

PHASE SPACE

Phase Space:

"A combination of position space and momentum space is known as phase space." Thus phase space has 6 dimensions, i.e., three position co-ordinates and three momentum co-ordinates, all mutually perpendicular to each other. Since 6-dimensional diagram can not be drawn, Phase space is purely a mathematical concept.

To specify the state of a dynamical system of particles, we require the position and velocity (or more conveniently momentum) of each of its particles, i.e. we must specify six quantities x, y, z, p_x, p_y, p_z for each of the particles. As a purely mathematical concept we may imagine six dimensional space in which $dx dy dz dp_x dp_y dp_z$ is an element of volume and the state of a particle in this space will be described by a set of six-coordinates x, y, z, p_x, p_y, p_z . This six dimensional space for a single particle is called phase space or μ -space (mu-space). An element of volume in the phase space is called a 'Cell'.

- The instantaneous state of a particle in the phase space is represented by a point known as phase point or representative point.

- The phase space is divided into six dimensional cells whose sides are $dx, dy, dz, dp_x, dp_y, dp_z$. Such cells are called phase cells. A cell may contain a large number of phase points.

- For general case of 'f' degrees of freedom per molecule, we have -
(Particle)

- i) Position space - f - dimensional
- ii) Momentum Space - f - dimensional
- iii) μ -Space - $2f$ - dimensional
- iv) Γ -space (Gamma Space) - $2fN$ - dimensional
[If we are to deal with a system of N-particles]

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- Division of Phase Space into cells:

The phase space is divided into six dimensional cells whose sides are $dx, dy, dz, dp_x, dp_y, dp_z$. Such cells are called phase cells. Volume of each cell is

$$dT = dx dy dz dp_x dp_y dp_z.$$

- According to classical statistics there is no restriction on the volume of the phase cell; it may be reduced to any extent.

But- according to Uncertainty Principle,

$$dx dp_x \geq h$$

$$dy dp_y \geq h$$

$$dz dp_z \geq h$$

$$\text{Thus, } dT \geq h^3$$

Therefore Volume of a cell,
 $dT \approx h^3$

The Unit of Phase space Volume
 $= (\text{Joule-sec})^3$

Hence, minimum size of phase space cell according to quantum statistics is h^3 .

What is the minimum size of phase space cell in classical and quantum statistics ?

Ans. Minimum size of phase space cell in classical statistics is zero whereas in quantum statistics it is h^3 .

✓ PHASE SPACE DIAGRAM OF ONE DIMENSIONAL HARMONIC OSCILLATOR

corit

✓ Consider a one dimensional harmonic oscillator whose position coordinate is x and whose momentum is p_x . Then energy of the oscillator is given by

$$E = \frac{p_x^2}{2m} + \frac{1}{2} kx^2 \quad \dots (1)$$

where m is the mass of the oscillator.

The first term in eq. (1) is the kinetic energy of the oscillator in terms of its momentum p_x while second term represents its potential energy. k is the spring factor (force constant) of the restoring force acting on the oscillator. ~~Thus expression of energy has two quadratic terms.~~

Now Eq. (1) can be written as

$$\frac{p_x^2}{2mE} + \frac{kx^2}{2E} = 1$$

or

$$\frac{x^2}{(2E/k)} + \frac{p_x^2}{2mE} = 1 \quad \dots (2)$$

This equation represents an ellipse in the $x - p_x$ phase space as shown in Fig. Its semi-major axis

$$a = \sqrt{\frac{2E}{K}}$$

and semi-minor axis

$$b = \sqrt{2mE}$$

Thus the trajectory of the oscillator in the two dimensional position momentum phase space is an ellipse and the instantaneous state of the oscillator is represented by some point on the ellipse.

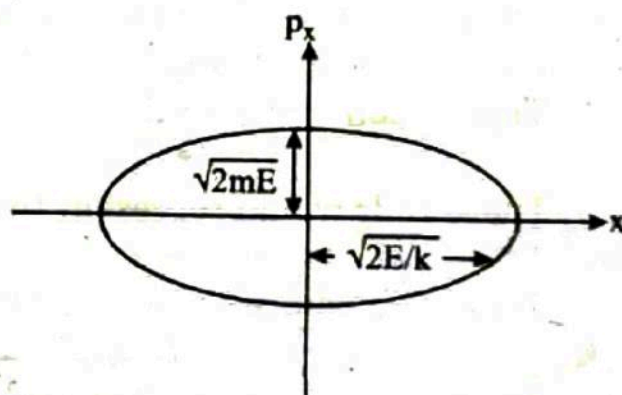
The area of the ellipse in phase space is given by

$$A = \pi ab = \pi \sqrt{\frac{2E}{k}} \cdot \sqrt{2mE}$$

$$= 2\pi E \sqrt{\frac{m}{k}} \quad \dots (3)$$

This area represents the phase space available to the oscillator having energy between 0 and E . Therefore, the phase space available to the oscillator having energy between E and $E + dE$ will be given by ~~the differential of the area given by eq. (3). It is~~

$$dA = 2\pi \sqrt{\frac{m}{k}} dE \quad \dots (4)$$



This represents the region of states accessible to the oscillator.

