Lecture 5, Statistical Mechanics: Concepts and applications 2017/18 ICFP Master (first year): Hard spheres and the Ising model in one dimension (Transfer matrix 1/2)

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In this lecture, we introduce, on the one hand, to the statistical physics of one-dimensional systems. We treat one particle system, namely the one-dimensioanal gas of hard spheres, and one spin systems, namely the one-dimensional Ising model. These models are both exactly solvable using, among others, the transfer matrix method.

We will thus introduce to the fundamental tool in classical statistical mechanics called the "Transfer Matrix". Knowing the eigenvalues of the transfer matrix constitutes the solution of the corresponding modle. At the end of the lecture, we will discuss the fundamental reasons why there is no phase transition. This will lead us to a discussion of the Frobenius-Perron theorem, on the one hand, but also to a discussion of domain walls, on the other.

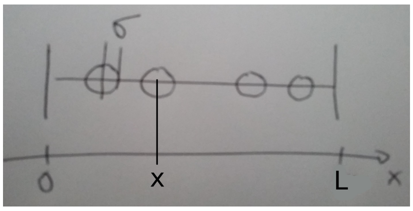

FIG. 1: $N = 4$ one-dimensional hard spheres of radius σ on an interval of length L, without periodic boundary conditions. Many of the properties of this model can be solved analytically. The position x of each sphere is taken to be the x-value of its center.

I. ONE-DIMENSIONAL HARD SPHERES

The one-dimensional hard-sphere model is exactly solvable (its thermodynamics and some of its structural properties can be obtained in closed form). We will compute the equation of state, check the equivalence of ensembles, introduce to the virial expansion, and compute (what amounts to) correlation functions. In a nutshell, the model can be mapped to non-interacting particles. It is amazing how such non-interacting variables can give rise to highly non-trivial correlation functions, that have a physical interpretation, and that are so intricate that not all is known analytically about them.

We consider, as in Fig. 2, N one-dimensional spheres in a box of finite volume L without any other interaction than the hard-sphere repulsion. This is the one-dimensional analogue of the 2D disks case repulsion. The particles have of course momenta, in addition to their positions.

A. One-dimensional hard spheres - partition function

We can write down the partition function of this system is given by

$$Z_{N,L} = \int_{\sigma}^{L-\sigma} dx_1 \cdots \int_{\sigma}^{L-\sigma} dx_N \pi(x_1, \ldots, x_N), \tag{1}$$

where the Boltzmann weight π

$$\pi(x_1, \ldots, x_N) = \pi(x_{P_1}, \ldots, x_{P_N}) = \begin{cases} 1 & \text{if legal} \\ 0 & \text{otherwise} \end{cases}$$

Note that it is symmetric under permutations. One often multiplies the partition function of eq. (1) by a factor $1/N!$, in order to avoid the socalled Gibbs paradox. The question of the presence or not of this factor $1/N!$ is very interesting, and it has nothing to do with quantum mechanics, see[1]. We will just leave it out.

B. Partition function, derivation by integration and mapping

The statistical weight π, as indicated, and also the integration domain, are totally symmetric under permutations $(P_1 \dots P_N)$, so that we are free to choose one of the $N!$ permutations, and multiply the integral with this same factor $N!$:

$$Z_{N,L} = N! \int_\sigma^{L-\sigma} dx_1 \cdots \int_\sigma^{L-\sigma} dx_N \pi(x_1, \dots, x_N) \Theta(x_1, \dots, x_N) \tag{2}$$

(the function Θ is equal to one if $x_1 < x_2 < \cdots < x_N$ and zero otherwise). Now, let us change variables $x \to y$ in the integral, but later apply it also to the samples

$$y_1 = x_1 - \sigma, \; \dots, \; y_k = x_k - (2k-1)\sigma, \; \dots, \; y_N = x_N - (2N-1)\sigma,$$

we obtain the integral

$$Z_{N,L} = N! \int_0^{L-2N\sigma} dy_1 \cdots \int_0^{L-2N\sigma} dy_N \Theta(y_1, \dots, y_N), \tag{3}$$

Look at this integral: the bounds for $y_1, y_2, \dots$ are again symmetric, and we can undo the trick that brought us from eq. (**??**) to eq. (**??**) by suppressing the ordering of the variables y and also the factor $N!$. We arrive at:

$$Z_{N,L} = \int_0^{L-2N\sigma} dy_1 \cdots \int_0^{L-2N\sigma} dy_N = \begin{cases} (L-2N\sigma)^N & \text{if } L > 2N\sigma \\ 0 & \text{otherwise} \end{cases}. \tag{4}$$

We may rewrite the partition function in terms of the density $\rho = 2\sigma N/L$

$$Z_{N,\rho} = \begin{cases} L^N(1-\rho)^N & \text{if } \rho < 1 \\ 0 & \text{otherwise} \end{cases}. \tag{5}$$

We see that this is an analytic function for all N and all ρ, and even that the free energy per particle $-\log Z/N$ is an analytic function, so that this model has no phase transition at finitie density.

