

COIN TOSSING EXPERIMENT – 1

1. What is a system?

ANS: A system is defined by the collection of a large number of particles.

2. What is ensemble?

ANS: A collection of a number of macroscopically identical but essentially independent systems.

Microscopically identical – each of the system constituting an ensemble satisfies the same macroscopic conditions like volume, energy, pressure and temperature and the total number of particles etc.

Essentially Independent – the system (in the ensemble) is mutually non-interacting to others i.e., the system differs in microscopic conditions like parity, symmetry, quantum states etc.

3. What is a microstate?

ANS: Each possible combinations of positions and velocities, momentum of all molecules refers to a microstate of the system.

4. What is Macrostate?

ANS: The macrostate of a system refers to its macroscopic properties such as its temperature, pressure, volume and density.

DISTRIBUTION FUNCTIONS EXPERIMENT – 2

1. Write the Distribution Functions for Maxwell-Boltzmann, Fermi-Dirac and Bose-Einstein.

ANS:

Maxwell-Boltzmann Distribution Function

The average number of particles in a state of energy ϵ is a system of particles at absolute temperature T is

$$f_{MB}(\epsilon) = Ae^{-\frac{\epsilon}{kT}} \quad \text{--- (2)}$$

A = Constant

= Depends on number of particle in the system

= It has the same role as that of normalization constant in case of wave function

k = Boltzmann's constant

$= 1.381 \times 10^{-23} \text{ J/K} = 8.617 \times 10^{-5} \text{ eV/K}$

Combining Eq. (1.a) and (2), we get

$$n(\epsilon) = g(\epsilon)f_{MB}(\epsilon)$$

$$n(\epsilon) = Ag(\epsilon)e^{-\frac{\epsilon}{kT}} \quad \text{--- (3)}$$

Let's apply MB statistics to find the distribution of energies among the molecules of an ideal gas

notes by sk sir

18.3 Bose–Einstein Condensation

- A gas of non-interacting particles (atoms & molecules) of relatively large mass.
- The particles are assumed to comprise an ideal B-E gas.
- Bose – Einstein Condensation: phase transition
- B – E distribution:
$$f(\varepsilon) = \frac{N(\varepsilon)}{g(\varepsilon)} = \frac{1}{e^{\frac{(\varepsilon - \mu)}{kT}} - 1}$$

Fermi-Dirac distribution and the Fermi-level

Density of states tells us **how many states exist at a given energy E** . The **Fermi function $f(E)$** specifies how many of the existing states at the energy E will be filled with electrons. The function $f(E)$ specifies, **under equilibrium conditions**, the **probability** that an available state at an energy E will be occupied by an electron. It is a **probability distribution function**.

$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

(2.7)

E_F = Fermi energy or Fermi level

k = Boltzmann constant = 1.38×10^{-23} J/K
= 8.6×10^{-5} eV/K

T = absolute temperature in K

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Boltzmann	Bose Einstein	Fermi Dirac
$\bar{n}_k = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right)}$	$\bar{n}_k = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) - 1}$	$\bar{n}_k = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) + 1}$
indistinguishable $Z = (Z_1)^N / N!$ $n_k \ll 1$	indistinguishable integer spin 0, 1, 2 ...	indistinguishable half-integer spin 1/2, 3/2, 5/2 ...
spin doesn't matter	bosons	fermions
localized particles Ψ don't overlap	wavefunctions overlap total Ψ symmetric	wavefunctions overlap total Ψ anti-symmetric
gas molecules at low densities	photons ^4He atoms	free electrons in metals electrons in white dwarfs
"unlimited" number of particles per state $n \ll 1$	unlimited number of particles per state	never more than 1 particle per state

2. Explain Fermi energy and chemical potential and their importance/significance.

Fermi energy and chemical potential are two related concepts in the field of condensed matter physics that are crucial for understanding the behaviour of electrons in materials.

Fermi energy, also known as the Fermi level, is the highest energy level occupied by electrons in a material at absolute zero temperature. It is named after Enrico Fermi, the Italian physicist who first proposed the concept. The Fermi energy is a fundamental parameter that determines many electronic properties of materials, such as their electrical conductivity, thermal conductivity, and optical properties.