NUMBER OF PHASE CELLS IN GIVEN ENERGY RANGE OF HARMONIC OSCILLATOR

For one dimensional oscillator, the area of a phase cell in phase space is given by

$$\delta_x \delta p_x = h \quad \because \text{phase space is two dimensional } (x-p_x)$$

The energy E of the oscillator with mass m is given by

$$E = \frac{p_x^2}{2m} + \frac{1}{2} kx^2$$

or
$$\frac{x^2}{(2E/k)} + \frac{p_x^2}{2mE} = 1 \quad \dots(1)$$

This equation represents an ellipse with semi major axis $a = \sqrt{(2E/k)}$ and semi-minor axis $b = \sqrt{(2mE)}$

The phase space area of the oscillator having energy between 0 and E is

$$\pi a b = \pi \sqrt{(2E/k)} \sqrt{(2mE)} = 2\pi E \sqrt{(m/k)} \quad \dots(2)$$

We know that the frequency ν of the oscillators is given by

$$\nu = \frac{1}{2\pi} \sqrt{\left(\frac{k}{m}\right)} \quad \text{or} \quad \sqrt{\left(\frac{m}{k}\right)} = \frac{1}{2\pi\nu} \quad \dots(3)$$

From eqs. (2) and (3), area of phase space $= 2\pi E \times \frac{1}{2\pi\nu} = \frac{E}{\nu}$

$$\begin{aligned} \therefore \text{number of phase cell} &= \frac{\text{area of phase space}}{\text{area of phase cell}} \\ &= \frac{E/\nu}{h} = \frac{E}{h\nu} \end{aligned}$$

I. VOLUME IN PHASE SPACE :

Consider the volume of the momentum space lying between the values of total momentum p and $p+dp$. A small element of momentum space with coordinates in the range p to $p+dp$, θ to $\theta+d\theta$ and ϕ to $\phi+d\phi$ is shown in fig 2. The element is considered in polar coordinates p , θ and ϕ like the polar coordinates of position r , θ and ϕ .

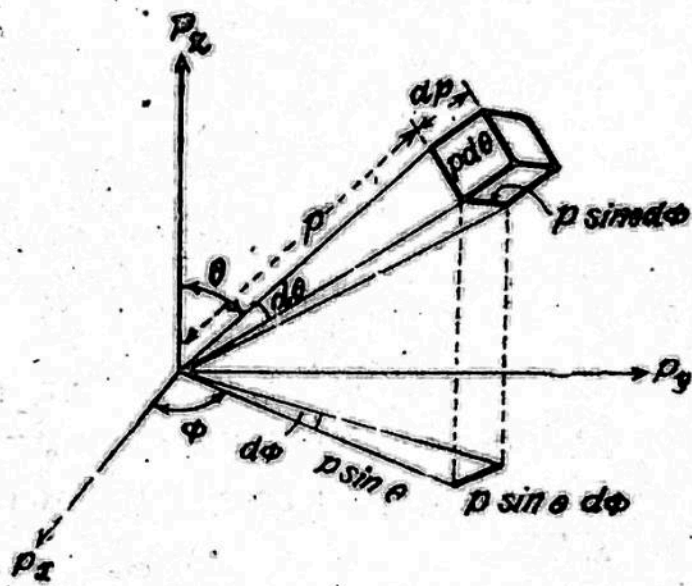


Fig. 2.

The volume of the element is given by

$$\begin{aligned} d\tau_p &= dp \cdot p d\theta \cdot p \sin \theta d\phi \\ &= p^2 dp \sin \theta d\theta d\phi \end{aligned} \quad \dots(1)$$

Again, the volume of momentum space lying between p and $p+dp$ and independent of direction is given by

$$\Delta\tau_p = p^2 dp \cdot \int_0^\pi \sin \theta d\theta \cdot \int_0^{2\pi} d\phi = 4\pi p^2 dp. \quad \dots(2)$$

This volume is the same as the volume of a spherical shell of thickness dp lying between p and $p+dp$.

