

## MODERN PHYSICS

### 1) State Planck's quantum hypothesis.

Max Planck postulated the following assumptions.

i) the atomic oscillator in a body cannot have any arbitrary amount of energy. They have only discrete units of energy  $E_n = n h \nu$  where  $n$  is quantum number that can take only positive integer values  $n = 1, 2, 3, \dots$ ;  $\nu$  is the frequency of the oscillator and  $h$  is Planck's constant  $h = 6.62 \times 10^{-34}$  Joules-sec. This equation shows that the oscillator energy is quantized.

ii) The atoms absorb or emit energy when they move from one quantum state to the other in indivisible discrete units. The amount of radiation energy in each unit is called a 'quantum' of energy of radiation of that frequency. Each quantum carries an energy  $E = h \nu$

The energy of each quantum is the smallest quantity of energy of radiation of that frequency. The energy of an oscillator changes only by multiples of  $h \nu$ . The hypothesis that radiation energy is emitted or absorbed in a discontinuous manner and in the form of quantum is called 'Planck's hypothesis'.

### 2) State the de-Broglie concept of matter waves

Electromagnetic radiation displays a dual character, behaving as a wave and a particle. Louis de Broglie in 1923 extended the wave-particle dualism to all fundamental particles such as electrons, protons, neutrons, atoms and molecules etc..

**According to de Broglie hypothesis, a moving particle is associated with a wave which is known as de Broglie wave or a matter wave. These waves are associated with particles like electrons, protons, neutrons etc. The wavelength of the matter wave is given by**

$$\lambda = h / p = h / m v$$

**where  $m$  is the mass of the particle,  $v$  its velocity and  $p$  its momentum.  $h$  is called Planck's constant given by  $6.63 \times 10^{-34}$  J-sec.**

Considering the Planck's quantum theory of radiation, the energy of a photon (quantum) is given by  $E = h \nu = h c / \lambda$  .....(1)

where  $c$  is the velocity of light,  $\nu$  is the frequency and  $\lambda$  its wavelength. The radiation interacts with matter in the form of photons or quanta. Thus the radiation behaves like a particle..

According to Einstein's mass-energy relation  $E = m c^2$  .....(2)

From eqns (1) and (2),  $m c^2 = h c / \lambda$  or  $\lambda = h / m c = h / p$

$p$  is the momentum associated with the photon. If we consider the case of a material particle of mass  $m$  and moving with a velocity  $v$  i.e., momentum  $m v$ , then the wavelength associated with this particle is

$$\lambda = h / p = h / m v$$

If  $E$  is the kinetic energy of the material particle, then  $E = m v^2 / 2 = p^2 / 2m$  or  $p = \sqrt{2mE}$

Therefore the de Broglie wavelength of a material particle moving with momentum  $p$  is given by

$$\lambda = h / \sqrt{2mE}$$

In the case of electrons accelerated by a potential  $V$  volts from rest to velocity  $v$ , the  $E = V e$  or

$$\lambda = h / \sqrt{2 m_0 V e}$$

Because of the smallness of  $h$ , we observe the wave nature only for particles of atomic or nuclear size. For ordinary objects the de Broglie wavelength is very small and so it is not possible to observe wave nature of these macroscopic objects.

**For electrons, the de-Broglie wavelength  $\lambda = 12.26 / \sqrt{V}$  Å**

### 3) Write a note on de-Broglie concept of matter waves

Electromagnetic radiation displays a dual character, behaving as a wave and a particle.

Louis de Broglie in 1923 extended the wave-particle dualism to all fundamental particles such as electrons, protons, neutrons, atoms and molecules etc..

According to de Broglie hypothesis, a moving particle is associated with a wave which is known as de Broglie wave or a matter wave. These waves are associated with particles like electrons, protons, neutrons etc. The wavelength of the matter wave is given by

$$\lambda = h / p = h / mv$$

where 'm' is the mass of the particle, v its velocity and p its momentum. h is called Planck's constant given by  $6.63 \times 10^{-34}$  J-sec

Because of the smallness of h, we observe wave nature for only particles of atomic or nuclear size. For ordinary objects the de Broglie wavelength is very small and so it is not possible to observe wave nature of these macroscopic objects.

