Exam: Statistical Mechanics 2015/16, ICFP Master (first year)

Werner Krauth, Maurizio Fagotti

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I. INTRODUCTION

The exam has four parts, of which the part II and V carry some calculations that may take awhile. Parts III and IV review course material.

II. BASIC STATISTICS

In the lecture, we treated the maximum likelihood approach as one of the key methods for estimating the parameters of a distribution. Here we treat two examples. The second one was of great historical importance on the battlefields of WW2 although it proved necessary to go one step farther than we will do here.

A. Point estimate for the parameters of a Gaussian distribution

Suppose that we have n data points $x_1, x_2, x_3, , ..., x_n$ (these points are real numbers between $-\infty$ and ∞), and we know that they are drawn from a Gaussian distribution with unknown values of the variance σ^2 and the mean value $\langle x \rangle$:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-(x - \langle x \rangle)^2/(2\sigma^2)). \tag{1}$$

What is the maximum likelihood estimator for the mean value $\langle x \rangle$ and variance σ^2 of this Gaussian distribution from the data?

Hint1 Remember (from the first lecture) that the likelihood function is given by $p(x_1)p(x_2)....p(x_n)$.

Hint2 If you use the log likelihood function, explain why this can be done.

Carefully explain your calculation.

B. German tank (char) problem

1. Preparation

Consider N balls numbered $1, 2, 3, ..., N$, and take k out them (urn problem without putting them back). What is the probability $p_N(m)$ that the largest of them is equal to m?

Hint0 How many ways are there to pick k (different) balls out of N?

Hint1 To solve this simple combinatorial problem, consider that m must be contained in $k, k+1, k+2, ...N$.

Hint2 Count the number of ways to pick $(k-1)$ balls so that they are smaller than m.

Carefully explain your calculation.

2. Application

From an urn with an unknown number N of balls (tanks), the following $k = 4$ balls were drawn (without putting them back):

$$1, 2, 4, 14$$

What is the maximum likelihood estimater of the total number N of balls (tranks) (based on the probability distribution of the sample maximum m, here 14) that are contained in the urn (destroyed tanks left on the battlefield)?

The (disappointing) result of the maximum likelihood estimator (here in the famous "German tank problem") points to one of the limitations of the maximum likelihood method, namely that it presents a bias. Comment on this property. Be assured, a simple trick allows to arrange the situation.

III. CORRELATION LENGTHS

In this section, we ask a few simple question about phase transitions.

- Explain the concept of a correlation length within equilibrium statistical physics (one formula, one or two sentences).

- Explain in a few word what differenciates the low-temperature and the high-temperature phases of the two-dimensional Ising model. Explain carefully what happens to the correlation length in the low-temperature phase (does it exist, is it finite or infinite?). What does mean-field theory say about the correlation length in Ising-type models?

- Contrast the situation of the two-dimensional Ising model with the one of the two-dimensional XY model. Explain carefully the behaviour of the correlation length in the low-temperature phase (is it finite or infinite, does it vary in some essential way).

IV. BOSE-EINSTEIN CONDENSATION.

In a physical system with partition function of non-interacting particles, almost all particles populated the groundstate as the temperature $T \to 0$.

In Bose-Einstein condensation (of non-interacting particles), almost all particles populate the ground state as the temperature $T \to 0$.

So, what is the difference between the behavior of distinguishable and bosonic quantum particles? In explaining this, please use as an example the results for a three-dimensional trap with frequencies $\omega_x = \omega_y = \omega_z = 1$. Discuss this case both for distinguishable and for bosonic ideal particles. In two sentences, explain why there can be a difference between bosons and distinguishable ideal particles, after all.

V. QUASI ONE-DIMENSIONAL DISKS AND THE TRANSFER MATRIX

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

NB Lucas sequence ($L_0 = 2, L_1 = 1, L_2 = 3, 4, 7, 11, ...$)

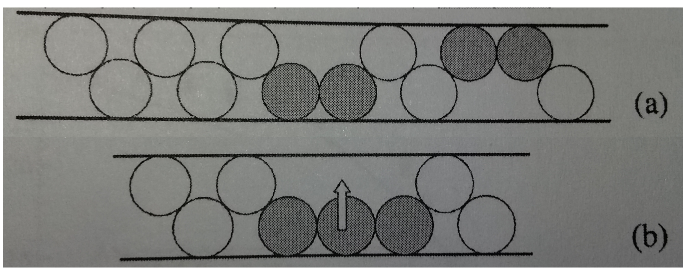

FIG. 1: A jammed (upper) and an unjammed (lower) configuration

In this problem, we consider hard disks of diameter σ, but at a difference with the lecture, we study jammed configurations (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.

- Sketch the longest jammed configuration of N disks, and the shortest jammed configuration of N disks.