Now we shall express the volume of phase space $\Delta\tau$ in terms of a volume $\Delta\tau_p$ of momentum space and the volume V of ordinary space. The relationship is given by

$$\Delta\tau = 4\pi p^2 dp \int_V dx dy dz$$

or

$$\Delta\tau = 4\pi p^2 dp \cdot V \quad \dots(3)$$

The element of phase space can also be expressed in terms of kinetic energy. We know that $\epsilon = p^2/2m$, where m is the mass of the particle

$$\therefore p = \sqrt{2m\epsilon} \text{ and } dp = (m/2\epsilon)^{1/2} d\epsilon$$

Substituting these values in equation (3), we get

$$d\tau = 4\pi (2m\epsilon) \left(\frac{m}{2\epsilon}\right)^{1/2} d\epsilon.V$$

or

$$d\tau = 2\pi (2m)^{3/2} \epsilon^{1/2} d\epsilon.V$$

..(4)

***** For the phase space representing a single particle of mass m in volume V , calculate the number of phase cells in energy range E to $E + \delta E$. Given that volume of each phase cell is h^3 . What will be the number of microstates in this energy range?

(Bohll: band 1993, 77; Agra 79; Lucknow 81)

Ans: Consider a region of phase space having momentum between p and $p + dp$ in the energy range E and $E + dE$.

For a single particle we have six dimensional phase space. Three position co-ordinates q_x, q_y, q_z and three momentum co-ordinates p_x, p_y, p_z specify the microstate of a particle in the phase space. An element of volume in the phase space is

$$\delta q_x \delta q_y \delta q_z \delta p_x \delta p_y \delta p_z = h^3 \quad (\text{since } h = \delta p_i \delta q_i)$$

The total volume of the phase space is

$$\iiint \iiint \iiint dq_x dq_y dq_z dp_x dp_y dp_z$$

where the limits of integration are to be specified.

$$\text{We have } \iiint dq_x dq_y dq_z = \iiint dx dy dz = \text{given volume } V$$

$$\text{So the volume of phase space} = V \iiint dp_x dp_y dp_z$$

Volume of momentum space containing momentum between p and $p+dp$ will be given by the volume of a spherical shell of radius p and thickness dp

$$\text{Therefore } \iiint dp_x dp_y dp_z = 4\pi p^2 dp$$

If energy corresponding to momentum p is ϵ , then

$$\begin{aligned} p^2 &= 2m\epsilon \text{ or } p = \sqrt{2m\epsilon} \\ \therefore dp &= \sqrt{2m} \cdot \frac{1}{2} \epsilon^{-1/2} d\epsilon \\ &= \sqrt{\left(\frac{m}{2\epsilon}\right)} d\epsilon \end{aligned}$$

Therefore volume of phase space

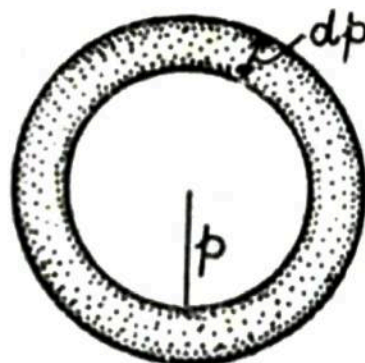
$$\begin{aligned} &= V \cdot 4\pi (2m\epsilon) \sqrt{m/2\epsilon} d\epsilon \\ &= 4\sqrt{2} \pi V m^{3/2} \epsilon^{1/2} d\epsilon \end{aligned}$$

$\therefore$ The number of cells in the phase space

$$\phi(\epsilon) d\epsilon = \frac{4\sqrt{2} \pi V}{h^3} m^{3/2} \epsilon^{1/2} d\epsilon$$

For a single particle the number of accessible microstates will be equal to the number of cells in the phase space. Therefore, the number of microstates in this energy range ϵ to $\epsilon+\delta\epsilon$ is given by

$$\phi(E) d\epsilon = \frac{4\sqrt{2} \pi V}{h^3} m^{3/2} \epsilon^{1/2} d\epsilon$$



Ensembles:

A system is defined as a collection of a number of particles. An ensemble is defined as a collection of a large number of microscopically identical but essentially independent systems. By the term *macroscopically identical* we mean that each of the systems constituting an ensemble satisfies the same macroscopic conditions e.g., volume, energy, pressure, total number of particles, etc. By the term *independent systems* we mean that the systems constituting an ensemble are mutually non-interacting. In an ensemble the systems play the same role as the non-interacting molecules do in a gas. The macroscopic identity of the systems constituting an ensemble may be achieved by choosing the same values of some set of macroscopic parameters which uniquely determine the equilibrium state of the system. Accordingly there may be many types of ensembles, out of them the most widely used are the microcanonical, canonical and grand canonical ensembles.

Microcanonical ensemble. It is the collection of a large number of essentially independent systems having the same energy E , volume V and the number of particles N . For simplicity we assume that all the particles are identical. The individual systems of a microcanonical ensemble are separated by rigid, impermeable and well insulated walls (Fig. 3-1) such that the values of E , V and N for a particular system are not affected by the presence of other systems.

