Homework 5, Statistical Mechanics: Concepts and applications 2019/20 ICFP Master (first year)

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With solutions. NB: Exercise 3 was an exam question in the final exam of the 2015/16 course

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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

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

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

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

- What is the interpretation of eq. (2) in physical terms (one sentence)?

  A three-particle system is equivalent to two one particle systems, whose lengths add up to the length of the three-particle system.

- 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).

$$
\begin{aligned}
Z_{3,L}^{indist} &= \int_{3\sigma}^{L-3\sigma} dx Z_{1,x-\sigma} Z_{1,L-x-\sigma} \\
&= \int_{3\sigma}^{L-3\sigma} dx (x-\sigma-2\sigma)(L-x-\sigma-2\sigma) \\
&= \int_{0}^{L-6\sigma} dx x (L-6\sigma-x) \\
&= \frac{1}{3!}(L-6\sigma)^3
\end{aligned}
$$

- 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).

$$
Z_{N+1,L}^{indist} = \int_{(2N-1)\sigma}^{L-3\sigma} dx Z_{N-1,x-\sigma}^{indist} Z_{1,L-x-\sigma}
$$

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:

$$
\begin{aligned}
\pi(x) = \frac{\{\text{partition function, restricted to having one particle at } x\}}{Z_{N,L}} \\
= \frac{1}{Z_{N,L}} \sum_{k=0}^{N-1} \binom{N-1}{k} Z_{k,x-\sigma} Z_{N-1-k,L-x-\sigma}, \quad (3)
\end{aligned}
$$

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)?

  The probability of having one disk at position x is the sum of the probabilities of having k particle to the left of it and $N-k-1$ particles to the right of it.

- 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.

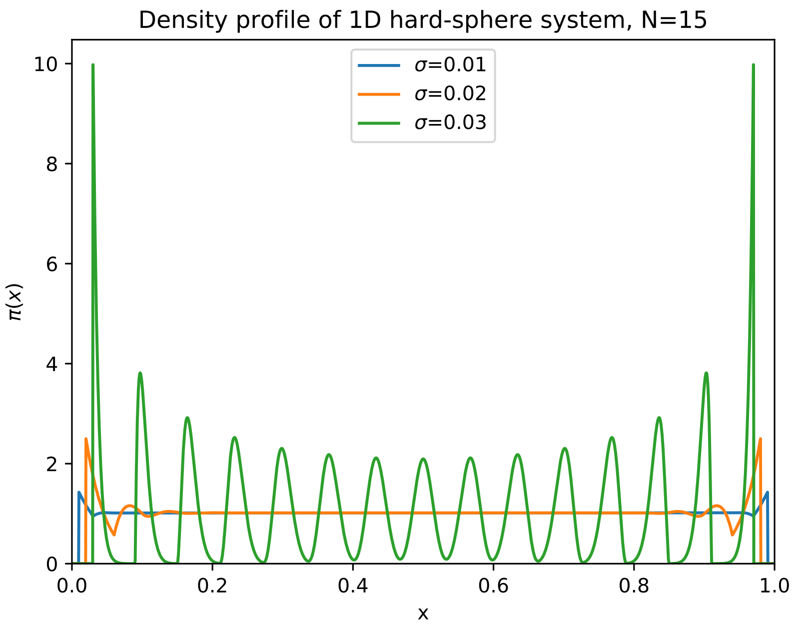

FIG. 1: The density profile of the 1D hard-sphere system, with different radius of the disks.

The density profile is in Fig. 1. When the radius is small ($\sigma = 0.01$), the PDF is almost flat. There are two prohibited region, due to the non-trivial size of the spheres. At the boundaries, the PDF is dominated by the first(last) particle in the system, and this is why there are peaks. When the radius is larger, for example $\sigma = 0.03$, only 10% of the system is empty and the free space for each sphere to move is smaller than the size of the spheres. Thus, the spheres are stuck at where they are supposed to be and there are peaks in the PDF. The full understanding of the structure is the object of the famous Asakura–Oosawa theory of depletion, and it is non-trivial.

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

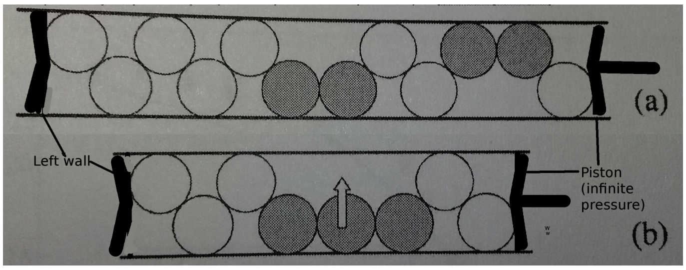

FIG. 2: A jammed (upper) and an unjammed (lower) configuration. We may imagine a piston pushing from the right side, with infinite pressure. Notice the slight wedge shape of the piston and bottom (left) plate.

- 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).

  As shown in Fig. 3, for two neighbouring disks, the distance in the x direction is shorter when the configuration is 1 or 3. These configurations will be referred to as short bonds, and configuration 2, 4 will be referred to as long bonds. As shown in the Fig. 3, in the shortest jammed configuration, there are only short bonds. However, if there are more than two long bonds in a row, the configuration is no longer jammed. Thus, the longest jammed configuration has a short bond every long bond.

- Starting from the four jammed configurations with two disks (see Fig. 4), 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 $Z^{\downarrow}$).

