Statistical Physics: Weekly Problem 5 (SP5)

(1) (a) With $\beta = 1/(k_B T)$ the one particle partition function is

$$Z = e^{\beta\epsilon} + e^{\beta 0} + e^{-\beta\epsilon} = 1 + 2\cosh(\beta\epsilon).$$

[2 marks]

(b) The internal energy is

$$U = -N\frac{\partial \ln Z}{\partial \beta} = -N\,\epsilon\,\frac{e^{\beta\epsilon} - e^{-\beta\epsilon}}{1 + e^{\beta\epsilon} + e^{-\beta\epsilon}} = -N\epsilon\,\frac{2\sinh(\beta\epsilon)}{1 + 2\cosh(\beta\epsilon)}.$$

The heat capacity is

$$C_V = \frac{\partial U}{\partial T} = -k_B\,\beta^2\,\frac{\partial U}{\partial \beta} = Nk_B\beta^2\epsilon^2\left[\frac{e^{\beta\epsilon} + e^{-\beta\epsilon}}{1 + e^{\beta\epsilon} + e^{-\beta\epsilon}} - \frac{(e^{\beta\epsilon} - e^{-\beta\epsilon})^2}{(1 + e^{\beta\epsilon} + e^{-\beta\epsilon})^2}\right].$$

The term in square brackets doesn't simplify to a very compact expression. Any sensible simplification is fine, for example,

$$C_V = Nk_B\beta^2\epsilon^2\left[\frac{1}{1 + e^{\beta\epsilon} + e^{-\beta\epsilon}} + \frac{3}{(1 + e^{\beta\epsilon} + e^{-\beta\epsilon})^2}\right].$$

The free energy is

$$F = -Nk_BT\ln Z = -Nk_BT\ln\left[1 + e^{\beta\epsilon} + e^{-\beta\epsilon}\right].$$

The entropy is

$$S = \frac{U - F}{T} = -Nk_B\,\frac{\epsilon}{k_BT}\,\frac{e^{\beta\epsilon} - e^{-\beta\epsilon}}{1 + e^{\beta\epsilon} + e^{-\beta\epsilon}} + Nk_B\ln\left[1 + e^{\beta\epsilon} + e^{-\beta\epsilon}\right].$$

[2 marks]

(2) (a) Each single-particle energy ϵ_i can hold up to $g_i \times \eta$ particles. Therefore we have $g_i \times \eta$ "boxes" in which to distribute n_i particles, i.e. n_i boxes are full and $\eta \times g_i - n_i$ are empty. The number of ways we can do this for each energy ϵ_i is

$$\Omega_{\epsilon_i} = \frac{(\eta \times g_i)!}{n_i!\,(\eta \times g_i - n_i)!}.$$

Since the number of ways, Ω_{ϵ_i}, to distribute the n_i particles in the various levels, ϵ_i, are independent, the total number of microstates for the distribution $(n_1, n_2, \ldots)$ is the product

$$\Omega(\{n_i\}) = \prod_j \frac{(\eta \times g_j)!}{n_j!\,(\eta \times g_j - n_j)!}.$$

[2 marks]

(b) To find the most probable distribution $(n_i, n_2, \ldots)$, maximize the entropy under the usual constraints of fixed N, U, i.e. maximize

$$\frac{S}{k_B} - \alpha N - \beta U =$$

$$= \sum_i \left[[(\eta \times g_i) \ln(\eta \times g_i) - \eta \times g_i] - (n_i \ln n_i - n_i) - [(\eta \times g_i - n_i) \ln(\eta \times g_i - n_i) - (\eta \times g_i - n_i)] - \alpha n_i - \beta n_i \epsilon_i \right]$$

$$= \sum_i \left[(\eta \times g_i) \ln(\eta \times g_i) - n_i \ln n_i - (\eta \times g_i - n_i) \ln(\eta \times g_i - n_i) - \alpha n_i - \beta n_i \epsilon_i \right].$$

The derivative with respect to any of the n_j is zero, so

$$\begin{aligned}
\frac{\partial}{\partial n_j} \left\{ \frac{S}{k_B} - \alpha N - \beta U \right\} &= 0 \\
-\ln n_j - 1 + \ln(\eta \times g_j - n_j) + 1 - \alpha - \beta \epsilon_j &= 0 \\
\ln(\eta \times g_j / n_j - 1) &= \alpha + \beta \epsilon_j \\
\eta \times g_j / n_j &= e^{\alpha}\, e^{\beta \epsilon_j} + 1 \\
\frac{n_j}{g_j} &= \frac{1}{(e^{\alpha}/\eta)\, e^{\beta \epsilon_j} + (1/\eta)} \\
&= \frac{1}{A\, e^{\beta \epsilon_j} + (1/\eta)}
\end{aligned}$$

where $A = e^{\alpha}/\eta$. [2 marks]

(c) This distribution function reduces to the Fermi Dirac distribution for $\eta = 1$. It reduces to the Maxwell-Boltzmann distribution for large η ($\eta \to \infty$). [2 marks]