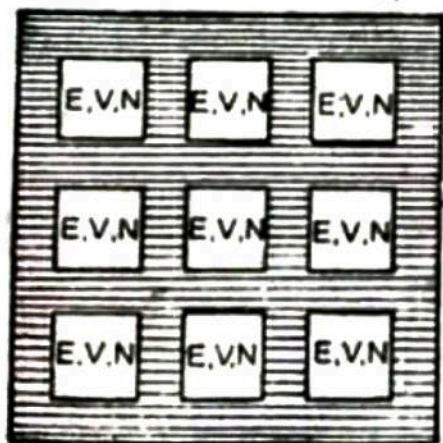


Fig. 3-1

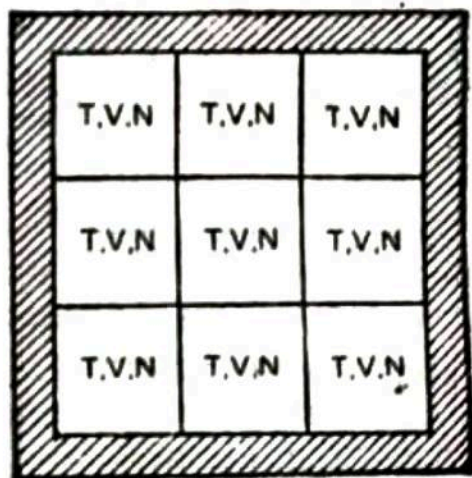


Fig. 3-2

Canonical ensemble It is the collection of a large number of essentially independent systems having the same temperature T , volume V and the same number of identical particles N . The equality of temperature of all the systems can be achieved by bringing each in thermal contact with a large heat reservoir at constant temperature T or bringing all of the systems in thermal contact with one another. The individual systems of a canonical ensemble are separated by rigid, impermeable but conducting walls.

As the separating walls are conducting, heat can be exchanged between the systems. As a result all the systems will arrive at the common temperature T .

Grand-canonical ensemble. It is the collection of a large number of essentially independent systems having the same temperature T , volume V and chemical potential μ . The individual systems of a grand canonical ensemble are separated by rigid, permeable and conducting walls (Fig. 3.3). As the separating walls are conduction and permeable, the exchange of heat energy as well as that of particles between the systems takes place in such a way that all the systems arrive at common temperature T and chemical potential μ . The detailed information regarding the characteristics of these ensembles can be had after a complete study of Liouville's theorem.

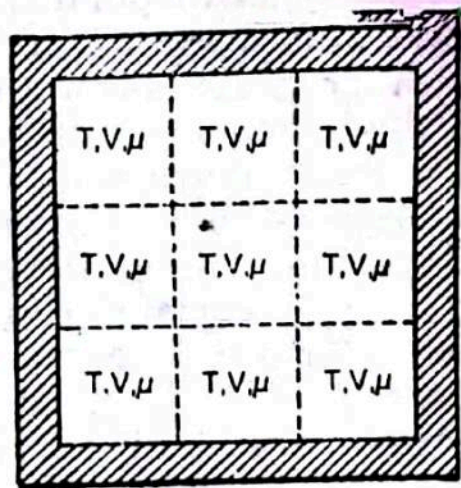


Fig. 3-3

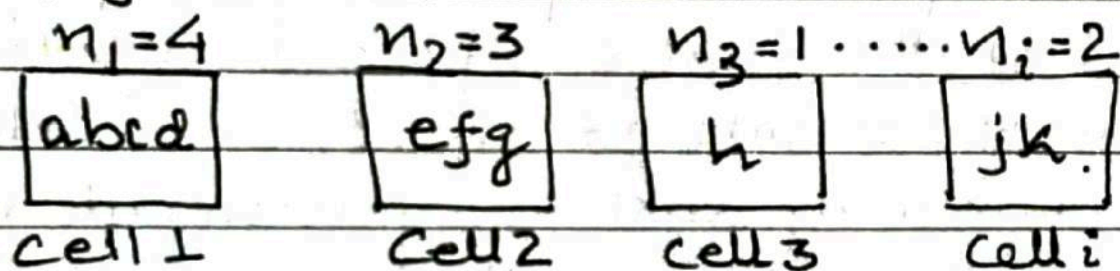
Microstates and Macrostates:

Let us consider an ensemble consisting of a large number of independent systems or a gas consisting of a large number of molecules, in the phase space. Each system or molecule may be represented by a point known as phase point or representative point in the phase space. Let the phase space be divided into cells numbered $1, 2, 3, \dots, i$ etc. A phase point for any system or molecule may reside in one of these cells.

- A microstate of the ensemble may be defined by the specification of the individual position of phase points for each system or molecule of the ensemble. Thus in a microstate we have to state to which cell each system or molecule belongs temporarily.
- A macrostate of the ensemble may be defined by the specification of phase points in each cell, i.e., specifying the numbers only and overlooking the

identities of the systems or molecules.

