19. Particle number fluctuations in the grandcanonical ensemble

In the grandcanonical ensemble, the expected values of a quantity $A(\{n_{\boldsymbol{p},s}\})$, which depends on the occupation numbers $n_{\boldsymbol{p},s}$, are calculated according to the relation

$$\langle A\rangle = \frac{1}{\mathcal{Q}(V,\beta,z)}\sum_{N=0}^{+\infty} z^N \sum_{\substack{\{n_{\boldsymbol{p},s}\}\\ \sum n_{\boldsymbol{p},s}=N}} A(\{n_{\boldsymbol{p},s}\})e^{-\beta\sum_{\boldsymbol{p}}\epsilon_{\boldsymbol{p}}n_{\boldsymbol{p},s}} \tag{1}$$

The grandcanonical partition function is given here by

$$\mathcal{Q}(V,\beta,z) = \prod_{\boldsymbol{p},s}[1\mp ze^{-\beta\epsilon_{\boldsymbol{p}}}]^{\mp 1} \tag{2}$$

with a minus in the case of Bose-Einstein statistics and a plus for Fermi-Dirac statistics. Here the occupation numbers $n_{\boldsymbol{p}}$ run through the values $n_{\boldsymbol{p},s}\in\{0,1,2,3,\dots\}$ for bosons and $n_{\boldsymbol{p},s}\in\{0,1\}$ for fermions.

(a) First, using Eq.(1), show the validity of the relation

$$\langle n_{\boldsymbol{p}}\rangle = \sum_{s=-S}^{S}\langle n_{\boldsymbol{p},s}\rangle = -\frac{1}{\beta}\frac{\partial}{\partial\epsilon_{\boldsymbol{p}}}\ln\mathcal{Q} \tag{3}$$

and determine from this the mean occupation numbers

$$\langle n_{\boldsymbol{p}}\rangle = (2S+1)\frac{ze^{-\beta\epsilon_{\boldsymbol{p}}}}{1\mp ze^{-\beta\epsilon_{\boldsymbol{p}}}} \tag{4}$$

with a minus for Bose-Einstein statistics and a plus for Fermi-Dirac statistics. (2 points)

(b) Now derive the relation

$$-\frac{1}{\beta}\frac{\partial\langle n_{\boldsymbol{p}}\rangle}{\partial\epsilon_{\boldsymbol{p}}} = \langle n_{\boldsymbol{p}}^2\rangle - \langle n_{\boldsymbol{p}}\rangle^2 \tag{5}$$

and show that the following holds for the relative particle number fluctuations

$$\frac{\langle n_{\boldsymbol{p}}^2\rangle - \langle n_{\boldsymbol{p}}\rangle^2}{\langle n_{\boldsymbol{p}}\rangle^2} = \frac{1}{\langle n_{\boldsymbol{p}}\rangle}\pm 1, \tag{6}$$

with a plus for Bose-Einstein statistics and a minus for Fermi-Dirac statistics.
(2 points)

20. Ideal Boltzmann gas in the grandcanonical ensemble

Let us consider an ideal of gas of N non-interacting particles of mass m with energy

$$E = \sum_{\boldsymbol{p}} \frac{p^2}{2m} n_{\boldsymbol{p}}. \tag{7}$$

Furthermore, we also assume that the gas is put in contact with a reservoir at the set temperature T and chemical potential μ.

(a) According to the previous exercise, the internal energy of an ideal gas in the grand canonical ensemble should read

$$U = \frac{1}{\mathcal{Q}(V,\beta,z)} \sum_{N=0}^{+\infty} z^N \sum_{\substack{\{n_{\boldsymbol{p}}\} \\ \sum n_{\boldsymbol{p}} = N}} E(\{n_{\boldsymbol{p}}\}) e^{-\beta E}. \tag{8}$$

Show that it can be written in terms of the grand canonical partition function as follows

$$U = -\frac{\partial}{\partial \beta} \ln \mathcal{Q} \tag{9}$$

(1 point)

(b) It was shown during the lecture that in the case of an ideal gas the grand canonical partition function is represented by the following form

$$\mathcal{Q} = \sum_{N=0}^{+\infty} \frac{z^N}{N!} V^N \left(\frac{m k_B T}{2\pi\hbar^2} \right)^{3N/2}. \tag{10}$$

Use the definition of the thermal wavelength $\lambda = \sqrt{\frac{m k_B T}{2\pi\hbar^2}}$, and show that the partition function is given by

$$\mathcal{Q} = e^{zV/\lambda^3} \tag{11}$$

(1 point)

(c) Use Eq(1) and the relation $\frac{PV}{k_B T} = \ln \mathcal{Q}$ to prove that the internal energy can be represented by the equation of state

$$U = \frac{3}{2}PV. \tag{12}$$

(1 point)