If we study the transformation from the x_i to the y_i, we notice that the y describe trivial non-interacting point-particles on an interval between 0 and $L - 2N\sigma$.

C. Partition function, Transfer-matrix derivation

The second derivation of the one-d hard-sphere partition function uses a transfer-matrix strategy. Let us first compute the partition function for $N = 1$. Evidently it is given by $Z_1 = L - 2\sigma$ (of course only if $L \geq 2\sigma$). It is zero otherwise. Now we immediately go from one to three spheres. The middle of the three can be transformed into a wall. We find that

$$\begin{aligned} Z_{3,L} &= \int_{3\sigma}^{L-3\sigma} Z_{1,x-\sigma} Z_{1,L-x-\sigma} && (6) \\ &= \int_{3\sigma}^{L-3\sigma} (x-3\sigma)(L-x-3\sigma) && (7) \\ &= \frac{1}{6}(L-6\sigma)^3 && (8) \\ &= \frac{1}{3!}(L-2N\sigma)^3 && (9) \end{aligned}$$

The general case is relegated to the homework session of this lecture.

D. Pressure and the equivalence of ensembles

E. The virial expansion

F. Correlation function

Computing[2] the probability to be at x, for one-dimensional hard spheres, is represented by the statistical weight of having a particle at x and then k more spheres to the left of x and $N-1-k$ spheres to its right. As, initially, we have to choose one sphere out of N to put it at x and then k spheres out of the remaining $N-1$, x is given by the sum of the statistical weights of putting k disks to the left (in the remaining left interval of length $x-\sigma$ and the $N-1$ remaining disks to the right (length of interval $L-x-\sigma$

$$\pi(x) = \sum_k \sum \tag{10}$$

Figures/One_d_hard_sphere_correlation_function.jpg

FIG. 2: Correlation function of the one-dimensional hard-sphere gas. It is computed by placing a first sphere at position x and by asking about the statistical weight of all possible configurations of k spheres to the left and $N-1-k$ spheres to the right.

The function $\pi(x)$ is easy to write down, and also to evaluate numerically (this is done in program. You will notice that this function is exactly equal t what we can obtain by the sampling approach of Section **??** (see Fig. **??**). It is also very interesting that, for$\rho < 1/2$, there is a central region, where the density $\pi(x)$ is strictly independent of . This not so simple problem was treated in a paper in Journal of Mathematical Physics (!)[?] , that provides a valid proof (in pp. to pp..), but that is not so easy to follow.

Computing the envelope of $pi(x)$, otherwise than by the explicit summation, is a hopeless endeavor for finite N, but it is easier to analyze in the $N \to \infty$ limit.

G. One-dimensional hard spheres - correlation functions

One might think that in the problem of one-dimensional hard spheres, all we did was to consider boundary effects close to a wall. After all, in the center of the system, the density is constant.

To nevertheless show that the problem that we just treated is very relevant to bulk systems, we look at the equivalence of N spheres on a ring (or on an interval of length L with periodic boundary conditions

II. ONE-DIMENSIONAL ISING MODEL

A. Partition function, Transfer-matrix derivation $h = 0$

We consider the Ising model in one dimensions (Ising chain), for the moment without a magnetic field. The hamiltonian (the energy) of the system is given by

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1}. \tag{11}$$

1. *Open boundary conditions*

Let us first compute the partition function for two sites ($N = 2$) without periodic boundary conditions. It is given by the following four configurations and the partition function is the sum of their statistical weights:

$$Z_2 = \sum \begin{matrix} \uparrow\uparrow & \mathrm{e}^{\beta J} \\ \uparrow\downarrow & \mathrm{e}^{-\beta J} \\ \downarrow\uparrow & \mathrm{e}^{-\beta J} \\ \downarrow\downarrow & \mathrm{e}^{\beta J} \end{matrix} = 2\left(\mathrm{e}^{\beta J} + \mathrm{e}^{-\beta J}\right) = 4\cosh(\beta J). \tag{12}$$

