Statistical mechanics

Lecture note: 2

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Topics in this Lectures:

- 1. Revision
- 2. Strongly degenerate F-D system (T<<T_F)
 - Relation of Fermi energy with chemical potential
 - Chemical potential in terms of temperature
 - Total internal energy
 - Specific heat capacity
 - Entropy
 - Pressure
- 4. Tutorial sheet.

Revision:

• The occupation no. for the ith energy level is given as

$$n = \frac{1}{e^{\frac{\varepsilon_i - \mu}{kT}} + 1}$$

• For the case of energy levels which are closely spaced, Fermi distribution function is given as

$$f(\varepsilon) = \frac{1}{e^{\frac{\varepsilon - \varepsilon_f}{kT}} + 1}$$

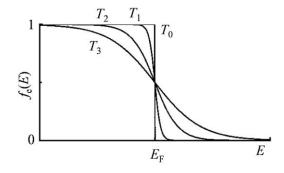


Figure 1: Representation of Fermi distribution function at various temperature.

• Completely degenerate F-D system (T=0)

1. Total no. of particles
$$N = \frac{2}{3}CV\varepsilon_f^{\frac{3}{2}}$$

2. Fermi energy
$$\qquad \epsilon_f = \frac{h^2}{2m} (\frac{3N}{4\pi g_s V})^{\frac{2}{3}}$$

3. Fermi Temperature
$$T_f = \frac{\varepsilon_f}{k} = \frac{h^2}{2mk} \left(\frac{3N}{4\pi g_s V}\right)^{\frac{2}{3}}$$

4. Electron gas in metals Fermi energy for electrons

$$\varepsilon_f = \frac{h^2}{8m} \left(\frac{3N}{\pi V}\right)^{\frac{2}{3}}$$

Fermi temperature can be written as:

$$T_f = \frac{\varepsilon_f}{k} = \frac{h^2}{8mk} \left(\frac{3N}{\pi V}\right)^{\frac{2}{3}}$$

Strongly degenerate F-D system (T<<T_F)

1. Relation between Fermi energy and chemical potential.

In fig 2 we have shown mean occupation no. as a function of ϵ for low as well as high temperature. Dashed lines are corresponding the curve at T=0 K and electron in tail has some freedom to move into unoccupied states. We will now derive N for T<<T_F.

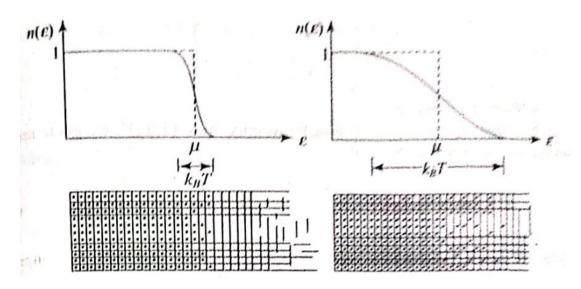


Figure 2: occupation number of strongly degenerate Fermi gas at two different temperatures.

From equation 5,

$$N = \int_0^\infty \frac{g_s 2\pi V(2m)^{\frac{3}{2}} \epsilon^{1/2}}{h^3} \frac{d\epsilon}{e^{\frac{\epsilon_i - \mu}{KT} + 1}}$$

$$N = CV \int_0^\infty \frac{\epsilon_s^{\frac{1}{2}} d\epsilon}{\exp \frac{\epsilon_r - \mu}{KT} + 1}$$
(18)

Where C has given earlier. Let $x = \varepsilon/kT$ and $x_0 = \mu/kT$, than eqn 18 can be modified as:

$$N = CV(kT)^{\frac{3}{2}} \int_0^\infty \frac{x^{\frac{1}{2}d\varepsilon}}{\exp(x-x_o)+1}$$
 (19)

Using sommerfled's lemma as:

$$\int_0^\infty f(x - x_0) x^s dx = \frac{x_0^{s+1}}{s+1} \left[1 + \frac{\pi^2}{6} \frac{s(s+1)}{x_0^2} + \dots \right]$$
 (20)

