Final Exam: Statistical Mechanics 2017/18, ICFP Master (first year)

Werner Krauth, Olga Petrova, Jacopo De Nardis
(Dated: 15 January 2018)

Introduction

Some general information:

- Starting time: 9:00 AM, finishing time: 12:00 PM
- External material is not allowed (no books, scripts, calculators, computers, etc.). Do not touch your phone during the entire duration of the exam, even to check the time.
- Use only paper provided by ENS.
- Do not forget to write your name onto the cover sheet.
- Please transfer your answers from the green scratch paper (brouillon) to the white exam paper.
- Please leave the scratch paper at your desk.
- Do not forget to sign the register ("feuille d'émargement").

NB: This exam sheet contains three exercises on pages numbered 2-6.

I. CHEBYCHEV INEQUALITY AND MILL'S INEQUALITY

In this exercise, we explore basic properties of four different probability distributions. For clarity, we summarize the following:

Random variable	Property	Comment
X, X_i	$\mathrm{Var}(X) = 1$, Mean $\mu(X) = 0$	General zero-mean distribution
$\overline{X}_N$	Average of N independent X_i	see eq. (1)
Y, Y_i		Normal distribution, see eq. (2)
$\overline{Y}_N$	Average of N independent Y_i	see eq. (3)

1. Recall the definition of the mean (expectation) of a probability distribution and of its variance. Now consider a random variable X taken from a probability distribution π with zero mean and unit variance and the average of N such independent random variables:

$$\overline{X}_N = \frac{X_1 + \cdots + X_N}{N} \tag{1}$$

What is the variance of $\overline{X}_N$, and what is its mean?

Mean $\mu = \int z\pi(z)dz$, Variance $\int (z-\mu)^2 \pi(z)dz$. Mean of $\overline{X}_N$ is zero, $\mathrm{Var}(\overline{X}_N) = 1/N$.

2. Chebychev's inequality states that the probability to be more than t away from the mean $\mathbb{P}(|z - \mu(X)| \geq t)$ satisfies

$$\mathbb{P}(|z-\mu| \geq t) \leq \mathrm{Var}(X)/t^2 \quad \text{(Chebychev inequality; for arbitrary distribution)}$$

Prove Chebychev's inequality (Hint: You may suppose that the mean $\mu = 0$).

From the definition of the variance (for zero mean),

$$\mathrm{Var} X = \int_{-\infty}^{\infty} dz z^2 \pi(z) > \int_{|z|>t} dz z^2 \pi(z) > t^2 \int_{|z|>t} dz \pi(z) = t^2 \mathbb{P}(|z| \geq t)$$

The Chebychev inequality follows by dividing through t^2.

3. For the normal distribution

$$\pi(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right), \tag{2}$$

the much stronger Mill's inequality holds. It is given by:

$$\mathbb{P}(|z| > t) < \sqrt{\frac{2}{\pi}} \frac{\mathrm{e}^{-t^2/2}}{t} \quad \text{(Mill's inequality; normal distribution)}$$

Prove Mill's inequality and generalize it for a Gaussian distribution with zero mean, but standard deviation σ (Hint: note that $\mathbb{P}(|z| > t) = 2\mathbb{P}(z > t)$).

From the definition, we have that

$$\begin{aligned}
\mathbb{P}(|z| > t) = 2\mathbb{P}(z > t) = & \sqrt{\frac{2}{\pi}} \int_t^{\infty} dz \exp\left(-z^2/2\right) = \\
& \sqrt{\frac{2}{\pi}} \exp\left(-t^2/2\right) \int_t^{\infty} dz \exp\left(-(z^2/2 - t^2/2)\right) = \\
& \sqrt{\frac{2}{\pi}} \exp\left(-t^2/2\right) \int_t^{\infty} dz \exp\left[-\frac{1}{2}(z+t)(z-t)\right] < \\
& \sqrt{\frac{2}{\pi}} \exp\left(-t^2/2\right) \int_t^{\infty} dz \exp\left[-t(z-t)\right] = \\
& \sqrt{\frac{2}{\pi}} \exp\left(-t^2/2\right) \int_0^{\infty} du \exp\left[-tu\right]
\end{aligned}$$

and Mill's inequality follows immediately. For a Gaussian with standard deviation σ, one simply changes $\mathbb{P}(|z| > t)$ into $\mathbb{P}(|z| > t\sigma)$. The rhs of the above eqs remains unchanged.

