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## C14T ( Statistical Mechanics) , Topic :- Fermi- Dirac Statistics

### Fermi- Dirac Statistics

#### Basic features:

The basic features of the Fermi-Dirac statistics:

1. The particles are all identical and hence indistinguishable.
2. The fermions obey (a) the Heisenberg's uncertainty relation and also (b) the exclusion principle of Pauli.
3. As a consequence of 2(a), there exists a number of quantum states for a given energy level and because of 2(b) , there is a definite a priori restriction on the number of fermions in a quantum state; there can be simultaneously no more than one particle in a quantum state which would either remain empty or can at best contain one fermion.

If , again, the particles are isolated and non-interacting, the following two additional condition equations apply to the system:

$$\sum \partial N_i = 0 ; \sum \partial U = 0$$

#### ❖ Thermodynamic probability:

Consider an isolated system of N indistinguishable, non-interacting particles obeying Pauli's exclusion principle. Let  $N_1, N_2, N_3, \dots, N_i$  ...particles in the system have energies  $E_1, E_2, E_3, \dots, E_i$  ... respectively and let  $g_i$  denote the degeneracy  $E_i$ . So the number of distinguishable arrangements of  $N_i$  particles among  $g_i$  eigenstates in the  $i^{\text{th}}$  energy level is

$$W_i = \frac{g_i!}{N_i!(g_i - N_i)!} \quad \dots(1)$$

Therefore, the thermodynamic probability W, that is, the total number of eigenstates of the whole system is the product of  $W_i$  <sup>s</sup>

$$W = \sum_i^n \frac{g_i!}{N_i!(g_i - N_i)!} \dots\dots(2)$$

❖ **FD- distribution function : Most probable distribution :**

From eqn(2) above , taking logarithm and applying Stirling's theorem,

$$\begin{aligned} \ln W &= \sum [ \ln g_i! - \ln N_i! - \ln (g_i - N_i)! ] \\ &= \sum g_i \ln g_i - g_i - N_i \ln N_i + N_i - (g_i - N_i) \ln (g_i - N_i) + (g_i - N_i) \\ &= \sum g_i \ln g_i - N_i \ln N_i - (g_i - N_i) \ln (g_i - N_i) \end{aligned}$$

For this distribution to represent the most probable distribution , the entropy S or  $\ln W$  must be maximum, i.e.  $\partial S = 0$  or  $\partial \ln W = 0$  for small changes  $\partial N_i$  in of individual  $N_i$  's.

$$\partial \ln W_{max} = \sum [ -\ln N_i + \ln (N_i - g_i) ] \partial N_i = 0 \dots\dots(3)$$

Taking into account the conservation of particles and of energy,

$$\sum \partial N_i = 0 \quad (4)$$

$$\sum E_i \partial N_i = 0 \quad (5)$$

Multiplying eqn(4) by  $-\alpha$  and eqn(5) by  $-\beta$  and adding to eqn (3) , we get

$$\sum [ -\ln N_i + \ln (N_i - g_i) - \alpha - \beta E_i ] \partial N_i = 0 \quad (6)$$

Where  $-\alpha$  and  $-\beta$  are Langrange's undetermined multipliers.

Since the  $\partial N_i$ 's are now in effect independent, the expression in the bracket of eqn. (6) is zero for each value of  $i$ .

$$\begin{aligned} \therefore \ln \frac{g_i - N_i}{N_i} &= \alpha + \beta E_i \\ \Rightarrow \frac{g_i}{N_i} - 1 &= e^{\alpha + \beta E_i} \end{aligned}$$

$$\Rightarrow N_i = \frac{g_i}{e^{\alpha + \beta E_i} + 1} \quad (7)$$

The general form of FD- distribution function for an assembly of fermions among the various energy levels of a system.

It can be shown, as before , that  $\beta = \frac{1}{kT}$

$$\therefore f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{\alpha + \frac{E_i}{kT}} + 1} \quad (9)$$

Where  $f(E_i)$  is the occupation index of a state energy  $E_i$ , that is, the average number of particles in each of the quantum states of that energy. The right hand side of eqn.(9) is sometimes called **Fermi factor**.