Chemical potential, on the other hand, is a thermodynamic quantity that describes the energy required to add or remove a particle from a system. It is defined as the partial derivative of the internal energy of a system with respect to the number of particles in the system, at constant temperature and volume. In condensed matter physics, the chemical potential is often used to describe the energy required to add or remove an electron from a material.

The importance of Fermi energy and chemical potential lies in their ability to describe the behaviour of electrons in materials. In particular, the Fermi energy determines whether a material is a metal, an insulator, or a semiconductor. Metals have a Fermi energy that lies within the conduction band, which allows electrons to move freely throughout the material and conduct electricity. Insulators have a large energy gap between the valence and conduction bands, which prevents electrons from moving freely and thus they do not conduct electricity.

Chemical potential also plays a crucial role in determining the behaviours of electrons in materials. For example, the chemical potential of a material can affect its response to an external electric field or magnetic field. It can also determine the direction of electron flow in a circuit, and can be used to predict the behaviours of electron transport in a wide range of materials, from metals to semiconductors and beyond.

PARTITION FUNCTION EXPERIMENT 7

1. Connection between State function and Partition function?

State functions and partition functions are both important concepts in thermodynamics that describe different aspects of a system.

A state function is a thermodynamic property that depends only on the current state of a system and not on how that state was reached. Examples of state functions include temperature, pressure, internal energy, and entropy. The value of a state function depends only on the current state of the system, and not on the path by which the system reached that state.

A partition function, on the other hand, is a mathematical function that is used to calculate the thermodynamic properties of a system in equilibrium. Specifically, the partition function is used to calculate the probabilities of the different possible states of a system, and from these probabilities, the thermodynamic properties of the system can be determined.

There is a connection between state functions and partition functions in that the partition function depends on the state of the system. Specifically, the partition function is a function of the energy levels and the number of particles in the system, which are state functions. By calculating the partition function for a system, we can determine the probabilities of the different possible states of the system, and from these probabilities, we can calculate the average values of state functions like energy, entropy, and temperature.

In summary, the partition function is a mathematical function that depends on the state of a system, which is described by state functions. By using the partition function, we can determine the probabilities of different possible states of the system and calculate the average values of state functions for the system.

2. Difference between Micro-Canonical, Canonical and Grand-Canonical ensemble?

Microcanonical, canonical, and grand canonical ensembles are three different ways of describing a system in statistical mechanics, each with its own set of assumptions and constraints.

1. Microcanonical ensemble:

The microcanonical ensemble is a theoretical construct that describes a closed system in which the total energy, volume, and number of particles are fixed. The microcanonical ensemble assumes that the system is completely isolated and that it can exchange energy, but not particles or volume, with its surroundings. In the microcanonical ensemble, the system is described by a single macrostate, which corresponds to a specific combination of energy, volume, and number of particles.

2. Canonical ensemble:

The canonical ensemble describes a system in contact with a heat bath, which can exchange energy with the system. The total energy of the system and the heat bath is conserved, but the number of particles and volume of the system can fluctuate. In the canonical ensemble, the system is described by a distribution of microstates, which correspond to different energy levels that the system can occupy. The probability distribution of the microstates is determined by the temperature of the heat bath and the energy levels of the system.

3. Grand canonical ensemble:

The grand canonical ensemble is used to describe a system that can exchange both energy and particles with a reservoir. The total energy, volume, and chemical potential of the system and reservoir are conserved, but the number of particles in the system can fluctuate. In the grand canonical ensemble, the system is described by a distribution of microstates, which correspond to different energy levels and particle numbers that the system can occupy. The probability distribution of the microstates is determined by the temperature, chemical potential, and energy levels of the system and reservoir.

In summary, the microcanonical ensemble describes a completely isolated system, the canonical ensemble describes a system in contact with a heat bath, and the grand canonical ensemble describes a system that can exchange both energy and particles

with a reservoir. The different ensembles are used to describe different types of systems and to calculate different thermodynamic properties.