<u>FERMI DIRAC GASSES</u>

<u>Fermions</u>: Are particles of half-integer spin that obey Fermi-Dirac statistics. Fermions obey the Pauli exclusion principle, which prohibits the occupancy of an available quantum state by more than one particle.

<u>Ideal fermion gas</u>: Consisting of *N* non-interacting and indistinguishable fermions in a container of volume *V* held at absolute temperature *T*.

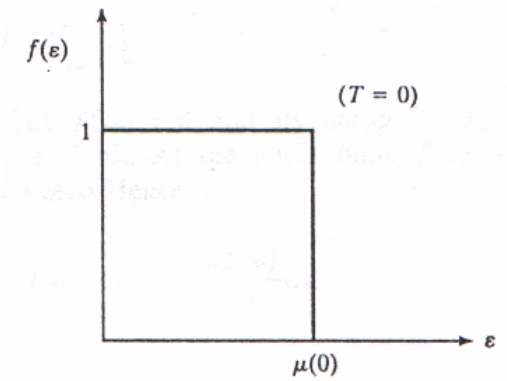
<u>Fermi-Dirac distribution</u>: For an ideal FD gas (non-interactions between the indistinguishable particles) of N molecules in a volume V, the most probable number of particles with ε_i energy is:

$$f(\varepsilon_i) = \frac{n_i^*}{g_i} = \frac{1}{e^{\beta(\varepsilon_i - \mu)} + 1}$$

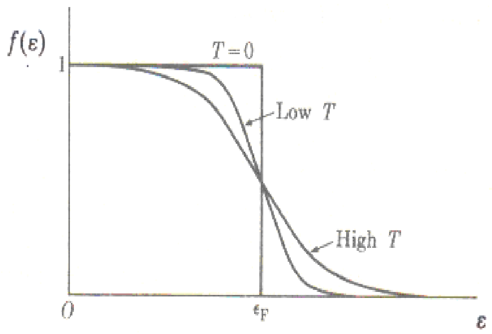
and the continuum is:

$$f(\varepsilon) = \frac{N(\varepsilon)}{g(\varepsilon)} = \frac{1}{e^{y} + 1}, \qquad y = \beta(\varepsilon - \mu)$$

Fermi function gives the probability that a single particle state ε_i will be occupied by a fermion. Clearly, $0 \le f(\varepsilon) \le 1$.



The Fermi function at $T = 0$.



Distribution function $f(\varepsilon)$ at three temperatures in Fermi-Dirac statistics.

Notes:

1- μ no need to be negative, due to the +1 in the denominator. μ may be positive or negative.

2- If $\mu\beta << 0$, then $e^{\beta(\varepsilon-\mu)} >> 1$, and $f(\varepsilon)$ reduces to the Maxwell-Boltzmaan distribution.

3- If $\mu\beta >> 1$

i- if $\varepsilon << \mu \;\Rightarrow\; \beta(\varepsilon - \mu) << 0 \;\Rightarrow\; f(\varepsilon) = 1$

ii- if $\varepsilon >> \mu \;\Rightarrow\; \beta(\varepsilon - \mu) >> 0 \;\Rightarrow\; f(\varepsilon) = e^{-\beta(\varepsilon-\mu)}$ and fall off exponentially like Maxwell-Boltzmaan distribution.

iii- if $\varepsilon = \mu \quad \Rightarrow \quad f\ (\varepsilon) = \frac{1}{2}$

iv- In the limit of $T \to 0$ we have sharp drop and

$$f\ (\varepsilon) = \begin{cases} 1 & \varepsilon < \mu_o \\ 0 & \varepsilon > \mu_o \end{cases} \quad \Rightarrow \quad N = \begin{cases} \int_0^{\mu_o} g\,(\varepsilon) d\,\varepsilon & T = 0 \\ \int_0^{\mu_o} g\,(\varepsilon) f\ (\varepsilon) d\,\varepsilon & T \neq 0 \end{cases}$$

Where

$$g\,(\varepsilon) = g_s \left(\frac{2\pi V}{h^3}\right)(2m)^{3/2}\sqrt{\varepsilon}, \qquad\qquad g_s = 2s + 1$$

$$= 4\pi V \left(\frac{2m}{h^2}\right)^{3/2}\sqrt{\varepsilon}, \qquad \text{for electrons}$$

Exclusion principle implies that a FD gas has a large mean energy even at absolute zero, $0 < \varepsilon < \mu_o (\equiv \varepsilon_f\ (0))$

$$T = \begin{cases} 0 & \mu_o > 0, \quad \varepsilon < \mu_o & \text{Very low temperature} & \text{Completely degenerate} \\ T << T_f & \mu_o > 0 & \text{Low temperature} & \text{degenerate} \\ T \approx T_f & \mu_o = 0 & \text{Intermediate temperature} & \text{Slightly degenerate} \\ T >> T_f & \mu < 0 & \text{High temperature} & \text{Classical limit} \end{cases}$$

At absolute zero, due to exclusion principle, all the states with $0 < \varepsilon \le \mu_o (\equiv \varepsilon_f\ (0))$ are completely filled and all the states with $\varepsilon > \mu_o$ are completely empty.

Completely Degenerate Gas

Total number of particles:

$$N = \int_0^{\mu_o} g\,(\varepsilon) f\ (\varepsilon) d\,\varepsilon$$

$$= 4\pi V \left(\frac{2m}{h^2}\right)^{3/2} \int_0^{\mu_o} \sqrt{\varepsilon}\ d\,\varepsilon = \frac{8\pi V}{3}\left(\frac{2m}{h^2}\right)^{3/2} \mu_o^{\ 3/2}$$

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

For convenience, we introduce a Fermi temperature T_f such that $\mu_o = \varepsilon_F = k_B T_f$. This can be written as:

$$T_f = \frac{\mu_o}{k_B} = \frac{h^2}{2mk_B}\left(\frac{3}{8\pi}\frac{N}{V}\right)^{2/3}$$

Example: Metallic potassium has $\rho = 0.86\times10^3\,\text{kg/m}^3$ and atomic weight of $M = 39$ kg/kmole. Find μ_o, T_f, and v_f.