If we consider $f(x-x_0) = 1/\{exp(x-x_0)+1\}$ and s = 1/2, we get

$$\int_0^\infty \frac{x^{\frac{1}{2}} d\varepsilon}{\exp(x - x_0) + 1} = \frac{2}{3} x_0^{\frac{3}{2}} \left[1 + \frac{\pi^2}{8x_0^2} + \cdots \right]$$
$$= \frac{2}{3} \left(\frac{\mu}{kT} \right)^{\frac{3}{2}} \left[1 + \frac{\pi^2}{8} \left(\frac{kT}{\mu} \right)^2 + \cdots \right]$$

Using the above result in eqn 18 we get,

$$N = \frac{2}{3}CV(\mu)^{\frac{3}{2}} \left[1 + \frac{\pi^2}{8} \left(\frac{kT}{\mu} \right)^2 + \cdots \right]$$
 (21)

From eqn. 8 and 21 we get

$$\varepsilon_f^{\frac{3}{2}} = (\mu)^{\frac{3}{2}} \left[1 + \frac{\pi^2}{8} \left(\frac{kT}{\mu} \right)^2 + \cdots \right]$$
 (22)

Eqn 22 represents relation between Fermi energy and chemical potential and it says at T=0, Fermi energy is equal to chemical potential and it starts deviating for higher T. thus we can say that $\varepsilon_i = \mu(T)$

$$\mu(T) = \varepsilon_f \left[1 + \frac{\pi^2}{8} \left(\frac{kT}{\mu} \right)^2 + \dots \right]^{\frac{2}{3}}$$
 (23)

$$\mu(T) = \varepsilon_f \left[1 + \frac{\pi^2}{8} \left(\frac{T}{T_f} \right)^2 + \cdots \right]^{\frac{2}{3}}$$
 (24)

using binomial expansion

$$\mu(T) = \varepsilon_f \left[1 - \frac{\pi^2}{12} \left(\frac{T}{T_f} \right)^2 + \frac{\pi^4}{80} \left(\frac{T}{T_f} \right)^4 \dots \right]$$
 (25)

the above equation gives the variation of chemical potential with respect to temperature. This is represented by following graph.

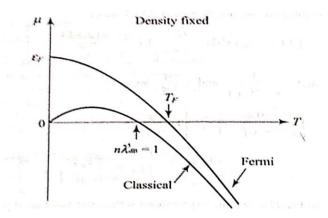


Figure 3: Temperature variation of chemical potential of Fermi gas

2. Total internal energy

The total energy of FD statistic can be written as:

$$E = CV \int_0^\infty \frac{\varepsilon^{\frac{3}{2}} d\varepsilon}{\exp\frac{\varepsilon - \mu}{kT} + 1}$$
 (26)

Let $x = \varepsilon/kT$ and $x_0 = \mu/kT$, than eqn 26 can be modified as:

$$E = CV(kT)^{\frac{5}{2}} \int_0^\infty \frac{x^{\frac{3}{2}} d\varepsilon}{\exp(x - x_o) + 1}$$
 (27)

Using the sommerfled's lemma as we used earlier to get eq. 21, the eqn 27 can be written as

$$E = \frac{2}{5}CV(\mu)^{\frac{5}{2}} \left[1 + \frac{5\pi^2}{8} \left(\frac{T}{T_E} \right)^2 + \cdots \right]$$
 (28)

Substituting the value of μ from eqn 25 we get

$$E = \frac{2}{5}CV \left(\varepsilon_f \left[1 - \frac{\pi^2}{12} \left(\frac{T}{T_f} \right)^2 + \frac{\pi^4}{80} \left(\frac{T}{T_f} \right)^4 \dots \right] \right)^{\frac{5}{2}} \left[1 + \frac{5\pi^2}{8} \left(\frac{T}{T_F} \right)^2 + \dots \right]$$
 (29)

$$E = \frac{2}{5}CV(\varepsilon_f)^{\frac{5}{2}} \left[1 - \frac{5\pi^2}{24} \left(\frac{T}{T_f} \right)^2 + \dots \right] \left[1 + \frac{5\pi^2}{8} \left(\frac{T}{T_F} \right)^2 + \dots \right]$$
 (30)

