Homework 5, Statistical Mechanics: Concepts and applications
2018/19 ICFP Master (first year)

Werner Krauth, Victor Dagard

(Dated: October 7, 2018)

In lecture 05 (physics in one dimension) we treated the one-dimensional hard-sphere model and the one-dimensional Ising model. In this homework session, you will study variations on these two themes.

I. "TRANSFER MATRIX" SOLUTION OF THE ONE-DIMENSIONAL HARD-SPHERE MODEL

In lecture 5, we determined the partition function of the (distinguishable-particle) one-dimensional hard-sphere model, using two transformations of variables. For spheres of radius σ, the result obtained was

$$Z^{\text{dist.}}_{N,L} = \begin{cases} (L-2N\sigma)^N & \text{if } L-2N\sigma \geq 0 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

(see also SMAC section 6.1, p. 270, note that we consider the distinguishable-particle partition function. The indistinguishable is defined by $Z^{\text{indist.}}_{N,L} = Z^{\text{dist.}}_{N,L}/N!$). We also used a recursion-type argument to obtain the same result for $N = 3$. In fact, we obtained:

$$Z^{\text{indist.}}_{3,L} = \int_{3\sigma}^{L-3\sigma} dx Z_{1,x-\sigma} Z_{1,L-x-\sigma}. \tag{2}$$

- What is the interpretation of eq. (2) in physical terms (one sentence)?
- Evaluate eq. (2), and check that the value of $Z_{3,L}$ it produces is compatible with what we obtained by the transformation method (use mathematica or sage or Wolfram alpha, etc).
- Generalize to arbitrary N, that is, express $Z^{\text{indist.}}_{N+1,L}$ through $Z_{1,..}$ and $Z^{\text{indist.}}_{N-1,...}$, and evaluate the corresponding one-dimensional integral (use mathematica or sage or Wolfram alpha, etc). please indicate the command line you programmed).

II. DENSITY PROFILE OF THE ONE-DIMENSIONAL HARD-SPHERE MODEL

In lecture 5, we obtained the density profile $\pi(x)$, the probability to have a disk of the one-dimensional hard-sphere model at position x as follows:

$$\pi(x) = \frac{\{\text{partition function, restricted to having one particle at } x\}}{Z_{N,L}}$$
$$= \frac{1}{Z_{N,L}} \binom{N-1}{k} Z_{k,x-\sigma} Z_{N-1-k,L-x-\sigma}, \quad (3)$$

where all the partition functions are distinguishable (as in eq. (1)).

- What is the interpretation of eq. (3) in physical terms (one or two sentences)?
- Write a computer program to evaluate eq. (2) (make sure to program both cases in eq. (1), so that you can take the unrestricted sum over k for all x). Plot $\pi(x)$ for different densities, for example for $N = 15$. Comment what you see. You can also use larger N, if you want to.

III. QUASI ONE-DIMENSIONAL JAMMED DISKS AND THEIR TRANSFER MATRIX

In lecture 5, we introduced the concept of a transfer matrix. In the present short exercise, you will study the concept of a transfer matrix as a general tool to set up an iteration. We consider hard disks of diameter σ in a closed channel with a piston that exerts infinite pressure so that, at a difference with what we considered in the lecture, all configurations are jammed (see fig. 1): Each disk touches one of the walls, and each inner disk touches two other disks and it cannot make an infinitesimal local move. The channel width is smaller than $\sigma(1 + \sqrt{3/4})$, so all disks are truly jammed. Clearly, temperature plays no role in this problem.

NB Fibonacci sequence ($F_0 = 0, F_1 = 1, F_2 = 1, 2, 3, 5, 8, ...$)

- Sketch the longest jammed configuration of N disks, and the shortest jammed configuration of N disks (shortest and longest are with respect to the length of the channel).
- Starting from the four jammed configurations with two disks (see fig. 2), compute the number of jammed configurations with three disks (two bonds), and the number of jammed configurations with four disks (three bonds) (Hint: this is analogous to the transfer matrix calculation in lecture 5 for the open Ising chain (without periodic boundary conditions) that used $Z^{\uparrow}$ and $Z^{\downarrow}$).

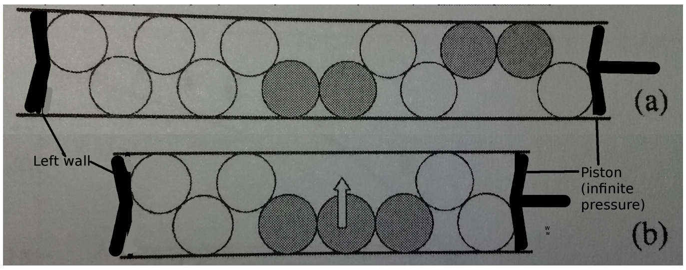

FIG. 1: A jammed (upper) and an unjammed (lower) configuration. We may imagine a piston pushing from the right side, with infinite pressure. Notice the slight wedge shape of the piston and bottom (left) plate.

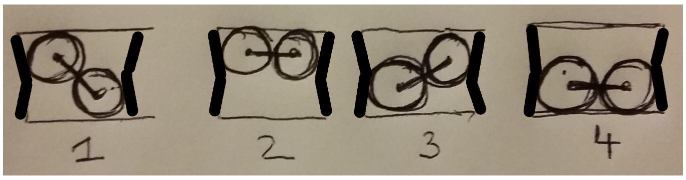

FIG. 2: The four jammed configurations with two disks (one bond). Notice again the slight wedge shape of the piston and bottom (left) plate.

- What is the total number of jammed configurations of N disks, in terms of a famous sequence?
- Write down the transfer matrix for this simple problem, and interprete the above findings in terms of the transfer matrix. What is the largest eigenvalue of this transfer matrix? Do you know the name of this number?
- Use the transfer matrix to compute the number of jammed configurations of N disks, but now starting from only a single configuration to the left, namely the configuration "1" of fig. 2.