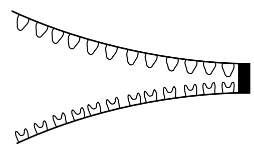
Statistical Physics
Assignment 4

Lecture: Prof. Dr. Otfried Gühne
Tutorial: Leonardo Novo, Tobias Moroder, Fri 8–10, Room: D115

Due to: Tue, 08.05

1. **Zipper molecule** (4 Points)
   Consider two chain molecules A and B with different reaction center $k = 0, \ldots, N$. The molecules are connected at $k = 0$ such that at most N of these center are free. Both chains close like a zipper, *i.e.*, the center k can only bind if already all previous groups $l < k$ are closed. The binding energy between a single group is ε.

   (a) Compute the mean number of open bindings $\langle G \rangle$ as a function of the temperature. (Hint: Start with the Hamiltonian – the quantum states for g and j open bounds satisfy $\langle g|j \rangle = \delta_{gj}$.)
   (b) Consider $\langle G \rangle$ for the high and low temperature regime.
   (c) Consider $\langle G \rangle$ and $\langle G \rangle / N$ for large chains.
   (d) Consider $\langle G \rangle$ for fixed temperature T but vanishing binding energy ε with (i) N fixed or (ii) εN fixed.

2. **Pressure ensemble** (4 Points)
   The grand canconical ensemble describes the situation of fluctuating particle number at constant volume. Now let us consider the opposite case of fluctuating volume but fixed particle number. In this scenario the partition function becomes
   $$Z_p = \sum_i \exp[-\beta(E_i + pV_i)] \tag{1}$$
   summed over all micro-states with energy E_i and volume V_i. The mean volume V is now controlled by the pressure p.

   As an example consider a linear molecule consisting of N building blocks. Each block can take two possible sizes, a small s or large one l. The configuration with length l comes at zero energy, while length s requires $\varepsilon > 0$.

   (a) Compute the partition function Z_p as a function of the temperature and the pressure.
   (b) Compute the mean length and discuss the two cases $p \to \pm\infty$.

3. **Electron in a box** *
   An electron of a threadlike molecule on a ring of length L (electron in a box of length L with periodic boundary conditions) takes on the energies
   $$E_n = \frac{\hbar^2}{2m} \left(\frac{2\pi n}{L} \right)^2 \tag{2}$$
   with $n \in \mathbb{Z}$.

   (a) Our first goal is the partition function for the case of large L. This can be evaluated using the first order approximation of the infinite sum via an integral, that can be derived from
   $$\int_0^\infty dx f(x) = \sum_{n=0}^{\infty} \int_0^1 ds f(n+s), \tag{3}$$
   using Taylor expansion of $f(n+s)$ around n. Note that electrons are spin-$\frac{1}{2}$ particles.
   (b) Compute the mean energy of the system as a function of the temperature.