4. Now consider $Y_1, \ldots Y_N$ independent normally distributed random variables and their average:

$$\overline{Y}_N = \frac{Y_1 + \cdots + Y_N}{N} \tag{3}$$

What is the variance of $\overline{Y}_N$, and what is its distribution? What are the bounds $\mathbb{P}(|\overline{Y}_N| > t)$ that you can obtain from the Chebychev inequality and from Mill's inequality?

$\overline{Y}_N$ is a Gaussian, because the sum of Gaussians is a Gaussian. Its variance equals $1/N$, so that its standard deviation is $\sigma = 1/\sqrt{N}$. For a Gaussian, Chebychev's inequality says that the probability to be more than $p\sigma$ away from the mean is smaller than $1/t^2$, whereas Mill's inequality states that this probability is smaller than $\sqrt{2/\pi} \exp\left(-t^2/2\right)/t$. For all $t > 1$, this is better than Chebychev, and it is quite sharp, already for $t \gtrsim 1$.

5. Does the central limit theorem make a statement about the relation between the distributions of $\overline{X}_N$ and of $\overline{Y}_N$? If yes, are there other conditions on the X_i for the central limit theorem to apply?

Yes, the Gnedenko-Kolmogorov theorem states that for iid random variables with finite variance the distribution of $\overline{X}$ converges to the distribution of $\overline{Y}$, for $N \to \infty$. There are no other conditions on the X_i. The finiteness of the variance is the only one.

II. BRAGG–WILLIAMS APPROXIMATION FOR THE 3-STATE POTTS MODEL, LANDAU THEORY

The three-state Potts model (that we already considered in the mid-term exam) has the following Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} \delta_{s_i,s_j}, \tag{4}$$

where δ_{s_i,s_j} is the Kronecker delta: it is equal to 1 when $s_i = s_j$ and zero otherwise. The spins can take on three values, namely A, B, and C. J is positive, and the term $\langle i,j \rangle$ indicates that i and j are neighbors. There are N sites in total and each spin (site) has q neighbors (for the cubic lattice in 3D, $q = 6$). We write down the free energy as a function of the density of spins $n_A = N_A/N$, $n_B = N_B/N$ and $n_C = N_C/N$, where N_A is the number of spins of type A, etc.

1. Recall that the entropy of a state is defined as k_B times the logarithm of the number of microscopic configurations. What is the number of microscopic configurations of the N spins, given N_A, N_B, and N_C, if we suppose that all these configurations are equally probable? Use Stirling's formula $\log(x!) = x \log x - x$ to obtain the entropy for large N, as a function of n_A, n_B, n_C.

   The number of different configurations is

   $$\left\{\text{\# of configs}\right\} = \frac{N!}{N_A! N_B! N_C!}$$

   Using Stirling's formula for the logarithm of this expression, we find

   $$N \log N - N_A \log N_A - N_B \log N_B - N_C \log N_C. \tag{5}$$

   We write $N_A = N\, n_A$ etc, so that the above equation becomes (noticing that $N_A + N_B + N_C = N$):

   $$-N(n_A \log n_A + n_B \log n_B + n_C \log n_C). \tag{6}$$

   The entropy is k_B times the last equation

2. Likewise, what is the energy of the system for large N if it is supposed that any site is equally likely to have value A, B, or C, under the condition that N_A, N_B, and N_C are fixed?

   There are $Nq/2$ edges. The total interaction is

   $$-\frac{NqJ}{2}(n_A^2 + n_B^2 + n_C^2)$$

3. From the above, write down the free energy in Bragg–Williams approximation as a function of n_A, n_B, n_C as a function of temperature. Do not forget to state the constraint equation on n_A, n_B, and n_C.