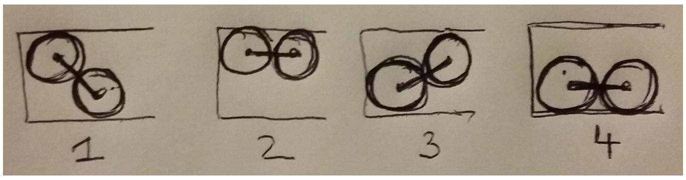

FIG. 2: The four jammed configurations with two disks (one bond)

- 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).
- 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. Relate your results to the sequences F_n and L_n.
- To check your transfer matrix calculation, use a combinatorial argument to obtain an explicit sum formula for the number of jammed configurations of N disks starting from the configuration "1" in fig. 2. Express this combinatorial formula in terms of the L_N and F_N.

SOLUTIONS

SOLUTIONS

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I. COMMENTS, BUGS

Here is what was written on the blackboard during the exam

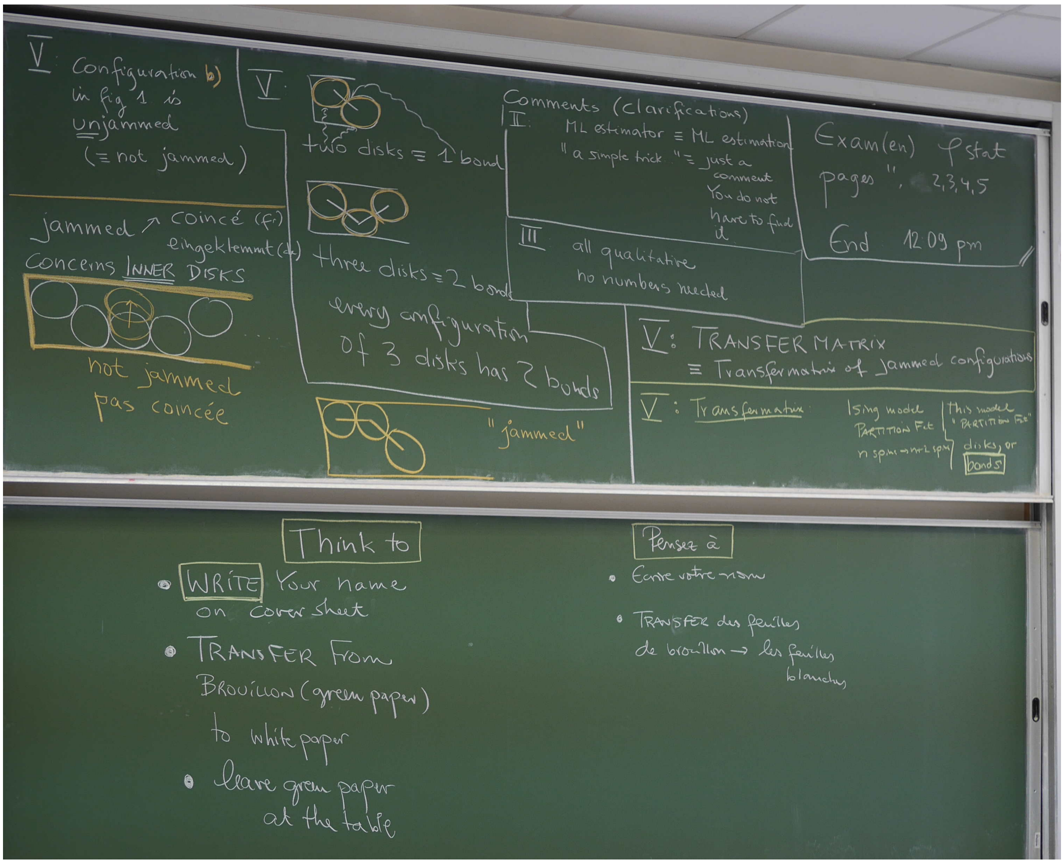

FIG. 3: Blackboard notices during the 2015/16 exam.

Some notes were written onto the blackboard. These notes repeated all the questions posed by students taking the exam so that everyone could listen to them.

Bug1: I had sent a message to students telling them that they could use their personal notes, and I think I mentioned this at the beginning of the exam, but without writing it on the blackboard. A student wrote to me saying he was unaware of the fact that the course material could be used.

Bug2: In the definition of the Fibonacci series, I dropped a 1.

II. SOLUTION OF PROBLEM II (BASIC STATISTICS)

A. First part, Gaussians

4 points (product, log monotone, deriv 1, deriv 2)

- The likelihood function is the product of the probabilities.
- We may take the logarithm of the likelihood function, as the logarithm is a monotonic function
- partial derivation with respect to the mean yields (we write μ for $\langle x \rangle$)

$$0 = \frac{\partial \log L}{\partial \mu} = \frac{1}{\sigma^2} \sum_i (x_i - \mu) \tag{2}$$

$$\mu = \frac{1}{N} \sum_i x_i \tag{3}$$

- partial derivation with respect to the variance yields

$$0 = \frac{\partial \log L}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum (x_i - \mu)^2 \tag{4}$$

$$\sigma^2 = \frac{1}{n} \sum (x_i - \mu)^2 \tag{5}$$

B. Second part, Tank problem

3 points (2 for formula, 1 for conclusion)

The probability that largest of k is equal to m is equal to the number of combinations of the $k-1$ other balls, in $1, \rightarrow, m-1$ divided by the total number of possibilities. This gives the likelihood function

$$L(N|k,m) = \frac{\binom{m-1}{k-1}}{\binom{N}{k}} \quad \text{for } N \geq m. \tag{6}$$

Here, k and m are known, and N is the unknown. But unfortunately, this decreases with N. The maximum likelihood value for N is thus m, and this does not seem right (the number of the largest tank shot down $\equiv$ the largest number ever produced).

