

Statistical Mechanics

Lecture 10

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Fermi Energy at absolute zero, $T = 0$:

We know that

$$\langle \epsilon(0) \rangle = \frac{\int_0^{\infty} \epsilon n(\epsilon) d\epsilon}{\int_0^{\infty} n(\epsilon) d\epsilon} \rightarrow (i)$$

$$\langle \epsilon(0) \rangle = \frac{\int_0^{\epsilon_F} \epsilon \sigma(\epsilon) d\epsilon}{\int_0^{\epsilon_F} \sigma(\epsilon) d\epsilon}$$

$$\langle \epsilon(0) \rangle = \frac{\frac{V(2s+1)(2m)^{3/2}}{4\pi^2 h^3} \int_0^{\epsilon_F} \epsilon^{3/2} d\epsilon}{\frac{V(2s+1)(2m)^{3/2}}{4\pi^2 h^3} \int_0^{\epsilon_F} \epsilon^{1/2} d\epsilon}$$

$$\langle \epsilon(0) \rangle = \frac{\int_0^{\epsilon_F} \epsilon^{3/2} d\epsilon}{\int_0^{\epsilon_F} \epsilon^{1/2} d\epsilon}$$

$$\langle \epsilon(0) \rangle = \frac{3}{5} \epsilon_F \rightarrow (ii)$$

Therefore the ground state or zero point energy is

$$E_0 = \frac{3}{5} N \epsilon_F \rightarrow (iii)$$

Substituting for N

$$E_0 = \frac{(2s + 1)}{10\pi^2} \left(\frac{2m}{h^2} \right)^{3/2} \epsilon_F^{5/2} \rightarrow (iv)$$

Ground state pressure of system is

$$P_0 = \frac{2}{3} \left(\frac{E_0}{V} \right) = \frac{2N}{5V} \epsilon_F = \frac{2}{5} n \epsilon_F \rightarrow (v)$$

Where $n = \frac{N}{V}$

Fermi Energy and Fermi Temperature (Alternate Method):

To derive Fermi energy this method is based on Heisenberg uncertainty Principle as we know

$$\Delta x \Delta P_x \approx h \rightarrow (i)$$

Equation (i) can be generalized to all three components as

$$(\Delta x \Delta P_x)(\Delta y \Delta P_y)(\Delta z \Delta P_z) \approx h^3 \rightarrow (ii)$$

$$\Delta P_x \Delta P_y \Delta P_z \approx \frac{h^3}{\Delta x \Delta y \Delta z} \rightarrow (iii)$$

Considering the momentum volume $(\Delta P_x \Delta P_y \Delta P_z)$ as sphere of radius ΔP , then we can write

$$(\Delta P_x \Delta P_y \Delta P_z) = \frac{4}{3} \pi \Delta P^3 = \frac{h^3}{\Delta V} \rightarrow (iv)$$

By virtue of uncertainty Principle, each electron occupies at least a volume ΔV and this electron can exist in either of two possible spin orientations. Therefore N is the number of electrons in a unit vector $\Delta V = \frac{2}{N}$. Therefore

$$\frac{4}{3} \pi (\Delta P)^3 = \frac{h^3 N}{2} \rightarrow (v)$$

Hence

$$\Delta P = h \left(\frac{3N}{8\pi} \right)^{1/3} \rightarrow (vi)$$

Since ΔV is the minimum volume needed to house an electron, ΔP is maximum as a consequence of uncertainty principle. Therefore

$$\epsilon_P = \frac{(\Delta P)^2}{2m} = \frac{h^2}{2m} \left(\frac{3N}{8\pi} \right)^{2/3} \rightarrow (vii)$$

Which agrees if $V = 1$ with equation as

$$\epsilon_P = \frac{h^2}{2m} \left[\frac{8N\pi^2}{(2s+1)V} \right]^{2/3} \rightarrow (viii)$$

And Fermi Temperature

$$T_F = \frac{\epsilon_F}{K} \rightarrow (ix)$$

Usually Fermi Temperature is higher than the ordinary temperature.

Bose-Einstein Principle:

Bose-Einstein statistics gives the statistical behaviour of an ensemble of indistinguishable particles which does not obey the Pauli's Exclusion Principle. Phonons and photons may be treated with the help of B-E statistics. The particles that obey the B-E statistics are called a boson.

The problem here is to distribute N_i particles among g_i quantum states of the energy level E_i keeping in mind that there is no restriction regarding the number of particles that may occupy a quantum state.

