Statistical Mechanics

Problem set 5 - Solutions

1) Entropy of a non-interacting system

$$\rho = \frac{e^{-\beta \sum_\alpha (\epsilon_\alpha - \mu)\hat{n}_\alpha}}{Q}$$

The thermodynamic potential is, as seen in class,

$$\Phi = -T \ln Q = \begin{cases} -T \sum_\alpha \ln\left(1 + e^{-\beta(\epsilon_\alpha - \mu)}\right) & (F) \\ T \sum_\alpha \ln\left(1 - e^{-\beta(\epsilon_\alpha - \mu)}\right) & (B) \end{cases}$$

We can write this in terms of

$$\bar{n}_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha - \mu)} \pm 1}$$

we have

$$\text{Fermions}: \quad \bar{n} = \frac{1}{e^{x}+1} \longrightarrow x = \ln\left(\frac{1-n}{n}\right) \longrightarrow 1 + e^{-x} = \frac{1}{1-\bar{n}}$$

$$\text{Bosons}: \quad \bar{n} = \frac{1}{e^{x}-1} \longrightarrow x = \ln\left(\frac{1+n}{n}\right) \longrightarrow 1 - e^{-x} = \frac{1}{1+\bar{n}}$$

Thus

$$\Phi = \begin{cases} -T \sum_\alpha \ln \dfrac{1}{1-\bar{n}_\alpha} \\ T \sum_\alpha \ln \dfrac{1}{1+\bar{n}_\alpha} \end{cases} = \begin{cases} T \sum_\alpha \ln (1-\bar{n}_\alpha) \\ -T \sum_\alpha \ln (1+\bar{n}_\alpha) \end{cases}$$

Moreover, we know that

$$\Phi = U - \mu N - TS$$

$$\Rightarrow \quad S = \frac{U - \mu N - \Phi}{T}$$

The 1^{st} term is

$$U - \mu N = \sum_\alpha (\epsilon_\alpha - \mu)\, \bar{n}_\alpha$$

Thus

$$\beta(U - \mu N) = \begin{cases} \sum_\alpha \ln \left(\dfrac{1-\bar{n}_\alpha}{\bar{n}_\alpha} \right) \bar{n}_\alpha & \text{(F)} \\ \sum_\alpha \ln \left(\dfrac{1+\bar{n}_\alpha}{\bar{n}_\alpha} \right) \bar{n}_\alpha & \text{(B)} \end{cases}$$

Combining everything, we get

Fermions :

$$S = \sum_\alpha \left\{ \ln\left(\frac{1-\bar{n}_\alpha}{\bar{n}_\alpha}\right)\bar{n}_\alpha - \ln(1-\bar{n}_\alpha) \right\}$$

$$= \sum_\alpha \left\{ \ln(1-\bar{n}_\alpha)(\bar{n}_\alpha - 1) - \bar{n}_\alpha \ln \bar{n}_\alpha \right\}$$

or

$$S = -\sum_\alpha \left\{ \bar{n}_\alpha \ln \bar{n}_\alpha + (1-\bar{n}_\alpha)\ln(1-\bar{n}_\alpha) \right\}$$

Bosons :

$$S = \sum_\alpha \left\{ \ln\left(\frac{1+\bar{n}_\alpha}{\bar{n}_\alpha}\right)\bar{n}_\alpha + \ln(1+\bar{n}_\alpha) \right\}$$

$$= \sum_\alpha \ln(1+\bar{n}_\alpha)(\bar{n}_\alpha + 1) - \bar{n}_\alpha \ln \bar{n}_\alpha$$

or

$$S = -\sum_\alpha \left\{ \bar{n}_\alpha \ln \bar{n}_\alpha - (1+\bar{n}_\alpha)\ln(1+\bar{n}_\alpha) \right\}$$

2) Ultra-relativistic Fermi-gas

$$\epsilon_k = \hbar c k \qquad \mathbf{k} = (k_1, \ldots, k_d)$$

$$k_i = \frac{2\pi l_i}{L}, \quad l_i = 0, \pm 1, \pm 2, \ldots$$

(a) DOS: following the same steps as Sec 2.1 of the notes:

$$\sum_{\mathbf{k}, s} f(\epsilon_k) = (2S+1)\left(\frac{L}{2\pi}\right)^d \int d^d k \, f(\epsilon_k)$$

$$= (2S+1)\left(\frac{L}{2\pi}\right)^d \frac{d\,\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)} \int_0^\infty dk \, k^{d-1} f(\epsilon_k)$$

Now things get different: changing variables to

$$\epsilon = \hbar c k$$

we get

$$d\epsilon = \hbar c \, dk$$

so

$$dk \, k^{d-1} = \frac{d\epsilon \, \epsilon^{d-1}}{(\hbar c)^d}$$

whence

$$\sum_{\mathbf{k}, s} f(\epsilon_k) = (2S+1)\left(\frac{L}{2\pi}\right)^d \frac{d\,\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)} \frac{1}{(\hbar c)^d} \int_0^\infty d\epsilon \, \epsilon^{d-1} f(\epsilon)$$