   The free energy is $F = U - TS$:

   $$F = -\frac{NqJ}{2}(n_A^2 + n_B^2 + n_C^2) + Nk_BT(n_A \log n_A + n_B \log n_B + n_C \log n_C). \tag{7}$$

   under the constraint $n_A + n_B + n_C = 1$.

4. Recall Viviani's theorem, which states that the sum of the distances from any interior point to the sides of an equilateral triangle equals the length of the triangle's altitude (see Fig. 1). Express the Bragg–Williams free energy in terms of the independent variables x and y. (Hint: $n_A = \frac{1}{3}(1 + 2y)$, etc.)

   We have for n_A:

   $$\begin{aligned} n_A &= 0 \quad \text{for} \quad y = -1/2 \\ n_A &= 1 \quad \text{for} \quad y = 1, \end{aligned}$$

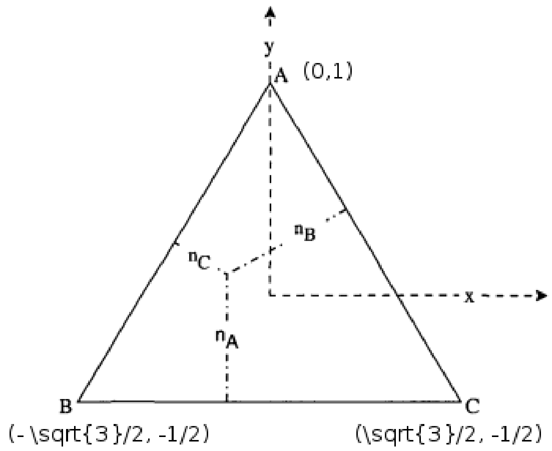

FIG. 1: Viviani's theorem (special case): $n_A + n_B + n_C = 1$ can be represented as points in the interior of this equilateral triangle.

so that it follows $n_A = \frac{1}{3}(1+2y)$. To obtain $n_B = c + dx + ey$, we can check the conditions in A and C, to obtain $n_B = \frac{1}{3}(1 - \sqrt{3}x - y)$, and by symmetry $n_C = \frac{1}{3}(1 + \sqrt{3}x - y)$. together therefore:

$$\begin{aligned} n_A =& \frac{1}{3}(1+2y) \\ n_B =& \frac{1}{3}(1-\sqrt{3}x - y) \\ n_C =& \frac{1}{3}(1+\sqrt{3}x - y) \end{aligned}$$

It suffices to plug these expressions into the original Bragg–Williams free energy.

5. Compute the values of x, y and, equivalently, of n_A, n_B, n_C that minimize the Bragg–Williams free energy in the limit $T \to 0$ and in the limit $T \to \infty$. Provide proof of why this is so, do not just plausibility arguements. What is the nature of the minimal-free-energy solution at small non-zero temperatures and at high finite temperatures?

   In the $T \to 0$ limit, the Bragg–Williams free energy is dominated by the energy term (the first term).

   $$F \propto (n_A^2 + n_B^2 + n_C^2) \propto (1+2y)^2 + (1 - \sqrt{3}x - y)^2 + (1 + \sqrt{3}x - y)^2$$

   The partial derivatives with respect to x and y of this function are zero only at $(x, y) = (0, 0)$, but this corresponds to a maximum. So the minimum is on the boundary. At the boundaries, one of the species is zero. Around the limiting line the free energy is proportional, for example, to $n_A^2 + (1 - n_A)^2$. Again the derivative is zero at $n_A = 1/2$, but this is a maximum. So the minimum is in the corner, and the solution is symmetric as is the triangle itself.

   In the $T \to \infty$ limit, the free energy is dominated by the entropy term. In this case, it is easy to show, through the partial derivatives, that the stable minimum is $(x, y) = (0, 0)$, corresponding to perfect symmetry of the species.

   At low temperature and at high temperature, the solution must preserve the symmetries of the $T = 0$ and $T = \infty$ limit.

6. From the above, further simplify the analysis of the Bragg–Williams free energy by writing it as a function of a single parameter m (Hint: use $m = y$, take into account one possible broken symmetry).

