Hand-in sheet 1 – Statistical Physics B

- *Please hand in your solution before Thursday 17 October 2024, 16:15.*
- *You can hand in your solutions in digital format as a pdf-file. Make sure to provide a file name which contains the hand-in number, your name, and your student number. You can send your solution to jeffrey.everts AT fuw.edu.pl. Also include your name and student number in the pdf file.*
- *In case of paper format, please do not forget to write your name and student number.*
- *Make sure to answer every question as completely as possible. When you do calculations, provide sufficient explanation for all steps.*
- *In total 100 points can be earned.*

A one-dimensional interacting gas

In some cases the partition function can be computed analytically, even for an interacting system. Consider a line of length L with N particles denoted with positions $x_1, ..., x_N$ and linear momenta $p_1, ..., p_N$, where $x_i \in [0, L]$ and $p_i \in (-\infty, \infty)$. There are fixed particles at $x_0 = 0$ and $x_{N+1} = L$, which effectively act as external potentials confining the particles to the line. The Hamiltonian is

$$H(p^N, x^N) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \Phi(x^N), \quad \Phi(x^N) = \sum_{i=1}^{N} \left[\sum_{j>i} v(|x_i - x_j|) + v(x_i) + v(L - x_i) \right]. \tag{1}$$

Observe that the second and third term in $\Phi(x^N)$ denote external potentials. Furthermore, we assume that $v(r)$ is of the form

$$v(x) = \begin{cases} \infty, & |x| < \sigma, \\ \varphi(x), & \sigma < |x| < 2\sigma, \\ 0, & |x| > 2\sigma. \end{cases} \tag{2}$$

This means all particles have a hard "core" and only interact with their immediate neighbours, i.e. we only include nearest-neighbour interactions (not the same as pair-wise additive).

(a) (*15 points*) Show that the canonical partition function can be written as

$$Z(N, L, T) = \frac{1}{\Lambda^N} \int_0^L dx_N \int_0^{x_N} dx_{N-1} ... \int_0^{x_2} dx_1 \exp\left[-\beta \sum_{i=1}^{N+1} v(x_i - x_{i-1}) \right]. \tag{3}$$

Give an expression for Λ and give a physical interpretation for this quantity.

(b) (*10 points*) Use the result of a. to derive the recursion relation

$$Z(N, L, T) = \frac{1}{\Lambda} \int_0^L dx_N \exp[-\beta v(L - x_N)] Z(N-1, x_N, T). \tag{4}$$

(c) (*15 points*) Define the Laplace transform $\mathcal{L}$ of a function f as $\mathcal{L}[f](s) = \hat{f}(s) = \int_0^\infty dx \exp(-sx) f(x)$. Specifically introduce $J(x) = \exp[-\beta v(x)]$ and show that

$$\hat{Z}(N, s, T) = \frac{1}{\Lambda^N} [\hat{J}(s)]^{N+1}. \tag{5}$$

(d) (*10 points*) Instead of performing the inverse Laplace transform of the result in (c), we perform an easier approach. Perform a Legendre transformation to go to the (N, p, T) ensemble (isobaric-isothermal ensemble). What is the relevant thermodynamic potential? Give an expression in terms of the chemical potential. Give an expression for the total differential of the thermodynamic potential.

(e) (*10 points*) The partition function in the (N, p, T) ensemble is

$$\Delta(N, p, T) = \frac{1}{\Lambda} \int_0^\infty dL \, \exp(-\beta p L) Z(N, L, T) \tag{6}$$

How does it relate to the thermodynamic potential in (d)? Show that for $N \to \infty$ that the fugacity is $z(p, T) = 1/\hat{J}(\beta p)$, with $z(p, T) = \exp(\beta\mu)/\Lambda$.

(f) (*10 points*) The average line density is $\rho = N/L$. Show that

$$\rho = -\frac{\hat{J}(\beta p)}{\hat{J}'(\beta p)}, \tag{7}$$

with a prime denoting differentiation to the argument.

(g) (*15 points*) Find the equation of state $p(\rho, T)$ for a hard-line system (the so-called Tonks gas), with $v(x) = \infty$ for $|x| < \sigma$ and zero otherwise.

(h) (*15 points*) Compute the isothermal compressibility κ_T and show that

$$\kappa_T = -\frac{1}{L}\left(\frac{\partial L}{\partial p}\right)_{N,T} = \frac{\beta N}{L}[\langle y^2 \rangle - \langle y \rangle^2]. \tag{8}$$

with $y = x_{i+1} - x_i$. Is it possible to have a long-range ordered lattice in one dimension?