In a typical "transfer-matrix" approach, we can now move from the partition function with $N - 1$ spins to the partition function with N spins and find:

$$Z_N = \sum \begin{matrix} \boxed{\ldots\uparrow}\downarrow & = \frac{1}{2} Z_{N-1} \exp(-\beta J) \\ \boxed{\ldots\uparrow}\uparrow & = \frac{1}{2} Z_{N-1} \exp(\beta J) \\ \boxed{\ldots\downarrow}\downarrow & = \frac{1}{2} Z_{N-1} \exp(\beta J) \\ \boxed{\ldots\downarrow}\uparrow & = \frac{1}{2} Z_{N-1} \exp(-\beta J) \end{matrix} = 2\left(\mathrm{e}^{\beta J} + \mathrm{e}^{-\beta J}\right) = 4\cosh(\beta J) \tag{13}$$

where each of the boxes contains all the configurations of $N - 1$ spins with the spin $N - 1$ oriented as indicated.

where we notice that the basic symmetry between up and down spins requires that the partition function of a system of $N - 1$ spins with the final spin in up position is simply $\frac{1}{2} Z_{N-1}$. We find

$$Z_N = Z_{N-1}\left[2\cosh(\beta J)\right] = Z_2\left[2\cosh(\beta J)\right]^{N-2} = 2\left[2\cosh(\beta J)\right]^{N-1} \tag{14}$$

so that one has

$$F = -kT \log Z_N = \frac{1}{\beta}\left[\log 2 + (N-1)\log\left[2\cosh(\beta J)\right]\right] \tag{15}$$

Clearly this is an analytic function at all temperatures and there is no phase transition.

We used in eq. (13) that the partition function $Z^{\downarrow}_{N-1} = \boxed{\ldots\downarrow}$ was the same as $Z^{\uparrow}_{N-1} = \boxed{\ldots\uparrow}$. More generally, we have that

$$Z^{\uparrow}_N = Z^{\uparrow}_{N-1} \times \uparrow\uparrow + Z^{\downarrow}_{N-1} \times \downarrow\uparrow \tag{16}$$

$$Z^{\downarrow}_N = Z^{\uparrow}_{N-1} \times \uparrow\downarrow + Z^{\downarrow}_{N-1} \times \downarrow\downarrow, \tag{17}$$

where we remember that $Z^{\uparrow}_N$ is the partition function of the Ising model with the restriction that the final spin (spin N) is "up".

We write eq. (17) as

$$\begin{bmatrix} Z^{\uparrow}_N \\ Z^{\downarrow}_N \end{bmatrix} = \underbrace{\begin{bmatrix} \mathrm{e}^{\beta J} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta J} \end{bmatrix}}_{\text{Transfer Matrix } T} \begin{bmatrix} Z^{\uparrow}_{N-1} \\ Z^{\downarrow}_{N-1} \end{bmatrix} \tag{18}$$

where the 2×2 matrix here is called the transfer matrix. Clearly we have:

$$\begin{bmatrix} Z^{\uparrow}_N \\ Z^{\downarrow}_N \end{bmatrix} = T^{N-1} \begin{bmatrix} Z^{\uparrow}_1 \\ Z^{\downarrow}_1 \end{bmatrix} \tag{19}$$

With $Z^{\uparrow}_1 = Z^{\downarrow}_1 = 1$, you easily check the value of eq. (**??**) for Z_2.

2. Periodic boundary conditions

Let us now consider the Ising chain of N spins with periodic boundary conditions. This is the same as an Ising chain on $N+1$ spins with open boundary conditions and two additional conditions:

1. If spin 1 is $\uparrow$, then spin $N+1$ is $\uparrow$.
2. If spin 1 is $\downarrow$, then spin $N+1$ is $\downarrow$.

We can impose these two condition separately by considering only $Z^{\uparrow}_{N+1}$ for the case where $[Z^{\uparrow}_1, Z^{\downarrow}_1] = [1, 0]$ and by considering only $Z^{\downarrow}_{N+1}$ for the case where $[Z^{\uparrow}_1, Z^{\downarrow}_1] = [0, 1]$. We find that the partition function is given by

$$Z^{\text{period}}_N = (T^N)(1,1) + (T^N)(2,2) = \text{Tr } T^N \tag{20}$$

where Tr stands for the trace of the matrix, the sum of its diagonal elements.