On simplifying we get:

$$E = \frac{2}{5}CV(\varepsilon_f)^{\frac{5}{2}} \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{T}{T_F} \right)^4 \dots \right]$$
 (31)

Using eqn 12 here, we get

$$E = E_0 \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{T}{T_F} \right)^4 \dots \right]$$
 (32)

$$E = \frac{3}{5} N \varepsilon_F \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{T}{T_F} \right)^4 \dots \right]$$
 (33)

Eqn 33 give total internal energy of Fermions in function of temperature, indicating with increase of temperature the total internal energy increases. Physically this is expected as with increase of temperature the particle will shift to higher energy states as indicated in Fig. 2, resulting in increase in internal energy. The internal energy of ideal monoatomic classical gas is 3/2NkT and Fig 4 represents that for T<T_F the energy of fermions deviates from classical value.

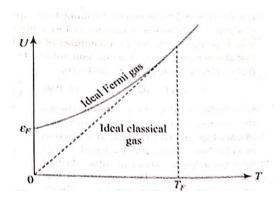


Figure 4: Internal energy of strongly Degenerate Fermi gas as function of Temperature.

3. Specific heat capacity

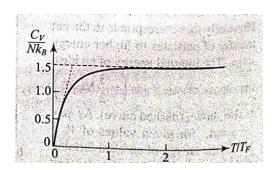


Figure 5 variation of constant volume heat capacity of ideal fermi gas with temperature.

The heat capacity of fermions system is given by

$$C_V = \left(\frac{dE}{dT}\right)_V = \frac{d}{dT} \left[\frac{3}{5} N \varepsilon_F \left[1 + \frac{5\pi^2}{12} \left(\frac{T}{T_F} \right)^2 - \frac{\pi^4}{16} \left(\frac{T}{T_F} \right)^4 \dots \right] \right]$$
(34)

$$C_V = \frac{3}{5} N \varepsilon_F \left[\frac{5\pi^2}{12} \left(\frac{2T}{T_F^2} \right) \right] \tag{35}$$

$$C_V = \frac{\pi^2}{2} \left(\frac{NkT}{T_F} \right) \tag{36}$$

$$C_V = \frac{\pi^2}{2} \left(\frac{kT}{\varepsilon_F}\right) R \tag{37}$$

$$C_V = \alpha T \tag{38}$$

Eqn 38 shows specific heat of fermions is directly proportional to temperature and it tends to zero as $T \rightarrow 0$. Earlier in Debye theory of lattice heat capacity we have studied that $C_v = \beta T^3$ where β is constant and from FD stat. we find that heat capacity due to fermions is given by eqn 38. Combining these results we conclude that heat capacity has two different contribution, electronic and lattice and can be written as:

$$C_V = \alpha T + \beta T^3 \tag{39}$$

Fig 5 shows the variation of heat capacity with temperature.

4. Entropy: Entropy is given as

$$S = \int_0^T \frac{c_V}{T} dT \tag{40}$$

From eqn 36 and 40

$$S = \frac{\pi^2}{2} \left(\frac{NkT}{\varepsilon_F} \right) \tag{41}$$

Thus entropy of strongly degenerate Fermi gas drops to zero at absolute zero of temperature.

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References:

- 1. Thermal Physics by S.C. Garg, R.M. Bansal and C. K. Ghosh.
- 2. Statistical Physics, Berkley series volume 5.
- 3. Fundaments of Statitical Mechanics and Thermal Physics, F. Rief.

Tutorial Problems:

1. Four weakly interacting particles are confined to a cubical box of volume V, with the energy of any one particle of the form

$$E = \frac{\pi^2 \hbar^2}{2mV^{2/3}} \left(n_x^2 + n_y^2 + n_z^2 \right)$$

Where $n_{x_i} n_y n_z$ are natural numbers. What is the energy of the system at absolute zero if the system is a)Fermionic b) bosonic? Ignore spin.

- 2. The Fermi energy of free electron in silver atom at 0 K is 5.51eV. what is the average energy per electron.
- 3. Given a Fermi gas what is the mean occupation number for a state with energy 2KT above the Fermi energy.