Solution: We will consider one free electron per atom for monovalent atoms. Thus the concentration is:

$$\frac{N}{V} = \frac{N_a\rho}{M} = \frac{(6.02\times10^{26}\text{ atoms/kmole})(0.86\times10^3\,\text{kg/m}^3)}{39\text{ kg/kmole}} = 1.33\times10^{28}\text{ atoms/m}^3,$$

$$\mu_o = \frac{h^2}{8m}\left(\frac{3}{\pi}\frac{N}{V}\right)^{2/3} = \frac{(hc)^2}{8mc^2}\left(\frac{3}{\pi}\frac{N}{V}\right)^{2/3} = \frac{(12.4\times10^{-7}\text{ eV.m})^2}{8\left(0.511\times10^6\text{ eV}\right)}\left(\frac{3}{\pi}\times1.33\times10^{28}\,\frac{\text{atoms}}{\text{m}^3}\right)^{2/3}$$

$$= 2.05\text{ eV}$$

Then

$$T_f = \frac{\mu_o}{k_B} = \frac{2.05\text{ eV}}{8.617\times10^{-5}\,\frac{\text{eV}}{\text{K}}} = 23790\text{ K}$$

So, even at room temperature we have to treat the metallic potassium quantum mechanically.

Use

$$\mu_o = \frac{p_f^2}{2m} \quad\Rightarrow\quad p_f^2 = 2m\,\mu_o$$

$$\Rightarrow\quad v_f^2 = \frac{2\mu_o}{m} = \frac{2\mu_o c^2}{mc^2} = \frac{2\left(2.05\text{ eV}\right)\times\left(3.0\times10^8\text{ m/s}\right)^2}{\left(0.511\times10^6\text{ eV}\right)} = 7.22\times10^{11}\text{ m}^2/\text{s}^2$$

$$\Rightarrow\quad v_f = 8.5\times10^5\text{ m/s}$$

Internal energy:

$$U_o = \int_0^{\mu_o} \varepsilon g(\varepsilon) f(\varepsilon)\, d\varepsilon$$

$$= 4\pi V\left(\frac{2m}{h^2}\right)^{3/2}\int_0^{\mu_o}\varepsilon^{3/2}\,d\varepsilon = \frac{8\pi V}{3}\left(\frac{2m}{h^2}\right)^{3/2}\mu_o^{5/2}$$

$$= \frac{3}{5}N\,\mu_o$$

Other thermodynamic functions are:

$S_o = 0,$

$\Omega_o = -PV = U_o - S_o - \mu_o N = -\frac{2}{5}\mu_o N$,

$P = -\frac{\Omega_o}{V} = \frac{2}{5}\mu_o\left(\frac{N}{V}\right) \quad = 2.71\times 10^7 \rho$ atm for electrons)

Thus at $T = 0$ K a fermion gas exerts a pressure. If the electrons in a metal were neutral they would exert a pressure of about 10^6 atm. The Coulomb attraction to the ions counterbalances the pressure. For $T = 0$ K the value of is positive and large.

H.W.

Prove that

$$\mu(T) \approx \mu_o\left[1 - \frac{\pi^2}{12}\left(\frac{T}{T_f}\right)^2\right], \qquad T << T_f$$

Notes:

1- $\mu(T)$ is positive for temperature below the Fermi temperature and negative for higher temperature.

2- As the temperature increases above, more and more of the fermions are in the excited states and the mean occupancy of the ground state falls below 1/2. In this region,

$$f(0) = \frac{1}{e^{-\beta\mu}+1} < \frac{1}{2}$$

which implies that

$$\frac{\mu}{k_B T} < 0$$

or $\mu < 0$.

For boson gas $\mu(T)$ is negative at all temperatures and is zero at absolute zero.

AT high temperature the fermion gas approximates the classical ideal gas. In the classical limit:

$$\mu = -k_B T \ln(z) = -k_B T \ln\left[\left(\frac{2\pi mkT}{h^2}\right)^{3/2}\frac{V}{N}\right]$$

Example: for kilo-mole of the fermion ^{3}He gas atoms at STP, $T_f = 0.069$ K, so that $\frac{T}{T_f} = 3900$, then classically

$$\frac{\mu}{kT} = -\ln\left(\frac{z}{N}\right) = -\ln\left[\left(\frac{2\pi mkT}{h^2}\right)^{3/2}\frac{V}{N}\right] = -12.7$$

And $e^{-\beta\mu} = 3.3\times10^5$. The average occupancy of single particle states is very small, as in the case of an ideal gas obeying the Maxwell-Boltzmann distribution.

The thermionic emission has been worked out (see Phatria chapter 8)

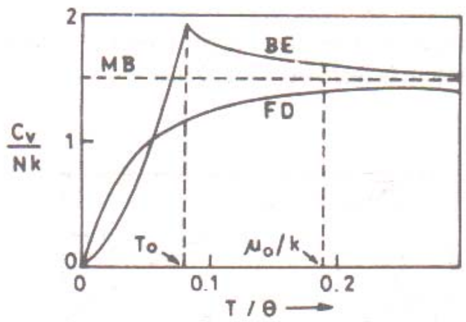


Fig. 7.5 Comparison of heat capacity of a gas according to the three statistics, $\theta = (h^2/mk)(\overline{N}/gV)^{2/3}$.