If the energy levels of the system are very close together, then the distribution function can be written in the form

$$N(E)dE = \frac{g(E)dE}{e^{\alpha + \frac{E_i}{kT}} + 1} \quad (10)$$

Where  $N(E)dE$  represents the number of particles energies between  $E$  and  $E+dE$ . The quantity  $\alpha$  is usually expressed in the form:  $\alpha = -\frac{E_F}{kT}$ , where  $E_F$  is called the Fermi energy of the system and its physical interpretation will shortly follow. The FD- distribution function then becomes

$$f(E_i) = \frac{1}{e^{\frac{(E_i - E_F)}{kT}} + 1} \quad (11)$$

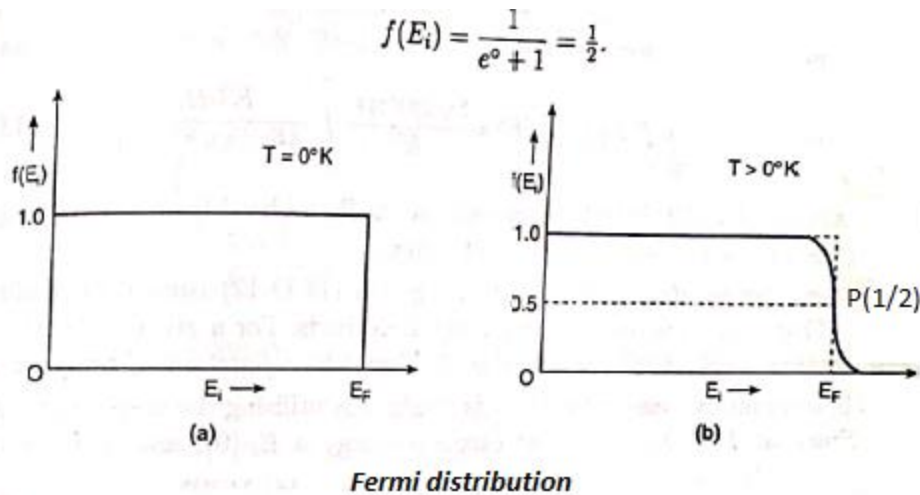
Since only one particle may occupy a quantum state, by the exclusion principle, the occupation index  $f(E_i)$  for FD-statistics also gives the probability that a quantum state of energy  $E_i$  is occupied.

#### ❖ Fermi energy or Fermi level :

At  $T = 0$  K we have from eqn. (11) above

$$\begin{aligned} f(E_i) &= \mathbf{1} \text{ when } E_i < E_F \\ &= \mathbf{0} \text{ when } E_i > E_F \end{aligned}$$

- At absolute zero, the Fermi energy or Fermi level represents the highest occupied energy level.
- The **Fermi level** is that energy level for which the probability of occupation at  $T > 0$  is  $\frac{1}{2}$ , that is, 50% of the quantum states are occupied and 50% are empty. This gives the physical interpretation of Fermi energy at a finite temperature.



### ❖ Determination of Fermi level : Electron Gas

Let us now apply FD-statistics to an electron gas and determine the Fermi level of the system. If the energy levels are closely spaced, the number of particles with energy between  $E$  and  $E+dE$  is given by

$$N(E)dE = f(E)g(E)dE$$

$$= \frac{8\sqrt{2}\pi V m^{\frac{3}{2}}}{h^3} \cdot \frac{E^{\frac{1}{2}}dE}{e^{\frac{(E-E_F)}{kT}} + 1}$$

∴ The total number of electrons is :

$$N(E) = \int_0^{\infty} N(E)dE = \int_0^{\infty} N(E)dE g(E)dE = \frac{8\sqrt{2}\pi V m^{\frac{3}{2}}}{h^3} \cdot \int_0^{\infty} \frac{E^{\frac{1}{2}}dE}{e^{\frac{(E-E_F)}{kT}} + 1} \quad (12)$$

The eqn.(12) is utilized to complete the Fermi level from a knowledge of  $N$  or  $N/V$ , the number of electrons per unit volume.

For non-zero temperature, ( $T \neq 0$ ), the integral in eqn.(12) can't be evaluated analytically. One is to take recourse to numerical methods. For a given concentration ( $N/V$ ) of electrons, (12) requires that  $E_F$  should be a function of temperature.

At  $T = 0$ , a simple expression for  $E_F(0)$  is obtained by utilizing the step-like property of  $f(E)$ . Since at  $T = 0$ , the highest occupied energy is  $E_F(0)$ , and  $f(E) = 1$  for  $E_i < E_F(0)$  and  $f(E) = 0$  for  $E > E_F(0)$ , equation (12) yields

$$\begin{aligned}
N &= \frac{8\sqrt{2}\pi V m^{\frac{3}{2}}}{h^3} \int_0^{E_F(0)} E^{\frac{1}{2}} dE \\
&= \frac{16\sqrt{2}\pi V m^{\frac{3}{2}}}{3h^3} [E_F(0)]^{\frac{3}{2}} \\
E_F(0) &= \frac{h^3}{8m} \left(\frac{3N}{\pi V}\right)^{\frac{2}{3}} = \frac{h^2}{8m} \left(\frac{3n_0}{\pi}\right)^{\frac{2}{3}} \quad (13)
\end{aligned}$$

The quantity  $n_0 = N/V$  is the density of free electrons. Hence  $E_F(0)$  is independent of the dimensions, whatever be the metal

