quantized and given by:

$E_n = n^2\pi^2 \cdot \hbar^2 \,/\, 2 \cdot m \cdot L^2$

where:

- n: Quantum number (integer values, n = 1, 2, 3, …),

- L: Length of the confinement region (e.g., 1 nm for nanomaterials),

-m: Mass of Electron.

5. Methodology

Step 1: Calculation of Density of States (DOS)

- Energy Calculation: We calculated the energy levels for a range of wave vectors \(k \) to simulate free electrons in a nanomaterial.
- Binning for DOS: We used a histogram-based approach to approximate the DOS. The number of states was counted within small energy intervals (bins) to approximate the DOS as a function of energy.
- Visualization: The DOS was plotted as a function of energy using Matplotlib.

Step 2: Calculation of Quantized Energy Levels E_n vs Quantum Number n

- Quantum Number Generation: We considered integer values of n from 1 to 20.
- Energy Levels Calculation: Using the particle-in-a-box formula, we found the energy E_n for each n.
- Visualization: The calculated energy levels were plotted against n to visualize the relationship between quantum number and energy levels.

Step 3: Combined Visualization

Both the DOS vs. Energy and E_n vs n plots were displayed side by side for a comprehensive view:

- Density of States: A smooth curve showing how DOS varies with energy.
- Energy Levels: Discrete points showing the quantization of energy levels as n increases.

6. Observations and Findings

1. Density of States (DOS):

In the plot of the density of states (DOS) versus energy on a **linear scale**:

- The **1D DOS** decreases steeply as energy increases due to the $g(E) \propto 1/\mathrm{sqrt}(E)$ relationship.
- The **2D DOS** remains constant, as expected.
- The **3D DOS** increases as energy increases, consistent with the $g(E) \propto \mathrm{sqrt}(E)$ relationship.

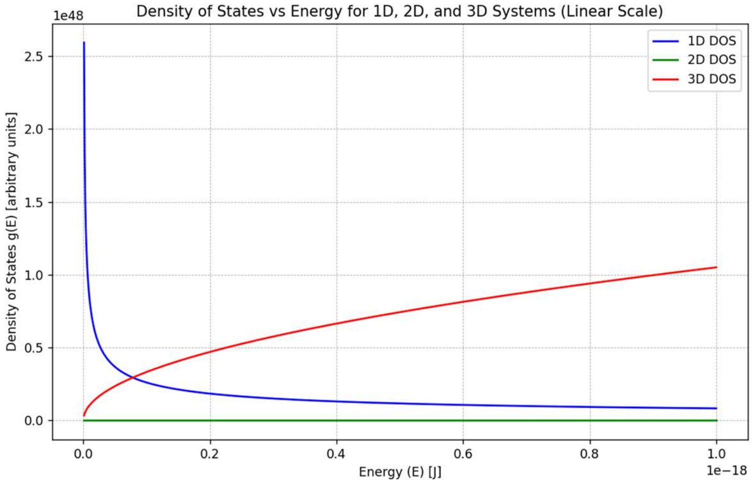

Figure 1: Relation observed between DOS and Energy

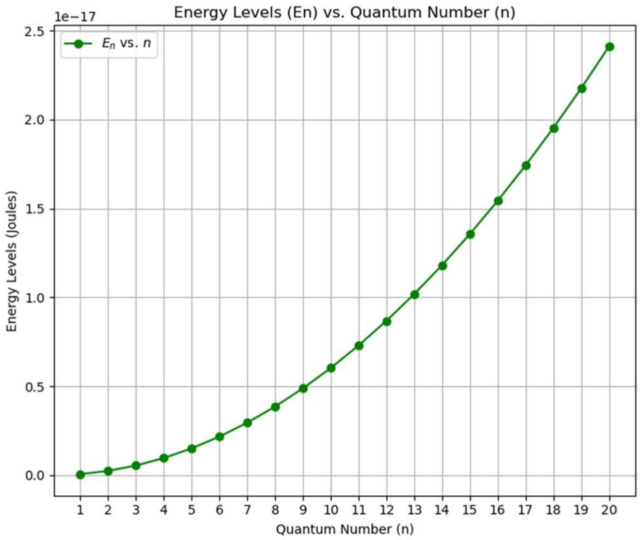

Figure 2: Relation Between Energy levels and Quantum Numbers

2. Energy Levels E_n vs. Quantum Number n:

- The energy levels increase quadratically with n, as evident from the plot.
- Each subsequent energy level is spaced further apart from the previous one, which aligns with the particle-in-a-box model where energy quantization grows with n^2.
- Adjusting the x-axis ticks allowed distinct visualization of each quantum number n, confirming the spacing effect in quantum confinement.

7. Conclusion

This project provides a fundamental approach to understanding the electronic properties of nanomaterials through the calculation of DOS and energy levels. The findings indicate:

- The quadratic growth of quantized energy levels, affirming quantum confinement principles.
- The dependency of DOS on energy, dimensionality, and material properties.

Quantized energy states due to spatial confinement is nothing but a hallmark of quantum mechanics in nanoscale systems. An increasing density of states with energy, which is crucial for understanding electronic behavior in materials where the free electron model is applicable.

8. References

1. Griffiths, D. J. (2005). Introduction to Quantum Mechanics. Pearson Prentice Hall.

2. Kittel, C. (2004). Introduction to Solid State Physics. John Wiley & Sons.

3. Online Resources: [NumPy Documentation] (https://numpy.org/doc/), [Matplotlib Documentation] (https://matplotlib.org/stable/contents.html)