Quiz 1: Gibbs Distribution

1. Consider a two-level system with energies 0 and $\varepsilon > 0$ populated by N particles at temperature T. Neglecting quantum exchange effects and interactions between the particles, find

   (a) average occupation numbers of the levels

   (b) entropy per particle and show that it is consistent with $S = \langle \log w(E_n) \rangle$

   (c) average energy per particle

   (d) specific heat

   (e) rms fluctuation of energy per particle

   Investigate all of the above answers in the limits of high and low temperature.

   Solution

   Partition function

$$Z = \sum_{M=0}^{N} \frac{N!}{M!\,(N-M)!} \exp\left(-\frac{M\varepsilon}{T}\right) = \left(1 + \exp\left(-\frac{\varepsilon}{T}\right)\right)^N = Z_1^N$$

   where Z_1 is the one-particle partition function. Average number of particles in each level

$$\frac{n(0)}{N} = \frac{1}{1+\exp(-\varepsilon/T)} = \begin{matrix} 1,\ \varepsilon \gg T \\ 1/2,\ \varepsilon \ll T \end{matrix}$$

$$\frac{n(\varepsilon)}{N} = \frac{\exp(-\varepsilon/T)}{1+\exp(-\varepsilon/T)} = \frac{1}{1+\exp(\varepsilon/T)} = \begin{matrix} 0,\ \varepsilon \gg T \\ 1/2,\ \varepsilon \ll T \end{matrix}$$

   Free energy

$$F_1 = -T \log\left(1 + \exp\left(-\frac{\varepsilon}{T}\right)\right)$$

   Entropy

$$S_1 = -\frac{\partial F_1}{\partial T} = \log\left(1+\exp\left(-\frac{\varepsilon}{T}\right)\right) + \frac{\varepsilon \exp(-\varepsilon/T)}{T(1+\exp(-\varepsilon/T))}$$

$$= \begin{array}{c} (\varepsilon/T)\exp(-\varepsilon/T) \to 0,\ \varepsilon \gg T \\ \log 2 + \varepsilon/2T \to \log 2,\ \varepsilon \ll T \end{array}$$

This is consistent with

$$S_1 = -w(0)\log w(0) - w(\varepsilon)\log w(\varepsilon)$$
$$= \frac{1}{1+\exp(-\varepsilon/T)}\log(1+\exp(-\varepsilon/T)) + \frac{\exp(-\varepsilon/T)}{1+\exp(-\varepsilon/T)}\log\frac{(1+\exp(-\varepsilon/T))}{\exp(-\varepsilon/T)}$$

Notice also that for $\varepsilon \ll T$

$$S = \log\left(\frac{N!}{(N/2)!\,(N/2)!}\right) \approx N\log N - 2\frac{N}{2}\log\frac{N}{2} = N\log 2$$

Energy

$$E_1 = F_1 + TS_1 = \varepsilon\frac{\exp(-\varepsilon/T)}{1+\exp(-\varepsilon/T)} = \frac{\varepsilon}{2}\exp\left(-\frac{\varepsilon}{2T}\right)\mathrm{Sech}\left(\frac{\varepsilon}{2T}\right)$$
$$= \frac{\varepsilon}{1+\exp(\varepsilon/T)} = \begin{array}{c} \varepsilon\exp(-\varepsilon/T) \to 0,\ \varepsilon \gg T \\ \varepsilon/2\,(1-\varepsilon/2T) \to \varepsilon/2,\ \varepsilon \ll T \end{array}$$

Specific heat

$$c = \frac{\partial E_1}{\partial T} = \left(\frac{\varepsilon}{T}\right)^2 \frac{\exp(\varepsilon/T)}{(1+\exp(\varepsilon/T))^2} = \left(\frac{\varepsilon}{2T}\right)^2 \mathrm{Sech}^2\left(\frac{\varepsilon}{2T}\right)$$
$$= \begin{array}{c} (\varepsilon/T)^2\exp(-\varepsilon/T) \to 0,\ \varepsilon \gg T \\ (\varepsilon/2T)^2 + O\left((\varepsilon/2T)^4\right),\ \varepsilon \ll T \end{array}$$

Energy fluctuations

$$\mathrm{rms}\,E_1 = \sqrt{\overline{E_1^2} - \overline{E_1}^2} = \sqrt{\varepsilon^2\frac{1}{(1+\exp(\varepsilon/T))} - \left[\varepsilon\frac{1}{1+\exp(\varepsilon/T)}\right]^2}$$
$$= \varepsilon\sqrt{\frac{\exp(\varepsilon/T)}{(1+\exp(\varepsilon/T))^2}} = \frac{\varepsilon}{2}\mathrm{Sech}\left(\frac{\varepsilon}{2T}\right) = \begin{array}{c} \varepsilon\exp(-\varepsilon/2T) \to 0,\ \varepsilon \gg T \\ \varepsilon/2\,(1-\varepsilon^2/2T^2) \to \varepsilon/2,\ \varepsilon \ll T \end{array}$$

Notice that $\mathrm{rms}\,E_1/E_1 = \exp(\varepsilon/2T) > 1$. However $\overline{E^2} - \overline{E}^2 = N\left(\overline{E_1^2} - \overline{E_1}^2\right)$, while $\overline{E} = N\overline{E}_1$ so that $\mathrm{rms}\,E/\overline{E} = N^{-1/2}\,\mathrm{rms}\,E_1/\overline{E}_1 \to 0$ in the thermodynamic limit $N \to \infty$.

2. Find the Maxwell's distribution in the relativistic limit $\varepsilon = pc$ and evaluate the mean energy and its rms fluctuation.

Solution

$$dw_p = A\exp\left(-\varepsilon/T\right) = A\exp\left(-pc/T\right)d^3p$$

Normalizing

$$\int dw_p = 1 = 4\pi A\int_0^\infty \exp\left(-pc/T\right)p^2dp = 8\pi A\left(\frac{T}{c}\right)^3$$

so that

$$dw_p = \left(\frac{c}{2T\pi^{1/3}}\right)^3 \exp\left(-pc/T\right)d^3p$$

or

$$dw_\varepsilon = \left(\frac{1}{2T\pi^{1/3}}\right)^3 \exp\left(-\varepsilon/T\right)\varepsilon^2 d\varepsilon$$

Mean energy

$$\overline{\varepsilon} = \left(\frac{1}{2T\pi^{1/3}}\right)^3 \int_0^\infty \exp\left(-\varepsilon/T\right)\varepsilon^3 d\varepsilon = 3T$$

and mean squared energy

$$\overline{\varepsilon^2} = \left(\frac{1}{2T\pi^{1/3}}\right)^3 \int_0^\infty \exp\left(-\varepsilon/T\right)\varepsilon^4 d\varepsilon = 12T^2$$

give rms fluctuation

$$\mathrm{rms}\,\varepsilon = \sqrt{\overline{\varepsilon^2} - \overline{\varepsilon}^2} = \sqrt{3}T$$