

Using Schrödinger wave equation calculate the energy Eigen value and the wave function for a particle in this well potential. From symmetry point of view comment why you are getting odd and even wave-functions? **(10) [BL5]**

[**Hints:** Apply the concept of 1D box for the asymmetric 1D potential box in and using that knowledge calculate it.]

Module 6: Statistical Mechanics

Statistical mechanics is a branch of physics that connects the microscopic properties of individual atoms and molecules to the macroscopic or bulk properties of materials. It provides a framework for understanding thermodynamics, phase transitions, and various other phenomena in condensed matter physics, astrophysics, and beyond.

- **Microstate:**

A microstate refers to a specific detailed microscopic configuration of a system. For a given set of particles, a microstate specifies the position and momentum of each particle.

- **Macrostate:**

A macrostate is defined by macroscopic quantities such as temperature, pressure, volume, and energy, which describe the overall state of the system without specifying the details of individual particles. Multiple microstates can correspond to the same macrostate. For example, a gas in a box with a given temperature and pressure can have countless arrangements of individual molecules (microstates) that result in the same overall conditions (macrostate).

- **Phase Space:**

Phase space is a conceptual multidimensional space in which all possible states of a system are represented. Each state is a point in this space, with dimensions corresponding to all possible values of position and momentum coordinates. For a system of N particles in three dimensions, the phase space has $6N$ dimensions, consisting of $3N$ position coordinates and $3N$ momentum coordinates. Phase space provides a complete description of a system's state. By examining trajectories in phase space, we can study the evolution of a system over time. The density of points in phase space can also be used to determine thermodynamic properties.

- **Maxwell-Boltzmann (MB) Statistics:**

Maxwell-Boltzmann statistics describe the distribution of particles in classical systems where quantum effects are negligible. It is applicable to ideal gases and assumes that the particles are distinguishable.

Properties:

1. The MB distribution applies to non-quantum, distinguishable particles.
2. It describes the distribution of molecular speeds in gases.
3. At higher temperatures, particles have higher kinetic energies.

Maxwell-Boltzmann distribution function $f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{\alpha + \beta E_i}}$

- **Fermi-Dirac (FD) Statistics:**

Fermi-Dirac statistics apply to fermions, particles with half-integer spin that obey the Pauli Exclusion Principle, which states that no two fermions can occupy the same quantum state simultaneously.

Properties:

1. FD statistics apply to electrons in metals, neutrons in neutron stars, and other fermionic systems.
2. At absolute zero, all states up to the Fermi energy are occupied.
3. The distribution shows a sharp cutoff at the Fermi energy at low temperatures.

Fermi-Dirac distribution function $f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{\alpha + \beta E_i} + 1}$, here $\alpha = -\frac{E_f}{kT}$, $\beta = \frac{1}{kT}$

- **Bose-Einstein (BE) Statistics:**

Bose-Einstein statistics apply to bosons, particles with integer spin that do not obey the Pauli Exclusion Principle. Multiple Bosons can occupy the same quantum state.

Properties

1. BE statistics apply to photons, helium-4 atoms, and other Bosonic systems.
2. Bosons tend to cluster into the same state, leading to phenomena like Bose-Einstein condensation.
3. At low temperatures, a significant fraction of particles can occupy the lowest energy state.

Bose-Einstein distribution function $f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{\alpha + \beta E_i} - 1}$, here $\alpha = -\frac{\mu}{kT}$, $\beta = \frac{1}{kT}$

- **Applications and Implications:**

Classical Systems

In classical systems, such as ideal gases, MB statistics effectively describe the distribution of particle velocities and energies. These principles underpin the kinetic theory of gases and are essential for understanding macroscopic gas properties like pressure and temperature.

Quantum Systems

For quantum systems, FD and BE statistics are crucial. FD statistics explain the behavior of electrons in solids, leading to the development of semiconductor technology and our understanding of metals and insulators. BE statistics are vital for understanding superfluidity and the behavior of photons in blackbody radiation.

Thermodynamic Quantities

The different statistical distributions allow us to derive macroscopic thermodynamic quantities from microscopic properties:

Entropy (S): Measures the number of accessible microstates. Higher entropy corresponds to more disorder.

Internal Energy (U): The average energy of the system.

Heat Capacity (C): How much energy is needed to change the system's temperature. Pressure (P) and Volume (V): Relations derived from the distribution of particles and their interactions.

Questions:

1. Assume that the entropy (S) and the statistical number (No. of microstate = W) of a physical system are related through an arbitrary functional form $S = f(W)$, Deduce this functional form of entropy considering the additive character of S and the multiplicative character of W.

(5) [BL4]

[Hint: try to find the function, which gives $f(A.B) = f(A) + f(B)$]

2. Write a MATLAB code to check the validity of the postulate of equal a priori probability by tossing two coins many times. **(5) [BL6]**

[Hint: Probability of head in toss is 50%]

3. Find out the phase space trajectory of a Simple Harmonic Oscillator. **(5) [BL4]**

[Hint: Write down the total energy in terms of position and momentum and then plot that phase space]

4. A system has a single particle state with 0, 1, 2, and 3 energy units. Discuss the macrostates and microstates for three distinguishable particles to be distributed in these energy states such that the total energy of the system is 3 units. **(5) [BL5]**

[Hint: Use MB Statistics]

5. Determine the temperature at which the mean speed of hydrogen molecules will be same as that of oxygen molecules at 35°C. (Given, the molecular mass of hydrogen molecule is 2 and of oxygen molecule is 32.) **(5) [BL4]**

[Hint: Use the formula for Mean velocity from MB Statistics]

6. A cubic meter of atomic hydrogen at 0° C and at atmospheric pressure contains about 2.7×10^{25} atoms. Find the number of these atoms in their first excited states ($n=2$) at 0° C and 10000° C. **(5) [BL 4]**

[Hints: $\frac{n(\epsilon_2)}{n(\epsilon_1)} = \frac{g(\epsilon_2)}{g(\epsilon_1)} e^{-(\epsilon_2 - \epsilon_1)/kT}$]

7. Find the Fermi energy in copper on the assumption that each copper atoms contributes one free electron to the electron gas. The density of copper is $8.94 \times 10^3 \text{ kg/m}^3$ and its atomic mass is 63.5 u. **(5) [BL 5]**
8. If the Fermi energy of a metal at thermal equilibrium $T = 0 \text{ K}$ is 12 eV, find (i) the average energy of free electrons in the metal, (ii) the speed of electron corresponding to the above average energy.

[Hints: $\epsilon_{avg} = \frac{3}{5} \epsilon_f$] **(5) [BL 4]**