Let there are cell 1, cell 2, cell 3, ..., cell i in phase space. Consider there are four phase points $abcd$ in cell 1, three phase points efg in cell 2, one phase point h in cell 3 and two phase points jk in cell i as shown in below:



[Cells in phase space]

The macrostate of figure is specified by only giving the ^{number of} phase points $n_1=4$, $n_2=3$, ..., $n_i=2$ of different cells.

This also represents a particular microstate by specifying the positions of phase points $abcd$ in cell 1, efg in cell 2 and so on.

Maxwell-Boltzmann Distribution Law

Consider a system of N distinguishable molecules of a gas. Suppose n_1 of them have energy E_1 , n_2 have energy E_2 , ... n_i have energy E_i and so on. Thus the entire assembly of molecules can be divided into different energy states with energies $E_1, E_2, E_3, \dots, E_i$ and having $n_1, n_2, n_3, \dots, n_i$ molecules.

(1) The total number of molecules N is constant. Hence

$$N = n_1 + n_2 + n_3 + \dots + n_i + \dots = \text{constant}$$

$$\text{or } \delta N = \delta n_1 + \delta n_2 + \delta n_3 + \dots + \delta n_i + \dots = 0$$

$$\text{i.e., } \sum_i \delta n_i = 0 \quad \dots(1)$$

(2) The total energy E of the gas molecules is constant. Hence

$$E = E_1 n_1 + E_2 n_2 + E_3 n_3 + \dots + E_i n_i + \dots = \text{constant}$$

$$\text{or } \delta E = E_1 \delta n_1 + E_2 \delta n_2 + E_3 \delta n_3 + \dots + E_i \delta n_i + \dots = 0$$

$$\text{i.e., } \sum_i E_i \delta n_i = 0 \quad \dots(2)$$

(3) Suppose there are g_i cells with the energy E_i . The total number of ways in which n_i molecules can have the energy E_i is $(g_i)^{n_i}$. Hence the total number of ways in which N molecules can be distributed among the various energies is

$$W_1 = (g_1)^{n_1} (g_2)^{n_2} (g_3)^{n_3} \dots (g_i)^{n_i} \dots$$

The number of ways in which the groups of $n_1, n_2, n_3 \dots n_i \dots$ particles can be chosen from N particles is given by

$$W_2 = \frac{N!}{n_1! n_2! n_3! \dots}$$

The number of distinguishable ways in which N molecules can be distributed among the possible energy levels is

$$W = W_1 W_2 = \frac{N!}{n_1! n_2! n_3! \dots} (g_1)^{n_1} (g_2)^{n_2} (g_3)^{n_3} \dots = \frac{N!}{\prod_i \frac{n_i!}{g_i^{n_i}}}$$

The quantity W is called the *thermodynamic probability* for the system. For the most probable distribution, W is a maximum subject to the restriction that the total number of particles N and the total energy E are constants.

The natural logarithm of Eq. (3) is

$$\ln W = \ln N! - \sum \ln n_i! + \sum n_i \ln g_i$$

By Stirling's theorem, $\ln n! = n \ln n - n$ ✓

$$\ln W = N \ln N - N - \sum n_i \ln n_i + \sum n_i + \sum n_i \ln g_i$$

$$\ln W = N \ln N - \sum n_i \ln n_i + \sum n_i \ln g_i$$

$$\therefore \sum n_i = N \quad \dots(4)$$

From Eq. (4), we have for maximum W

$$\delta \ln W_{\max} = - \sum n_i \frac{1}{n_i} \delta n_i - \sum (\ln n_i) \delta n_i + \sum (\ln g_i) \delta n_i = 0$$

$$\text{or } - \sum (\ln n_i) \delta n_i + \sum (\ln g_i) \delta n_i = 0 \quad [\because \sum \delta n_i = 0] \quad \dots(5)$$

Eqs. (1) and (2) can be incorporated into Eq. (5) by making use of Lagrange's method of undetermined multipliers. Multiplying Eq. (1) by $-\alpha$ and Eq. (2) by $-\beta$ and adding to Eq. (5), we get

$$\sum (-\ln n_i + \ln g_i - \alpha - \beta E_i) \delta n_i = 0 \quad \dots(6)$$

$$\text{or } -\ln n_i + \ln g_i - \alpha - \beta E_i = 0 \quad \dots(7)$$

$$\text{or } \boxed{n_i = g_i e^{-\alpha} e^{-\beta E_i}} \quad \dots(7)$$

Eq. (7) is called Maxwell-Boltzmann distribution law.