### Properties of de-Broglie waves or matter waves

i) Matter waves consists of group of waves or a wave packet each having the wavelength  $\lambda$ , is associated with the particle. **This group travels with the particle velocity v**

ii) Each wave of the group of matter waves travels with a velocity known as phase velocity of the wave  $v_{\text{phase}} = c^2 / v$  is greater than c

iii) Lighter is the particle, greater is its wavelength. Smaller is the velocity, greater is the wavelength associated with it. When  $v = 0$  then  $\lambda = \infty$  which means that the wave becomes indeterminate. This shows *that matter waves are generated by the motion of the particles.*

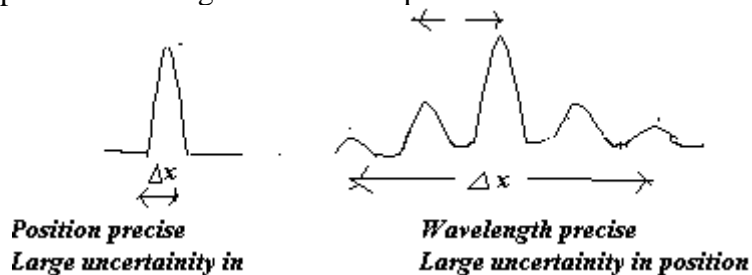
iv) The wave and particle aspects of a moving body can never appear together in the same experiment

v) The wave nature of matter introduces an uncertainty in the location of the particle because the wave is spread out in space.

### 5) State and explain Heisenberg's uncertainty principle

The concept of dual particle and wave nature of matter leads to another important principle called Heisenberg's Uncertainty principle. In wave mechanics the particle is described in terms of a wave packet and the particle may be found any where with in the wave packet at a given time.

The particle is located within the region  $\Delta x$ , the spread in the wave packet. Therefore there is an uncertainty  $\Delta x$  in the position of the particle. Further the wave packet is constituted by waves having a range of wavelengths. As the momentum of the particle is related to the wavelength ( $p = h / \lambda$ ), there arises an uncertainty in momentum  $\Delta p$ . The spread in wavelength  $\Delta \lambda$  is related to the spread in dimension  $\Delta x$ . The two uncertainties are interrelated because the spread in momentum depends on the spread in the length of the wave packet.



The narrower the wave packet, the more precisely a particle position can be specified. . However, the wavelength of the wave in a narrow packet is not well defined. This means that the particle's momentum  $p = h / \lambda$  is not a precise quantity. On the other hand, the uncertainty in the location of the particle is more in a wide wave packet but has a clearly well defined wavelength. The momentum that corresponds to this wavelength is therefore a precise quantity

Thus the certainty in position involves uncertainty in momentum and conversely certainty in momentum involves uncertainty in position. Thus we have the uncertainty principle proposed by Heisenberg in 1927. It is one of the most significant physical laws.

**Heisenberg's Uncertainty Principle:** It states that it is impossible to make simultaneous determination of the position and momentum of a particle precisely and that the product of the uncertainties in determining the position and momentum of a particle is approximately equal to Planck's constant  $h/2\pi$ .

Thus if  $\Delta x$  is the uncertainty in the determination of the position, and  $\Delta p$  is the uncertainty in the momentum, then according to Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta p \approx h/2\pi \quad (h = 6.63 \times 10^{-34} \text{ J}\cdot\text{sec})$$

Similarly, if we wish to measure the energy  $E$  emitted during the time interval  $\Delta t$  in an atomic process, then

$$\Delta E \cdot \Delta t \approx h/2\pi = 1.05 \times 10^{-34} \text{ J}\cdot\text{sec}$$

Thus, it is impossible to make a simultaneous determination of the energy and the time precisely and the product of the uncertainties in energy and time is greater than or equal to  $h$