  Two methods can be used to build the transfer matrix:

  Method 1:

  All the jammed configurations are divided into 4 classes: the configurations end with 1,

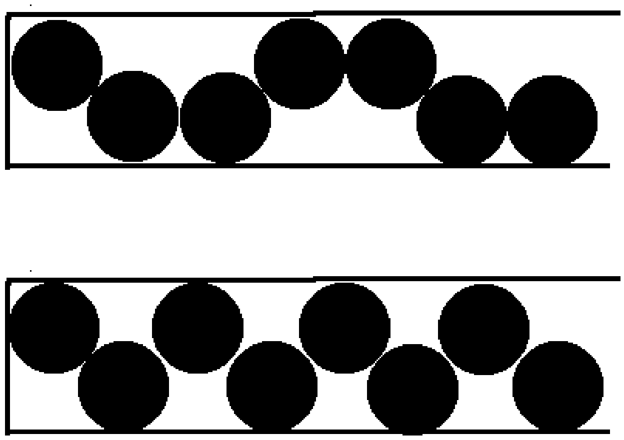

FIG. 3: The longest and shortest jammed configuration.

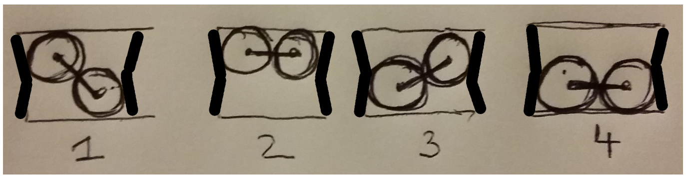

FIG. 4: The four jammed configurations with two disks (one bond). Notice again the slight wedge shape of the piston and bottom (left) plate.

2, 3, and 4 (Fig. 2). The number of configurations in a N particle system in each class could be written in a vector $(n_{N,1}, n_{N,2}, n_{N,3}, n_{N,4})^T$. When adding a new particle in the system, all of the jammed configurations could be found by adding a particle to the existing jammed configurations. For a configuration end with 1, adding a particle yields configurations of $N+1$ particles which ends with 3 or 4. For a configuration which ends with 2, adding a particle yields a configuration which ends with 1. (There should be another configuration, however, it is not jammed.) Expressing these relation using vector and matrix:

$$\begin{pmatrix} n_{N+1,1} \\ n_{N+1,2} \\ n_{N+1,3} \\ n_{N+1,4} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} n_{N,1} \\ n_{N,2} \\ n_{N,3} \\ n_{N,4} \end{pmatrix}$$

And the matrix here is the transfer matrix.

Method2:

With all of the jammed configurations of the N-1 and N-particle system, the jammed configurations of a N+1-particle system can always be found in two steps. Firstly, for each of the configurations in a N-particle system, there is always a corresponding jammed configuration in a N+1-particle system. All the new configurations, which end with a short bonds, can be found by adding particles which form short bonds at the end of the N-particle systems. Thus, there are n_N *jammed configuration in a N+1-particle system which end with short bonds. (Here the number of jammed configurations in a N-particle system is denoted by* n_N*). The rest of jammed configurations can be found by adding a particle, which creates a long bound, at the end of the systems, which end with short bonds. The number of jammed configurations, which end with short bonds, is exactly* n_{N-1}*. Thus, there is following relation:*

$$n_{N+1} = n_N + n_{N-1}$$

Expressing this relation by matrix,

$$\begin{pmatrix} n_{N+1} \\ n_N \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} n_N \\ n_{N-1} \end{pmatrix} \tag{4}$$

This is also the recursive formula for the Fibonacci sequence.

For a one particle system, there are 2 jammed configurations. Thus,

$$\begin{pmatrix} n_2 \\ n_1 \end{pmatrix} = 2\begin{pmatrix} F_3 \\ F_2 \end{pmatrix}$$

Since n_N *and* F_N *have identical recursive formula,*

$$n_N = 2F_{N+1}$$

Thus, $n_3 = 6$ *and* $n_4 = 10$*. These result can also be validated explicitly by finding out all the jammed configurations.*

- What is the total number of jammed configurations of N disks, in terms of a famous sequence?

  Starting from configuration 1, 2, 3, and 4, the total number of jammed configurations in a N-particle system is $2F_{n+1}$*.*

- 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?

The transfer matrix is

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$$

The eigenvalues are $(1 \pm \sqrt{5})/2$. *The larger one is also known as golden ratio. For the* 4×4 *transfer matrix, the largest eigenvalue is also* $(\sqrt{5}+1)/2$.

- 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. 4.

The eigenvectors of the transfer matrix are (not normalized)

$$e_{\pm} = \begin{pmatrix} \frac{1 \pm \sqrt{5}}{2} \\ 1 \end{pmatrix}$$

And,

$$\begin{pmatrix} F_1 \\ F_0 \end{pmatrix} = \frac{1}{\sqrt{5}}(e_+ - e_-)$$

Thus,

$$\begin{pmatrix} F_N \\ F_N - 1 \end{pmatrix} = \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^{N-1} e_+ - \left(\frac{1-\sqrt{5}}{2} \right)^{N-1} e_- \right]$$

and

$$F_N = \frac{1}{\sqrt{5}} \left[\left(\frac{1+\sqrt{5}}{2} \right)^{N} - \left(\frac{1-\sqrt{5}}{2} \right)^{N} \right]$$

Adding one particle to configuration 1 gives 3-particle systems which end with configuration 3 and 4. And, due to the symmetry of the problem, the jammed configuration, produced by adding particles to configuration 3 and 4 account for a half of the jammed configurations. Thus, the number of jammed configuration is F_N.