Thus the DOS reads

$$\mathcal{D}(\epsilon) = \alpha\, \epsilon^{d-1}$$

$$\alpha = (2S+1)\left(\frac{L}{2\pi}\right)^d \frac{d\,\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)} \frac{1}{(\hbar c)^d}$$

For $d = 1, 2, 3$, we get

$$\mathcal{D}(\epsilon) \sim \begin{cases} 1 & d=1 \\ \epsilon & d=2 \\ \epsilon^2 & d=3 \end{cases}$$

(b) Fermi level

$$N = \int_0^{\epsilon_F} d\epsilon\, \mathcal{D}(\epsilon) = \alpha \int_0^{\epsilon_F} d\epsilon\, \epsilon^{d-1} = \alpha \frac{\epsilon_F^{\,d}}{d}$$

$$\therefore \qquad \epsilon_F = (dN/\alpha)^{1/d}$$

(c) Ground-state energy

$$E_{gs} = \int_0^{\epsilon_F} d\epsilon\, \epsilon\, \mathcal{D}(\epsilon) = \alpha \int_0^{\epsilon_F} d\epsilon\, \epsilon^d = \frac{\alpha\, \epsilon_F^{\,d+1}}{d+1}$$

Now we use the fact that $\epsilon_F^d = dN/\alpha$, to write

$$E_{gs} = \frac{\alpha\,\epsilon_F}{d+1}\,\epsilon_F^d = \frac{\alpha\,\epsilon_F}{d+1}\,\frac{dN}{\alpha}$$

Thus

$$E_{gs} = \frac{d}{d+1}\,N\,\epsilon_F$$

3) Bose - Einstein condensation for a generic DOS

$$D(\epsilon) = \Lambda_2 \, \epsilon^2$$

(a) As we have seen in class, the number of particles can be split as

$$N = N_0 + \int_0^\infty d\epsilon \, D(\epsilon) \, \bar{n}(\epsilon)$$

where N_0 is the condensate fraction. We then get

$$N = N_0 + \Lambda_2 \int_0^\infty d\epsilon \, \frac{\epsilon^2}{z^{-1} e^{\beta\epsilon} - 1} \qquad z = e^{\beta\mu}$$

changing variables to $x = \beta\epsilon$ yields

$$N = N_0 + \Lambda_2 \, T^{2+1} \int_0^\infty dx \, \frac{x^2}{z^{-1} e^{x} - 1}$$

we let

$$g_2(z) = \Lambda_2 \int_0^\infty dx \, \frac{x^2}{z^{-1} e^{x} - 1}$$

which yields the implicit equation

$$g_2(z) = \frac{N - N_0}{T^{2+1}}$$

Again, following the same steps as done in class, we look for solutions with $N_0 = 0$:

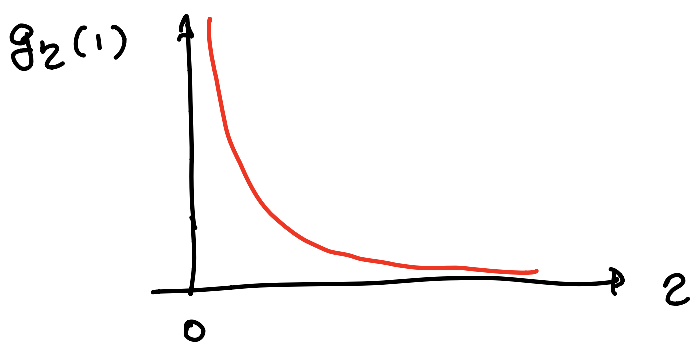
$$g_\nu(z) = \frac{N}{T^{\nu+1}}$$

Since $\nu > -1$, when we cool down, the RHS goes up. We must then ask whether there will be a solution $z(N,T)$ for all $T \neq 0$.

To check that, we analyze what happens when $\mu = 0$, or $z = 1$. In this case we get

$$g_\nu(1) = \Lambda_\nu \int_0^\infty dx \, \frac{x^\nu}{e^x - 1} = \Gamma(\nu+1)\, L_{1+\nu}(1)$$

where $L_n(z)$ is the PolyLog function. This result looks like



It is finite for all $\nu > 0$, but diverges when $\nu \leq 0$.

This divergence means that when $2 \leq 0$, for any $T > 0$, one can always find a solution of $g_2(z) = N/T^{2+1}$.

As a consequence, we never need to have a condensate fraction; BEC does not occur when $2 \leq 0$.

(b) The critical temperature is found from

$$g_2(1) = \frac{N}{T_c^{2+1}}$$

which yields

$$T_c = \left(\frac{N}{g_2(1)} \right)^{\frac{1}{1+2}}$$

If $2 = 1/2$ we get $T_c \sim N^{2/3}$, as found in class.

(c) Below T_c, N_0 is given by

$$N = N_0 + T^{2+1} g_2(1)$$

$$= N_0 + T^{2+1} \frac{N}{T_c^{2+1}}$$

Thus

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c} \right)^{2+1}$$

For $2 > -1$, this always looks like