## 6) Derive time independent and time-dependent Schrodinger wave equation

### Schrodinger's time independent wave equation :

According to de Broglie theory, a moving particle of mass  $m$  is always associated with a wave whose wavelength is given by  $\lambda = h/mv$ . If the particle has wave properties, it is expected that there should be some sort of wave equation which describes the behaviour of the particle. Consider a system of stationary waves associated with a particle. Let  $x, y, z$  be the coordinates of the particle and  $\psi$ , the wave displacement for the de Broglie wave at any time  $t$ . The classical differential equation of a wave motion is

$$\partial^2 \psi / \partial t^2 = v^2 (\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + \partial^2 \psi / \partial z^2) = v^2 \nabla^2 \psi \quad \dots\dots\dots(1)$$

where  $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$  is a Laplacian operator and  $v$  is the velocity of the particle. The solution of Eqn (1) gives as a periodic displacement in terms of time  $t$

$$\psi(x, y, z, t) = \psi_0(x, y, z) e^{-i \omega t} \quad \dots\dots\dots(2)$$

where  $\psi_0(x, y, z)$  is the spatial dependent part and  $e^{-i \omega t}$  is the time dependent part of the wave function.  $\psi_0(x, y, z)$  gives the amplitude at the point considered and  $\omega = 2\pi\nu$  is the angular frequency of the matter wave

Eqn (2) can be expressed as  $\psi(r, t) = \psi_0(r) e^{-i \omega t}$

In a time independent Schrodinger eqn, the P.E of a particle does not depend explicitly on time. It means that the forces that act upon the particle and thereby the potential energy  $V$  changes with position of the particle only. In such cases, time parameter  $t$  is eliminated from the equation and the resultant equation is called time independent wave equation

Differentiating twice with respect to  $t$

$$\partial^2 \psi / \partial t^2 = -\omega^2 \psi_0(r) e^{-i \omega t} = -\omega^2 \psi$$

Substituting the value of  $\partial^2 \psi / \partial t^2$  in Eqn (1), we have

$$\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + \partial^2 \psi / \partial z^2 + (\omega^2 / v^2) \psi = 0 \quad \dots\dots\dots(3)$$

$$\text{But } \omega = 2\pi\nu = 2\pi v/\lambda \quad \text{Hence } \omega/v = 2\pi/\lambda \quad \dots\dots\dots(4)$$

Substituting the value of  $\omega/v = 2\pi/\lambda$  in Eqn (3), we have

$$\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + \partial^2 \psi / \partial z^2 + (4\pi^2 / \lambda^2) \psi = 0 \quad \dots\dots\dots(5)$$

From de-Broglie relation, a particle of mass  $m$  moving with a velocity  $v$  is associated with wave whose wavelength  $\lambda = h/mv$

$$\text{Eqn (5) can be written as } \partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2 + \partial^2 \psi / \partial z^2 + (4\pi^2 m^2 v^2 / h^2) \psi = 0$$

$$\text{or } \nabla^2 \psi + (4\pi^2 / h^2) m^2 v^2 \psi = 0 \quad \dots\dots\dots(6)$$

If  $E$  and  $V$  are the total and potential energy of the particle respectively, then its

$$\text{K.E} = \frac{1}{2} mv^2 = E - V$$

$$m^2 v^2 = 2m (E - V)$$

Substituting this in Eqn (6)

$$\nabla^2 \psi + (4\pi^2 / h^2) 2m (E - V) \psi = 0$$

$$\text{or } \nabla^2 \psi + (8\pi^2 m / h^2) (E - V) \psi = 0 \dots\dots\dots(7)$$

**Eqn (7) is known as Schrodinger time independent wave equation.**

$$\text{Substituting } h = h / 2\pi . \text{ Eqn (7) is } \nabla^2 \psi + (2m / h^2) (E - V) \psi = 0$$

**For a free particle , potential energy  $V = 0$ . Hence the Schrodinger's time independent wave equation for a free particle can be expressed as**

$$\nabla^2 \psi + (8\pi^2 mE / h^2) \psi = 0$$

### **Schrodinger time - dependent wave equation:**

In time dependent Schrodinger wave Eqn., the P.E of a moving particle is both a function of time as well as the position of the particle. The Schrodinger time dependent wave equation may be obtained from Schrodinger time independent wave Eqn by eliminating E.