B. Partition function, Transfer-matrix derivation (finite field)

If we consider the short-range Ising model in a magnetic field, then the hamiltonian is given by

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{N} \sigma_i \tag{21}$$

and we may write the magnetic-field dependent term as $\frac{1}{2}h(\sigma_i + \sigma_{i+1})$, altough that is not a big deal. In any case, the transfer matrix is

$$\begin{bmatrix} \mathrm{e}^{\beta(J+h)} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta(J+h)} \end{bmatrix} \tag{22}$$

Example: For a two-site Ising chain with periodic boundary conditions, square the matrix and take the trace, and then check that this corresponds to the naive sum over the four terms. This is a useful exercise for next week. The outcome is

$$\text{Tr} Z_2 = \mathrm{e}^{2\beta(J+h)} + \mathrm{e}^{-2\beta J} \mathrm{e}^{2\beta(J-h)} \mathrm{e}^{-2\beta J}. \tag{23}$$

Also, using for a matrix $\left[\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right]$ that the eigenvalues are

$$\lambda_{1,2} = \frac{1}{2}\left(a + d \pm \sqrt{a^2 + d^2 = 4bc - 2ad}\right) \tag{24}$$

and using that the partition function with periodic boundary conditions is $Z_N = \lambda_1^N + \lambda_2^N$... you easily compute the free energy. One can also compute $m = -1/N \partial F / \partial h = \dots$ and one easily finds, with "un coup de Mathematica",

$$m = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + \mathrm{e}^{-4\beta J}}} \tag{25}$$

so that one obtains $m = 0$ for $h \to 0$ for all temperatures T.

C. Spin correlations

The two-point function $\langle s_i s_{i+\ell} \rangle$ can be computed within the transfer-matrix formalism with the insertion of $(-\sigma^z)$'s:

$$\begin{aligned} \langle s_i s_{i+\ell} \rangle = \frac{\text{tr}[T^i \sigma^z T^\ell \sigma^z T^{N-i-\ell}]}{Z} &\to \lambda_+^{-\ell} \langle \lambda_+ | \sigma^z T^\ell \sigma^z | \lambda_+ \rangle \\ &= \langle \lambda_+ | \sigma^z | \lambda_+ \rangle^2 + \left(\frac{\lambda_+}{\lambda_-}\right)^{-\ell} | \langle \lambda_+ | \sigma^z | \lambda_- \rangle |^2 \end{aligned} \tag{26}$$

The first term is nothing but the magnetization per unit length, so the connected correlation is given by

$$\langle s_i s_{i+\ell} \rangle - \langle s_i \rangle \langle s_{i+\ell} \rangle = \left(\frac{\lambda_+}{\lambda_-}\right)^{-\ell} | \langle \lambda_+ | \sigma^z | \lambda_- \rangle |^2 \tag{27}$$

and the correlation length is

$$\xi = \left(\log \frac{\lambda_+}{\lambda_-}\right)^{-1} . \tag{28}$$

We note that the correlation length depends on the subleading eigenvalue of the transfer matrix. Again, this is quite general.

More explicitly we find

$$\xi = \left(\log \frac{\cosh(\beta J h) + \sqrt{\sinh^2(\beta J h) + \mathrm{e}^{-4\beta J}}}{\cosh(\beta J h) - \sqrt{\sinh^2(\beta J h) + \mathrm{e}^{-4\beta J}}}\right)^{-1}$$

$$i = \left(2\mathrm{arctanh} \frac{\sqrt{\sinh^2(\beta J h) + \mathrm{e}^{-4\beta J}}}{\cosh(\beta J h)}\right)^{-1} . \tag{29}$$

III. ABSENCE OF PHASE TRANSITION IN ONE-DIMENSIONAL STATISTICAL SYSTEMS

We discuss two reasons why in one-dimensional statistical-physics systems a phase transition is often absent. One of the reasons is mathematical: The transfer matrix is irreducible, so that its dominant eigenvalue is non-degenerate (there is only a single one of them). Furthermore, one can prove that if the matrix elements are analytic functions, then so must be the largest eigenvalue. The second reason is more qualitative, often wrong, but essential to be known. It is related to domain walls.

A. Frobenius-Perron Theorem

The result obtained in Section II A is in fact rather general, indeed one can show that models with *finite-dimensional* transfer matrices can have phase transitions only if there are *forbidden* (infinite energy) configurations. This is a consequence of two theorems. The first is known as Perron-Frobenius theorem:

Theorem III.1 *Let A be an irreducible matrix with non-negative elements; the maximum eigenvalue is positive and non-degenerate.*

We remind that a matrix M is reducible if and only if it can be placed into block upper-triangular form by simultaneous row/column permutations. Clearly, a matrix with strictly positive elements is automatically irreducible.

$$P^t M P = \begin{pmatrix} X & Y \\ 0 & Z \end{pmatrix} , \tag{30}$$

where P is a permutation matrix and X and Z are square matrices.