M-B distribution in terms of temperature. It can be shown that $\beta = 1/kT$ where k = Boltzmann's constant and T = absolute temperature of the gas.

$$\therefore n_i = g_i e^{-\alpha} e^{-(E_i/kT)} \quad \dots(8)$$

Partition Function and its Relation with Thermodynamic Quantities:

(a) Partition Function (Z)

Let us consider an assembly of ideal gas molecules obeying classical statistics i.e., Maxwell-Boltzmann distribution law.

Using this distribution law, let n_i molecules occupy i^{th} state with energy between E_i and $E_i + dE_i$ and degeneracy g_i , then

$$\begin{aligned} n_i &= g_i e^{-\alpha} e^{\frac{-E_i}{kT}} \\ &= g_i A e^{-\beta E_i} \end{aligned} \quad \dots(i)$$

where $A = e^{-\alpha}$ and $\beta = \frac{1}{kT}$

So the total number of molecules in the system.

$$N = \sum_i n_i$$

$$= A \sum_i g_i e^{-\beta E_i}$$

$$\therefore \frac{N}{A} = \sum_i g_i e^{-\beta E_i} = Z \quad \dots(ii)$$

where Z is called the Boltzmann's partition function or simply the partition function. The term

$\sum_i g_i e^{-\beta E_i}$ represents the sum of all the $g_i e^{-\beta E_i}$ terms for every energy state of the given molecules. Consequently, the quantity Z indicates that how the gas molecules of a system are distributed or partitioned among the various energy levels and hence is called a partition function.

Thus,

$$\text{Partition function, } Z = \sum_i g_i e^{-\beta E_i} \quad \dots(10.60)$$

Taking $\sum_i g_i = 1$, we may write $Z = \sum_i e^{-\beta E_i}$

9.3 SYMMETRICAL AND ANTISYMMETRIC WAVE FUNCTIONS

The Schroedinger equation for n identical particles is written as

$$H(1, 2, \dots, n) \psi(1, 2, \dots, n, t) = i\hbar \frac{\partial}{\partial t} \psi(1, 2, \dots, n, t), \quad \dots(1)$$

where each of the numbers represents all the coordinates (positional and spin) of one of the particles. The Hamiltonian H is symmetrical in its arguments due to the identity of particles. The identity of particles means that they can be substituted for each other without changing H or indeed any other observable.

There are two kinds of solutions of wave function ψ of eqn. (1) that have symmetric properties of particular interest.

✓ (i) **Symmetric wave function ψ_s** : *A wave function is symmetric if the interchange of any pair of particles among its arguments leave the wave function unchanged.*

✓ (ii) **Antisymmetric wave function ψ_A** : *A wave function is antisymmetric if the interchange of any pair of particles among its arguments changes the sign of the wave function.*

If P is an exchange operator, then we must have

$$P\psi_s(1, 2) = \psi_s(2, 1).$$

$$P\psi_A(1, 2) = -\psi_A(2, 1).$$

* Bosons and Fermions:

1. The identical particles having an integral spin quantum number are described by symmetric wave function, *i.e.*,

$$P\psi_s(1, 2, 3, \dots, r, \dots, s, \dots, n) = +\psi_s(1, 2, 3, \dots, s, \dots, r, \dots, n)$$

This class of particles, *i.e.* the particles described by symmetric wave functions are known as Bose particles or Bosons and obey Bose-Einstein Statistics. The examples of Bosons are photons (spin 1), neutral helium atoms in normal state ($s = 0$) etc.

2. The identical particles having half odd integral spin quantum number are described by antisymmetric wave functions, *i.e.*

$$P\psi_A(1, 2, \dots, r, \dots, s, \dots, n) = -\psi_A(1, 2, \dots, s, \dots, r, \dots, n)$$

This class of particles *i.e.* the particles described by antisymmetric wave function obey Fermi-Dirac statistics and the particles are known as Fermi-particles or Fermions. The examples of Fermions are electrons, protons, neutrons, muons (all spin $\frac{1}{2}$).

Bose-Einstein Distribution Law

Bose used Planck's hypothesis, according to which radiation in a temperature enclosure is composed of light quanta known as photons, each of energy, $E = h\nu$. These photons in the enclosure are indistinguishable.

Basic Postulates :

In Bose-Einstein statistics, the conditions are:

1. The particles of the system are identical and indistinguishable.
2. Any number of particles can occupy a single cell in the phase space.
3. The size of the cell cannot be less than h^3 , where h is a Planck's constant ($h = 6.63 \times 10^{-34}$ Joule. sec).
4. The number of phase space cells is comparable with the number of particles, *i.e.*, the occupation index $f(E_i)$ is $\frac{n_i}{g_i} \approx 1$.
5. Bose-Einstein statistics is applicable to particles with integral spin angular momentum in units of $\frac{h}{2\pi}$. All particles which obey *B.E.* statistics are known as Bosons.