Differentiating  $\psi(r, t) = \psi_0(r) e^{-i \omega t}$  with respect to t

$$(\partial \psi / \partial t) = -i \omega \psi_0(r) e^{-i \omega t} = -i (2\pi \nu) \psi = -i (2\pi \nu) \psi$$

$$\text{or } (\partial \psi / \partial t) = -i (2\pi \nu) \psi = -i (E / h) \psi \quad (\text{since } E = h \nu)$$

$$\text{or } E\psi = -i (h / i) (\partial \psi / \partial t) = (i^2 h / i) (\partial \psi / \partial t) = i h (\partial \psi / \partial t)$$

Substituting the value of  $E\psi$  in the Schrodinger's time independent wave equation, we get

$$\nabla^2 \psi + (2m / h^2) [i h (\partial \psi / \partial t) - V\psi] = 0$$

$$\nabla^2 \psi = - (2m / h^2) [i h (\partial \psi / \partial t) - V\psi] = 0$$

$$-(h^2 / 2m) \nabla^2 \psi + V\psi = i h (\partial \psi / \partial t) \dots\dots \text{Schrodinger time-dependent Eqn } \dots\dots(8)$$

Eqn (8) can be written as

$$[(-h^2 / 2m) \nabla^2 + V]\psi = i h (\partial \psi / \partial t)$$

$$\text{or } H\psi = E\psi \dots\dots\dots(9)$$

where  $H = [(-h^2 / 2m) \nabla^2 + V]$  is called the **Hamiltonian operator** and  $E = i h (\partial / \partial t)$

Eqn (9) represents the motion of a material particle in terms of Hamiltonian operator

### **7) Write the physical significance the wave function $\Psi$**

Schrodinger introduced a quantity  $\Psi(x, t)$  that he called a 'wave function'. **The varying quantity that describes a matter wave is called the 'wave function'  $\Psi(x, t)$**

The wave function  $\Psi(x, t) = \psi_0 e^{-i \omega t}$  has no direct physical meaning since  $\Psi(x, t)$  is a complex quantity.. The physical interpretation of the wave function was given the German physicist Max Born. **The square of the absolute value of the wave function  $|\Psi|^2$  or  $\Psi\Psi^*$  ( $\Psi^*$  is the complex conjugate of  $\Psi$ ) is called the probability density. The product  $\Psi\Psi^*$  is a measure of the probability of finding the particle at that point at that time .**

$$P(x) = \Psi\Psi^* = |\Psi|^2$$

**Even though the wave function  $\Psi(x, t)$  is usually complex, the probability density will always be a real number ( positive or zero ).** A large value of  $|\Psi|^2$  means a strong possibility of the particle's presence while a small value of  $|\Psi|^2$  means a slight possibility of its presence. As long as  $|\Psi|^2 \neq 0$ , there is a definite chance of the presence of the particle.  $\Psi\Psi^* dx$  gives probability that the particle will be found between  $x$  and  $x+dx$

$$\int_{-\infty}^{+\infty} \Psi\Psi^* dV = 1 \quad \text{is called the normalization condition. It means that the particle exists some where at all times in the universe}$$

$$\text{If } \int_{-\infty}^{+\infty} \Psi\Psi^* dV = 0, \text{ then the particle does not exist}$$

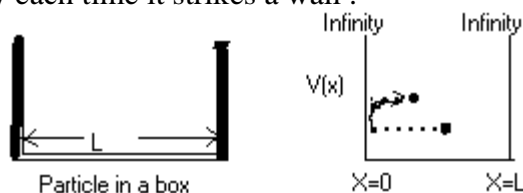
Besides being normalisable, the wave function should have the following properties:.

- i)  $\Psi$  must be single valued since  $\Psi\Psi^*$  can have only one value at a particular place and time
- ii)  $\Psi$  and its partial derivatives  $\partial\Psi/\partial x$ ,  $\partial\Psi/\partial y$  and  $\partial\Psi/\partial z$  must be continuous
- iii)  $\Psi$  must be finite for all values of  $x, y$  and  $z$

### 8) Give the quantum mechanical treatment of a particle in a box and hence obtain the expressions for energy eigen values and eigen functions of the particles .

Let us consider the application of Schrodinger's equation for a particle that is confined to a certain region of space instead of being able to move freely ( free particle but confined to certain region of space )

Consider a particle of mass  $m$  that can move only along the  $x$ -axis and bounces back and forth between the walls of a box. We shall assume that the walls of the box are infinitely hard, so the particle does not lose energy each time it strikes a wall .