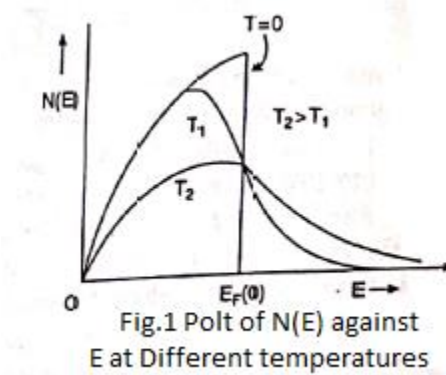


Fig.1 shows the distribution of particles  $N(E)$  as a function of energy  $E$  as given by (12). Since is the product  $f(E)$  and  $g(E)$ , since  $g(E) \propto \sqrt{E}$ , the step- character of  $f(E)$  at  $T=0$  shows that at this temperature  $N(E)$  ascends parabolically from zero at  $E = 0$  and increase in temperature, the sharp fall gradually smoothens out.

It can be shown that at temperature for which  $kT \ll E_F$ , the variation of  $E_F$  with temperature  $T$  is given by Sommerfeld equation.

$$E_F(T) = E_F(0) \left[ 1 - \frac{\pi^2}{12} \frac{k^2 T^2}{E_F^2(0)} \right] \quad (14)$$

Eq.(14) shows that with increasing temperature, the Fermi level decreases and vice versa. For metals samples,  $E_F(0)$  is a few  $eV$  and  $kT$  some ten milli- $eV$  at ordinary temperatures. The variation of Fermi level with temperature is thus quite small and may be neglected in many cases and, for all practical purposes,  $E_F(T)$  at temperature  $T$  may be considered constant and equal to  $E_F(0)$ .

❖ **Average electron energy at absolute zero :**

To determine the average energy electron at  $T = 0$  , we first obtain the total energy  $U_0$  of an electron gas at 0 K. We have

$$U_0 = \int_0^{E_F(0)} EN(E)dE = \frac{8\sqrt{2}\pi Vm^{\frac{3}{2}}}{h^3} \int_0^{E_F(0)} E^{\frac{3}{2}}f(E)dE$$
$$= \frac{8\sqrt{2}\pi Vm^{\frac{3}{2}}}{h^3} \frac{2}{5} [E_F(0)]^{\frac{5}{2}} = \frac{3}{5} NE_F(0)$$

$$[\therefore E_F(0) = \frac{h^2}{8m} \left(\frac{3N}{\pi V}\right)^{\frac{2}{3}}]$$

$\therefore$  Average electron energy  $\bar{U}_0$  (i.e. energy per particle ) is  $\frac{U_0}{N}$  given by

$$\bar{U}_0 = \frac{3}{5} E_F(0) \quad (15)$$

❖ **Comparison of MB, BE and FD- Statistics :**

An extensive discussion of MB, BE and FD statistical systems having been made, it would be worthwhile to make a comparison of the different important features of the three statistics. To highlight the differences, we present them here in table.

**Comparison of MB, BE and FD- Statistics**

Features	MB	BE	FD
1. Particles	Distinguishable, the uncertainty relation and the Pauli's exclusion principle do not apply. Ex. Gas particles at ordinary temperature.	Indistinguishable, called bosons that do not obey Pauli's exclusion principle but obey uncertainty relation. Ex. Photon and photon gas.	Indistinguishable, called fermions that obey Pauli's exclusion principle and also obey uncertainty relation. Ex. Electron gas in metals.
2. Particle spin	Spinless	0, 1, 2, .....	$\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$
3. Wave function	-	Symmetric under interchange of the coordinates of any two bosons.	Antisymmetric on interchange of the coordinates of any two fermions.
4. No. of particles Per energy state	No upper limit	No upper limit per quantum state, as Pauli principle is not obeyed.	At best, only one per quantum state is allowed as Pauli principle is obeyed.
5. Distribution function	$f(E) = e^{-\frac{E}{kT}}$	$f(E) = \frac{1}{e^{\alpha + \frac{E_i}{kT}} - 1}$	$f(E) = \frac{1}{e^{\frac{(E_i - E_F)}{kT}} + 1}$
6. Total energy	$U = \frac{3}{2}NKT$	$U = \frac{3}{2}NKT \left(1 - \frac{1}{5^{\frac{1}{2}} e^{-\alpha}}\right)$	$U = \frac{3}{2}NKT \left(1 + \frac{1}{5^{\frac{1}{2}} e^{-\alpha}}\right)$
7. Pressure	$P = \frac{NKT}{V}$	$\frac{NKT}{V} \left(1 - \frac{1}{5^{\frac{1}{2}} e^{-\alpha}}\right)$	$\frac{NKT}{V} \left(1 + \frac{1}{5^{\frac{1}{2}} e^{-\alpha}}\right)$

- MB is an approximation of BE and FD-statistics for  $E \gg E_F$  and  $E \gg kT_F$