BOSE-EINSTEIN DISTRIBUTION LAW

Consider an assembly of N bosons. They are identical and indistinguishable. No restriction is imposed as to the number of particles that may occupy a given cell. Let us now consider a box divided into g_i sections by $(g_i - 1)$ partitions and n_i indistinguishable particles to be distributed among these sections. The permutations of n_i particles and $(g_i - 1)$ partitions simultaneously is given by $(n_i + g_i - 1)!$. But this includes also the permutations of n_i particles among themselves and also $(g_i - 1)$ partitions among themselves, as both these groups are internally indistinguishable. Hence, the actual number of ways in which n_i particles are to be distributed in g_i sublevels is

$$\frac{(n_i + g_i - 1)!}{n_i! (g_i - 1)!},$$

Therefore, the total number of distinguishable and distinct ways of arranging N particles in the variable energy states is given by

$$W = \prod \frac{(n_i + g_i - 1)!}{n_i! (g_i - 1)!}, \quad \dots(1)$$

n_i and g_i are large numbers. Hence we may neglect 1 in the above expression.

$$W = \prod \frac{(n_i + g_i)!}{n_i! g_i!}, \quad \dots(2)$$

$$\ln W = \sum [\ln (n_i + g_i)! - \ln n_i! - \ln g_i!].$$

As n_i and g_i are large numbers, we can use Stirling approximation.

$$\ln W = \sum (n_i + g_i) \ln (n_i + g_i) - n_i \ln n_i - g_i \ln g_i. \quad \dots(3)$$

Here, g_i is not subject to variation and n_i varies continuously.

For most probable distribution, $\delta \ln W_{\max} = 0$.

Hence, if the W of Eq. (3) represents a maximum,

$$\delta \ln W_{\max} = \sum [\ln (n_i + g_i) - \ln n_i] \delta n_i = 0 \quad \dots(4)$$

The total number of particles and total energy are constants.

$$\sum \delta n_i = 0 \quad \dots(5)$$

$$\sum E_i \delta n_i = 0 \quad \dots(6)$$

Multiplying Eq. (5) by $-\alpha$, Eq. (6) by $-\beta$ and adding to Eq. (4),

$$\sum [\ln (n_i + g_i) - \ln n_i - \alpha - \beta E_i] \delta n_i = 0$$

The variations δn_i are independent of each other. Hence we get

$$\ln \left(\frac{n_i + g_i}{n_i} \right) - \alpha - \beta E_i = 0$$

or

$$n_i = \frac{g_i}{(e^{\alpha + \beta E_i}) - 1} \quad \dots(7)$$

or

$$n_i = \frac{g_i}{(e^{\alpha} e^{E_i/kT}) - 1} \quad \dots(8)$$

This is called Bose-Einstein distribution law.

43.8 FERMI-DIRAC DISTRIBUTION LAW

F-D statistics is obeyed by indistinguishable particles of half-integral spin (that have antisymmetric wave functions and obey Pauli exclusion principle). Consider N fermions with the total energy E , in which the i^{th} particle occupy the first energy level with energy E_1 , E_2 particles occupy the second energy level with energy E_2 and so on. Let g_i be the total number of states in which n_i particles can be distributed in g_i cells having the same energy E_i .

The number of distinguishable arrangements of n_i particles in g_i cells is

$$\frac{g_i!}{n_i!(g_i - n_i)!}$$

The total number of Eigen states for the whole system is given by

$$W = \prod_i \frac{g_i!}{n_i!(g_i - n_i)!} \quad (1)$$

Taking the natural logarithm of both sides,

$$\ln W = \sum [\ln g_i! - \ln n_i! - \ln (g_i - n_i)!]$$

Applying Stirling's approximation,

$$\ln W = \sum [g_i \ln g_i - g_i - n_i \ln n_i + n_i - (g_i - n_i) \ln (g_i - n_i) + (g_i - n_i)] \quad (2)$$

$$\ln W = \sum [g_i \ln g_i - n_i \ln n_i - (g_i - n_i) \ln (g_i - n_i)] \quad (2)$$

Here g_i is not subject to variation and n_i varies continuously.

For most probable distribution, $\delta \ln W_{\max} = 0$.

$$\delta \ln W_{\max} = \sum [-\ln n_i + \ln (g_i - n_i)] \delta n_i = 0 \quad (3)$$

$$\text{But} \quad \sum \delta n_i = 0 \quad (4)$$

$$\text{and} \quad \sum E_i \delta n_i = 0 \quad (5)$$

Multiplying Eq. (4) by $-\alpha$, Eq. (5) by $-\beta$ and adding to Eq. (3),

$$\sum [-\ln n_i + \ln (g_i - n_i) - \alpha - \beta E_i] \delta n_i = 0$$

As the variations δn_i are independent of each other, we get

$$\ln \left(\frac{g_i - n_i}{n_i} \right) - \alpha - \beta E_i = 0$$

$$\text{or} \quad n_i = \frac{g_i}{e^{\alpha} e^{\beta E_i} + 1} \quad (6)$$

This is known as Fermi-Dirac Distribution law.