The particle position at any instant is given by  $0 < x < L$  and the box is supposed to have walls of infinite height at  $x = 0$  and  $x = L$ . The walls of the box are infinite in height and rigid that the particle cannot penetrate or escape from the box. Since the particle is a free particle, the potential energy of the particle can be assumed to be zero between  $x = 0$  and  $x = L$ . and infinite at  $x = 0$  and  $x = L$ .. This situation is called '**particle in a box**'.

In terms of the boundary conditions imposed by the problem, the potential energy function  $V$  is

$$V = 0 \quad \text{for } 0 < x < L$$

Since the barrier or wall is infinitely tall, the particle cannot penetrate a wall. In such a case, the particle can rattle back rebounding from the wall. In quantum terms, the wave function  $\psi(x)$  is zero at the walls and at all points beyond the walls signifying that the probability of finding the particle in those locations is zero.

$$\psi(x) = 0 \quad \text{for } x \leq 0 \text{ and } x \geq L$$

Now we have to find out the magnitude of  $\psi$  between  $x = 0$  and  $x = L$  within the box.. The Schrodinger's Eqn in one dimension is

$$d^2\psi/dx^2 + (8\pi^2 m / h^2) (E - V) \psi = 0 \quad \dots\dots\dots(1)$$

Within the box, the potential energy  $V = 0$  and the Schrodinger's Eqn becomes

$$d^2\psi/dx^2 + (8\pi^2 m / h^2) E \psi = 0 \quad \text{or} \quad d^2\psi/dx^2 + (2m / h^2) E \psi = 0 \dots\dots\dots(2)$$

This is of the form  $d^2\psi/dx^2 + k^2 \psi = 0$  and the general solution of this equation is

$$A \sin kx + B \cos kx$$

where  $A$  and  $B$  are the constants which are to be evaluated using the boundary conditions imposed in the problem . The value of  $k^2 = 8\pi^2 m E / h^2$  and  $k = \sqrt{2mE} / h$ .

The solution to Eqn (2) is

$$\psi(x) = A \sin(\sqrt{2mE} / h)x + B \cos(\sqrt{2mE} / h)x \quad \dots\dots\dots(3)$$

**This solution is subject to the boundary conditions imposed in the problem;**

$$\psi(x) = 0 \quad \text{for } x = 0 \text{ and for } x = L$$

When  $x = 0$  ,the first term on RHS is zero and the second term reduces to  $B$  since  $\cos 0 = 1$ . This yields  $B = 0$  . Thus Eqn (3) reduces to

$$\psi(x) = A \sin(\sqrt{2mE} / h)x$$

$\psi(x)$  will be zero at  $x = L$  and the term on RHS will be zero only when

$$(\sqrt{2mE}/\hbar)L = n\pi \quad n=1,2,3 \dots \quad (4)$$

This result comes about because the sine of the angles  $\pi, 2\pi, 3\pi, 4\pi$  are all zero

### Eigen values and eigen functions of particle in a box:

From Eqn (4), it is clear that the energy of the particle can have only certain values. These eigen values constitute the energy of the particle of the system.

### The energy eigen values of the particle in a box are

$$E_n = n^2 \pi^2 \hbar^2 / 2mL^2 = n^2 \hbar^2 / 8mL^2 \quad n = 1,2,3,\dots \quad (5)$$

Since  $n$  can take only integer values, the energy is quantized.. The lowest energy state  $E_0$  corresponds to  $n = 1$ .

So  $E_0 = \pi^2 \hbar^2 / 2mL^2$  or  $E_0 = (\hbar^2 / 8mL^2)$ . This is called **zero point energy**

The allowed values of the energy states are  $E_1 = 4E_0$ ,  $E_2 = 9E_0$ ,  $E_3 = 16E_0$  and so on

$E_n$  depends on the values on  $n$ . Each value of  $E_n$  is called 'energy eigen value' or proper value. Since the energy is purely kinetic energy, that means only certain speeds are permitted for a particle

The wave function of a particle in a box whose energy is  $E_n$  is

$$\Psi_n = A \sin(\sqrt{2mE_n}/\hbar)x \quad (6)$$

Substituting for  $E_n$  from Eqn (5)

$$\Psi_n = A \sin(\sqrt{2m n^2 \pi^2 \hbar^2 / 2mL^2} / \hbar)x = A \sin(n\pi x / L) \quad (7)$$

$\Psi_n$  are called the 'eigen functions' corresponding to the energy eigen values  $E_n$ .

