Transfer matrix method

1 One dimensional lattice gas

Real interacting gas in one-dimension can be approximated by partitioning a line of length L into M cells of length $a = L/M$. We will moreover assume that the line has periodic boundary conditions and the cells are sufficiently small to only include 0 or 1 particles. We neglect the kinetic energy of the particles and assume that two particles in two nearby cells have an energy of $-\varepsilon$. The gas is found at a temperature T and chemical potential μ. The goal is compute *exactly* the grand-potential $\Omega(L, T, \mu)$, the entropy, and the pressure of the gas.

Solution We designate the index of the cells by α and the occupation of each cell by $n_\alpha \in 0, 1$. Then the grand partition function is given by

$$\Xi = \sum_{N=0}^{M} e^{\beta\mu N} \sum_{\{n_\alpha\}}' e^{\beta\varepsilon \sum_\alpha n_\alpha n_{\alpha+1}}, \tag{1}$$

where $\sum'$ designates the constraint, $\sum_\alpha n_\alpha = N$. We can write it as an unconstrained sum,

$$\Xi = \sum_{\{n_\alpha\}} \exp\left[\beta\mu \sum_\alpha n_\alpha + \beta\varepsilon \sum_{\alpha=1}^{M} n_\alpha n_{\alpha+1}\right]. \tag{2}$$

Unlike the partition functions we saw previously, this is an interacting partition function, which can be solved exactly in a handful of cases. Luckily this is one of them. We note that we can write

$$\exp\left[\beta\mu \sum_\alpha n_\alpha + \beta\varepsilon \sum_{\alpha=1}^{M} n_\alpha n_{\alpha+1}\right] = \exp\left[\beta\mu\frac{(n_1+n_2)}{2} + \beta\varepsilon n_1 n_2\right] \exp\left[\beta\mu\frac{(n_2+n_3)}{2} + \beta\varepsilon n_2 n_3\right] + \cdots \tag{3}$$

$$\times \exp\left[\beta\mu\frac{(n_M+n_1)}{2} + \beta\varepsilon n_M n_1\right],$$

where the last term uses the fact that the line is closed into a ring. We further note that for example for $M = 3$, the product

$$\sum_{n_1 n_2 n_3} \exp\left[\beta\mu\frac{(n_1+n_2)}{2} + \beta\varepsilon n_1 n_2\right] \exp\left[\beta\mu\frac{(n_2+n_3)}{2} + \beta\varepsilon n_2 n_3\right] \exp\left[\beta\mu\frac{(n_3+n_1)}{2} + \beta\varepsilon n_3 n_1\right], \tag{4}$$

can be written as the trace of three identical matrices,

$$\mathrm{Tr}\ T^3, \tag{5}$$

where

$$T_{n_1 n_2} = \exp\left[\beta\mu\frac{(n_1+n_2)}{2} + \beta\varepsilon n_1 n_2\right] = \begin{pmatrix} 1 & e^{\frac{1}{2}\beta\mu} \\ e^{\frac{1}{2}\beta\mu} & e^{\beta(\mu+\varepsilon)} \end{pmatrix}. \tag{6}$$

Therefore for generic M we have,

$$\Xi = \mathrm{Tr}\ T^M = \mathrm{Tr}\ UU^{-1}T^M = \mathrm{Tr}\ U^{-1}T^M U = \lambda_1^M + \lambda_2^M \tag{7}$$

where in the last two equalities we used U the matrix which diagonalizes T, and the cyclic property of the trace. The fundamental equation for T is given by,

$$\lambda^2 - \left(1 + e^{\beta(\mu+\varepsilon)}\right)\lambda + \left(e^{\beta(\mu+\varepsilon)} - e^{\beta\mu}\right) = 0 \tag{8}$$

Therefore,

$$\begin{aligned} \lambda_{1,2} &= \frac{1+e^{\beta(\mu+\varepsilon)}}{2} \pm \sqrt{\frac{\left(1-e^{\beta(\mu+\varepsilon)}\right)^2}{4} + e^{\beta\mu}} \\ &= e^{\frac{\beta(\mu+\varepsilon)}{2}}\left\{\cosh\frac{\beta}{2}(\mu+\varepsilon) \pm \sqrt{\sinh^2\frac{\beta}{2}(\mu+\varepsilon) + e^{-\beta\varepsilon}}\right\}, \end{aligned} \tag{9}$$

in the thermodynamic limit we have,

$$-P = \frac{\Omega}{L} = \lim_{M\to\infty}\frac{-\frac{1}{\beta}\ln\Xi}{Ma} = -\frac{(\mu+\varepsilon)}{2} - \frac{1}{\beta}\ln\left\{\cosh\frac{\beta}{2}(\mu+\varepsilon) + \sqrt{\sinh^2\frac{\beta}{2}(\mu+\varepsilon) + e^{-\beta\varepsilon}}\right\}, \tag{10}$$

where we used $\Omega = -PV$, which follows from the fundamental equation of thermodynamics. Therefore the pressure of the gas is,

$$P(\mu, T) = \frac{(\mu+\varepsilon)}{2} + \frac{1}{\beta}\ln\left\{\cosh\frac{\beta}{2}(\mu+\varepsilon) + \sqrt{\sinh^2\frac{\beta}{2}(\mu+\varepsilon) + e^{-\beta\varepsilon}}\right\}, \tag{11}$$

and the entropy is,

$$S = -\left(\frac{\partial\Omega}{\partial T}\right)_\mu. \tag{12}$$

Particle number fluctuations (which is proportional to isothermal compressibility) are given by,

$$\frac{\beta}{L}\left[\left\langle N^2\right\rangle - \left\langle N\right\rangle^2\right] = \left(\frac{\partial^2 P}{\partial\mu^2}\right)_{T,M} \tag{13}$$

We would like to note in passing that Ω/L is analytic for $T > 0$, and therefore there is not phase-transition in this model except at $T = 0$.