Let us consider the following way as $|\dots| \dots |\dots| |\dots| |\dots|$ where a line denotes a quantum state and the particles contained in a quantum are shown by points on the right of the quantum state. In the array there are $(g_i + N_i)$ objects consisting of the quantum states and the particles. Keeping the first quantum state i.e. the first line fixed in its place, the remaining $(g_i + N_i - 1)$ can be arranged in $(g_i + N_i - 1)!$ ways.

However among these the number of ways of permuting the quantum state among themselves i.e. $(g_i - 1)!$ and the number of ways of permuting the particles among themselves is $N_i!$ can not be regarded as independent arrangement. Therefore number of ways in which N_i particles can be distributed in g_i state is given by

$$A = \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!} \rightarrow (i)$$

The total number of ways W of distributing N_1, N_2, \dots, N_n particles in n –energy level is the product of terms represented by equation (i) over all the levels i.e.

$$W = \prod_{i=1}^n \frac{(N_i + g_i - 1)!}{N_i! (g_i - 1)!} \rightarrow (ii)$$

Applying Sterling theorem for large enough N_i and g_i in equation (ii), we get

$$\ln W = \sum_{i=1}^n [(N_i + g_i - 1)\{\ln(N_i + g_i - 1) - 1\} - N_i(\ln N_i - 1) - (g_i - 1)\{\ln(g_i - 1) - 1\}]$$

$$\ln W = \sum_{i=1}^n [(N_i + g_i - 1) \ln(N_i + g_i - 1) - N_i \ln N_i - (g_i - 1) \ln(g_i - 1)] \rightarrow (iii)$$

As the system is in equilibrium for the most probable distribution, W or $\ln W$ has to be maximised under the conditions that the total number of particles N and the total energy U are constant i.e.

$$N = \sum_{i=1}^n N_i = \text{Constant} \rightarrow (iv)$$

$$U = \sum_{i=1}^n N_i \epsilon_i = \text{Constant} \rightarrow (v)$$

Applying Lagrange's undetermined multiples we can write

$$\sum_{i=1}^n [\ln(N_i + g_i - 1) - \ln N_i + \alpha + \beta E_i] \delta N_i = 0 \rightarrow (vi)$$

Where α and β are constant. Since variations are arbitrary we get from equation (vi) as

$$\ln(N_i + g_i) - \ln N_i + \alpha + \beta E_i = 0 \rightarrow (vii)$$

Where $(N_i + g_i - 1)$ by $(N_i + g_i)$ assuming large enough $(N_i + g_i)$. Equation (vii) yields the Bose-Einstein distribution function as

$$f(E_i) = \frac{N_i}{g_i} = \frac{1}{e^{-\alpha - \beta E_i} - 1} \rightarrow (viii)$$

At very high temperature the particles are distributed over a wide range of energy so that the number of particles in any energy range would be much smaller than the number of quantum states in that range i.e. $g_i \gg N_i$. In that case equation (vii) reduces to

$$\ln g_i - \ln N_i + \alpha + \beta E_i = 0 \rightarrow (ix)$$

Which is the same equation as Maxwell-Boltzmann system. Thus at high temperature the Bose-Einstein distribution function reduced to Maxwell-Boltzmann distribution function and given by

$$f(E_i) = e^{\alpha + \beta E_i} \rightarrow (x)$$

It is then appreciated that the quantity β must be satisfied as

$$\beta = -\frac{1}{K_\beta T} \rightarrow (xi)$$

So equation (viii) can be written as

$$f(E_i) = \frac{1}{e^{-\alpha} \cdot e^{E_i/K_\beta T} - 1} \rightarrow (xii)$$

The quantity α can be determined in terms of the number of particles in the system as in the case of Maxwell-Boltzmann and Fermi-Dirac system. It is seen that at high temperature α must be very large negative number in order that equation (xii) may be reduced to the form of equation (x). As the temperature approaches to zero $\alpha = 0$ and equation (xii) reduced to

$$f(E_i) = \frac{1}{e^{E_i/K\beta T} - 1} \rightarrow (xiii)$$

It is seen from equation (xiii) that at the absolute zero temperature the particle tend to occupy the lowest energy state. This phenomenon is known as Bose Condensation. It is believed that Bose Condensation is responsible for the superfluid state of liquid helium.

It is noted that if $E_i \gg K_\beta T$, the Bose-Einstein distribution reduced to Maxwell-Boltzmann distribution.