These wave functions meet all the requirements i) for each quantum number  $n$ , the wave function  $\Psi_n$  is single valued function of  $x$  and ii)  $\Psi_n$  and  $d\Psi_n/dx$  are continuous. Applying the normalization condition between  $x = 0$  and  $L$ , we have

$$\begin{aligned} \int_{-\infty}^{+\infty} |\Psi_n|^2 dx &= \int_0^L A^2 \sin^2(n\pi x/L) dx = A^2 \int_0^L (1/2) [1 - \cos 2(n\pi x/L)] dx \\ &= (A^2/2) [x - (L/2\pi n) \sin 2(n\pi x/L)]_0^L = (A^2/2)(L) = A^2 L / 2 \end{aligned}$$

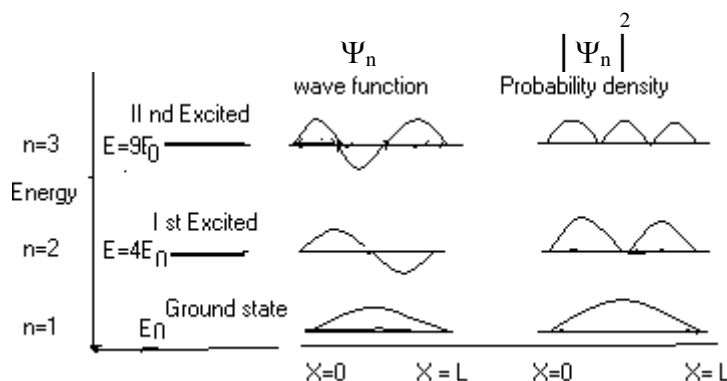
It is certain that the particle is somewhere inside the box. Hence for a normalized wave function

$$\int_0^L \Psi \Psi^* dx = \int_0^L |\Psi|^2 dx = 1 \quad \text{or} \quad A^2 L / 2 = 1 \quad \text{or} \quad A = \sqrt{2/L}$$

### The normalized wave functions of the particle in a box are

$$\Psi_n = \sqrt{2/L} \sin(n\pi x / L) \quad n = 1,2,3, \dots$$

The normalized wave functions  $\Psi_1, \Psi_2, \Psi_3 \dots$  with the probability densities  $|\Psi_1|^2, |\Psi_2|^2, |\Psi_3|^2$  are shown in Fig



While  $\Psi_n$  may be negative as well as positive,  $|\Psi_n|^2$  is always positive and since  $\Psi_n$  is normalized, its value at a given  $x$  is equal to the probability density  $P$  of finding the particle there. In every case  $|\Psi_n|^2 = 0$  at  $x = 0$  and  $x = L$ , the boundaries of the box.

We see that the lowest permitted energy of the particle is not zero but that corresponds to  $n=1$ . This lowest energy is called the **zero point energy** of the particle in the potential well

### 9) Distinguish between Maxwell-Boltzman, Bose-Einstein and Fermi-Dirac statistics

Maxwell-Boltzman	Bose – Einstein statistics	Fermi – Dirac statistics
Deals with a system of identical particles that are sufficiently far apart to be distinguishable	Deals with a system of identical particles that cannot be distinguished from one another	Deals with a system of identical particles that cannot be distinguished from one another
Deals with classical particles like molecules of a gas	Deals with <b>Bosons</b> such as photons, $\alpha$ - particles,	Deals with <b>Fermions</b> such as Electrons, protons , neutrons and neutrinos
Particles of any spin	Particles of integral spin $0 \text{ h}, 1 \text{ h}, 2 \text{ h}, 3 \text{ h}, \dots$	Particles of half-integral spin $\frac{1}{2} \text{ h}, (3/2) \text{ h}, (5/2) \text{ h} \dots$
No limit on the number of particles per state	Does not obey Pauli Exclusion Principle. No limit on the number of particles per state. The wave functions are symmetric to interchange of a pair of particles	Obeys Pauli Exclusion principle. Not more than one particle per quantum state. Wave functions are antisymmetric to interchange of pair of particles
$f_{MB} = A e^{-E/kT}$	$f_{BE} = 1 / (A e^{E/kT} - 1)$	$f_{FD} = 1 / [e^{(E - E_F)/kT} + 1]$