The second useful theorem is a well-known result in function theory and can be expressed as follows

Theorem III.2 *If $T(\beta)$ is a complex matrix with elements analytic functions of β, the eigenvalues are (branches) of analytic functions of β with only algebraic singularities localized at the points at which eigenvalues split or coalesce.*

We note that the elements of the transfer matrix are generally exponentials, therefore, if any configuration is allowed, all the elements of a finite transfer matrix are nonzero and the matrix is in turn irreducible. By the Perron-Frobenius theorem, the leading eigenvalue is non-degenerate and, from Theorem III.2, turns out to be an analytic function of β. This explains why the simplest one-dimensional (classical) models do not exhibit phase transitions.

B. Domain walls in the one-dimensional Ising model (local interactions)

Domain walls are excitations where the system of Ising spins is separated into one part with all up spins, followed by a part with all down spins. However, it is easy to see that the energy of a domain wall is J, but the entropy of a domain wall, the log of the number of possibilities, which is L/a, where L is the system size and $a = 1$ the lattice parameter. We find that the free energy is

$$\Delta F \sim -kT \log\left(\frac{L}{a}\right) \tag{31}$$

which is negative. It is therefore favorable to add a domain wall, or two domain walls, and destroy the ferromagnetic ground state. We should be warned that domain wall (or spin wave) arguments are in general easy, and very often they turn out to be wrong.

C. Domain walls in the one-dimensional Ising model with $1/r^2$ interactions

Notable work on the one-dimensional Ising model with $1/r^2$ interaction (all spins interacting, but with an energy decreasing with the square of the distance) is due to Fisher et al (1972)[3]. There was also the influential mathematical proof by Dyson[4], which showed that for interactions decaying slower than $1/r^2$, there had to be a phase transition, however this did not clear up the situation of the $1/r^2$ interaction.

Of particular interest is the two-page 1969 article by Thouless[5], which uses spin waves to explain that something unexpected must happen for the $1/r^2$ Ising model. This work cleared the way for the establishment of Kosterlitz–Thouless theory. Indeed, the one-dimensional Ising model with a $1/r^2$ interaction undergoes such a transition. There is also important work by Kosterlitz[6].

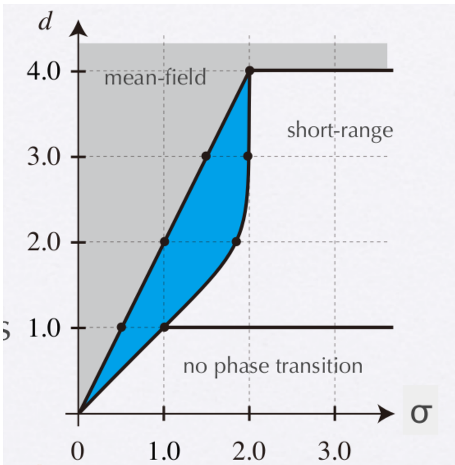

FIG. 3: Phase diagram of long-range Ising models in D dimensions with interaction $1/r^{D+\sigma}$ (Illustration from a talk by Synge Todo, Univ of Tokyo)

This is an example of where the domain wall argument is not easy, and (as much research has shown) not wrong. It goes back to Thouless[5]. Suppose a hamiltonian with interactions

$$H = -\sum_{i,j} \frac{\sigma_i \sigma_j}{(i-j)^2} \tag{32}$$

The cost of a domain wall at position x is

$$E = J \int_0^{x-a/2} \int_{x+a/2}^{L} \frac{dx_1 dx_2}{(x_1 - x_2)^2} \tag{33}$$

Integrating this energy twice, one may see that the energy of a domain wall on a system of length L with lattice parameter a is $\log L/a$. (This precise calculation will be the object of Homework 06). Both the energy of a domain wall and its entropy now scale like $\log L$. At low temperature, it becomes unfavorable to put a domain wall, while at high temperature, domain walls are favored. This result of Thouless[5] has been confirmed by much further research. See Fig. 3 for the general situation of long-range Ising models in D dimensions.

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[2] W. Krauth, *Statistical Mechanics: Algorithms and Computations*. Oxford University Press, 2006.

[3] M. E. Fisher, S.-k. Ma, and B. G. Nickel, "Critical Exponents for Long-Range Interactions," *Phys. Rev. Lett.*, vol. 29, pp. 917–920, 1972.

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