III. SOLUTION OF PROBLEM III (CORRELATION LENGTH)

4 points (def, Ising high, Ising low, XY low)

Here, we only want qualitative information.

- Correlation length

$$C(x) \sim \langle S(0)S(x)\rangle \sim \exp(-|x|/\xi) \tag{7}$$

  expectation value with respect to Boltzmann distribution, sometimes necessary to subtract mean value, $\langle S(0)\rangle \langle S(x)\rangle$

- Ising high temperature: correlation function finite, ξ finite, diverging on approach of critical point.

- Ising low temperature: connected correlation function finite, ξ finite (although magnetization finite), diverging on approach of critical point.

- XY model zero expectation value above and below critical point, finite correlation length above T_c, power-law decay below T_c, with temperature-dependent power.

IV. SOLUTION OF PROBLEM IV (BOSE-EINSTEIN CONDENSATION)

2 points $T \to 0$ groundstate; BEC: T/gap $\to \infty$

- $T \to 0$ groundstate, in both cases
- in BEC $T \sim N^{1/3}$, that is $T_{BEC}/T_{gap} \to \infty$

V. SOLUTION OF PROBLEM V (JAMMING)

7 points (1 per subsection, except Transfer matrix = 2 (one for writing, one for solution)

A. Longest and shortest jammed configuration

The longest jammed configuration and the shortest jammed configuration are shown in iFig. 4.

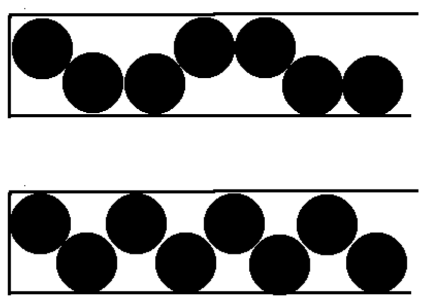

FIG. 4: The longest (upper) and shortest (lower) sequence of jammed disks

B. Number of jammed configurations

There are 4 configurations with two disks (one bond), and 6 configurations with three disks (two bonds).

C. Total number of configurations starting from 4.

The number of configurations of N disks is equal to $2F_{N+1}$

D. Transfer matrix

We can write down the transfer matrix (for multiplication of vectors from the rhs) in terms of the bonds 1-4 in the figure

$$T_{4\times4} = \begin{bmatrix} 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} \tag{8}$$

(bond 1 yields bonds $(3,4)$, bond 2 yields bond 1, etc) or alternatively in terms of the diagonal and horizontal bonds

$$T_{2\times2} = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \tag{9}$$

(diagonal bond yields straight or diagonal bond and straight bond yields diagonal bond). The largest eigenvalue is equal to $(1+\sqrt{5})/2$. This can be either computed explicitly in $T_{4\times4}$ or in

$T_{2\times 2}$, or else from the fact that the largest eigenvalue must turn out to be the ratio F_n/F_{n-1} for $n \to \infty$. This is called the golden mean. One gets it for the Fibonacci series in stating that for large n the ratio of subsequent numbers must be constant: $F_{n-1}, F_n, F_{n+1} = F_{n-1} + F_n$. This means that $1/\phi + 1 = (F_{n-1} + F_n))/F_n = F_n/F_{n-1} = \phi$. This gives the quadratic equation

$$\phi^2 - \phi - 1 = 0 \implies \phi = \frac{1 \pm \sqrt{5}}{2}. \tag{10}$$

The larger one is the golden mean.

E. Start with a diagonal configuration

Now, we start from the configuration 1, we obtain with both transfer matrices the sequence

$$1, 2, 3, 5, 8, 13, 21 \tag{11}$$

which can again be expressed as the Fibonacci series, or as a sum of the Fibonacci and the Lucas series.

F. Combinatorial formula

Let us call the diagonal bonds "0" and the straight bonds "1". We start with a "0". A possible configuration is 0100010101000010001 but we notice that the "1" bonds are always preceded by a "0". So let us write the 01 as x, so that each configuration is written as $000xxx000x0x0x0$, etc. If we have M x, then the total length is equal to $N - M$. We arrive at the formula:

$$F_{N+1} = \sum_{M=0}^{N/2} \frac{(N-M)!}{M!(N-2M)!}. \tag{12}$$

We can also write this as $(F_N + L_N)/2$, in honor of the French mathematician Lucas.