$\beta = 1/kT$ and $\alpha = -E_F/kT$ where E_F is called Fermi energy, $E_i = -akT$.

$$n_i = \frac{g_i}{e^{(E_i - E_F)/kT} + 1} \quad (7)$$

Definition of Fermi energy : It is the absolute zero of temperature the maximum kinetic energy that a free electron can have is called the Fermi energy, E_F .

$$n_i = \frac{g_i}{e^{(E_i - E_F)/kT} + 1}$$

Comparison of the Three Statistics

<i>Maxwell-Boltzmann</i>	<i>Bose-Einstein</i>	<i>Fermi-Dirac</i>
1. Particles are distinguishable. 2. Only particles are taken into consideration. 3. There is no restriction on the number of particles in a given state. 4. Volume of the state in six dimensional space is not known. 5. Number of distinguishable ways are given by $W = \prod_i \frac{g_i^{n_i}}{n_i!}.$ 6. Maximum probability distribution $\frac{1}{e^{(\alpha + \beta E_i)}}.$ 7. _____	1. Particles are indistinguishable. 2. Only quantum states are taken into consideration. 3. There is no restriction on the number of particles in a given quantum state. 4. Phase space is known $V = h^3.$ 5. Number of distinguishable ways are given by $W = \prod_i \frac{(n_i + g_i - 1)!}{n_i! (g_i - 1)!}.$ 6. Maximum probability distribution $\frac{1}{[e^{(\alpha + \beta E_i)}] - 1}.$ 7. At high temperatures, Bose-Einstein distribution approaches Maxwell-Boltzmann distribution.	1. Particles are indistinguishable. 2. Only quantum states are taken into consideration. 3. There is restriction on the number of particles in a given quantum state. 4. Phase space is known $V = h^3.$ 5. Number of distinguishable ways are given by $W = \prod_i \frac{g_i^{n_i}}{n_i! (g_i - n_i)!}.$ 6. Maximum probability distribution $\frac{1}{[e^{(\alpha + \beta E_i)}] + 1}.$ 7. At high temperatures, Fermi-Dirac distribution approaches Maxwell-Boltzmann distribution.

<i>Maxwell-Boltzmann</i>	<i>Bose-Einstein</i>	<i>Fermi-Dirac</i>
8. Applicable to ideal gas molecules. 9. Internal energy of an ideal monatomic gas depends only on its temperature. At absolute zero, energy is <u>zero</u>.	8. Applicable to photons and symmetrical particles <u>known as bosons</u>. 9. The energy at absolute zero is <u>taken to be zero</u>.	8. Applicable to electrons and antisymmetric particles <u>known as fermions</u>. 9. Due to Pauli's exclusion principle, all the electrons cannot occupy the lowest energy level. <u>Every absolute zero temperature, some of the electrons are distributed at higher energy levels</u>. Hence, <u>at absolute zero, the energy is not zero</u>. Therefore, at the complete degenerate state, the energy is in dependent of temperature.
10. $n_i = \frac{g_i}{e^{(\alpha + \beta E_i)}}$	10. $n_i = \frac{g_i}{[e^{(\alpha + \beta E_i)} - 1]}$	10. $n_i = \frac{g_i}{[e^{(\alpha + \beta E_i)} + 1]}$
11. All the three distributions can be represented by a single equation $\frac{g_i}{n_i} = [e^{(\alpha + \beta E_i)} + \delta]$ Here $\delta = 0$ Here $\delta = -1$ Here $\delta = +1$ If $\frac{g_i}{n_i} \geq 1$ or $n_i \leq g_i$, i.e. δ can be neglected. In the case of diluted systems, the three statistics lead practically to similar results. It means that at high temperatures, the three statistics give practically the same results.		

12.16. Difference between Classical and Quantum Statistics

The main points of difference between classical and quantum statistics are :

- Classical statistics is applied to a system of identical particles which obey the laws of classical mechanics, whereas quantum statistics is applied to a system of identical particles which obey the laws of quantum mechanics.
- In classical statistics the particles of the system are considered *distinguishable*, whereas in quantum statistics these are considered *indistinguishable*.
- In classical statistics the volume of the elementary cell in the phase space can be made as small as we please whereas in quantum statistics its value cannot be less than h^3 , where h is Planck's constant, given by 6.63×10^{-34} Joules second. In other words, the number of cells in the phase space can be made as large as we like in classical statistics but this is not so in quantum statistics.