   We discuss the Bragg–Williams free energy in the direction where $x = 0$, for $-1/2 < y < 1$. The first term is $-qNJ/6(1 + 2m^2)$. In the second term, the expression is

   $$Nk_BT \left[\frac{1}{3}(1+2m) \log \left[\frac{1}{3}(1+2m) \right] + 2\frac{1}{3}(1-m) \log \left[\frac{1}{3}(1-m) \right] \right]$$

Here, all the $\log \frac{1}{3}$ terms give a prefactor 1, and we obtain

$$F = -qNJ/6(1+2m^2) + Nk_BT\left[\frac{2}{3}(1-m)\log(1-m) + \frac{1}{3}(1+2m)\log(1+2m) - \log 3\right]$$

7. Expand the free energy as a function of m up to the m^4 term. The Bragg–Williams free energy, expanded for small m, has the structure of a Landau free energy. Explain why this is a Landau theory, and also explain the difference with the Landau theory for the Ising model (Hint: drop constant terms).

   Expanding up to fourth order in m, one obtains that the term in [ ] equals $m^2 - m^3/3 + m^4/2$, so that, forgetting terms in m^0, one has

$$F/N = \text{const} - \left(\frac{qJ}{3} - k_BT\right)m^2 - \frac{k_BT}{3}m^3 + \frac{k_BT}{2}m^4$$

   The m^3 term is absent in the Landau theory for the Ising model because of the $m \Leftrightarrow -m$ symmetry. It breaks this symmetry, and induces a first-order transition.

8. Landau theory (Bragg–Williams for small m) predicts a first-order phase transition for the three-state Potts model. Explain why this is so. Compute the temperature of the first-order phase transition within Landau theory to fourth order in m, and the jump of the value m (Hint: at the transition temperature, there are two local minima with zero free energy (if you neglect constants) and zero first derivative with respect to m).

   Forgetting again the constant term, the free energy per spin and its first derivative should both be zero, as this signals the competition of two stable solutions

$$f = 0 = -a_2m^2 - a_3m^3 + a_4m^4$$
$$f' = 0 = -2a_2m - 3a_3m^2 + 4a_4m^3$$

   We can devide the first equation by m^2 and the second by m, multiply the first one by 2, and obtain the jump in the magnetization to be equal to $m = 1/3$. It takes place at a temperature $k_BT = \frac{qJ}{3}\frac{18}{17}$. At this value of the temperature, the prefactor of m^2 is still positive, so the first-order transition effectively preempts the second-order phase transition consisting in the change of sign of the prefactor of m^2.

III. WEN'S PLAQUETTE MODEL

Wen's plaquette model is defined for spin 1/2 particles (referred to simply as *spins*), whose states are described by the three Pauli matrices, corresponding to the particle's spin in three spacial directions:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In this problem, you will be using the following properties of the Pauli matrices:

- Pauli matrices for *different* spins always commute.
- Each Pauli operator squared is equal to the identity matrix.
- Operators σ_i^x and σ_i^z, corresponding to the *same* spin i, anti-commute.
- Both operators σ_i^x and σ_i^z have eigenvalues $+1$ and -1, corresponding to the spin being *up* and *down*, respectively (in the two separate bases).
- Applying σ_i^x to a spin up in σ_i^z basis produces a spin down. In other words, σ_i^x flips the value of the σ_i^z operator.
- Equivalently, applying σ_i^z to a spin up in σ_i^x basis produces a spin down. In other words, σ_i^z flips the value of the σ_i^x operator.
- This can be generalized to more complex operators: e.g., σ_i^z flips the value of the $\sigma_i^x \sigma_j^x$ operator because it anti-commutes (= flips) σ_i^x and commutes (= does nothing to) σ_j^x.

  Another example: $\sigma_i^x \sigma_j^z$ *commutes* with $\sigma_i^z \sigma_j^x$ because σ_i^x anti-commutes with σ_i^z, σ_j^z anti-commutes with σ_j^x, and $(-1) \times (-1) = 1$.

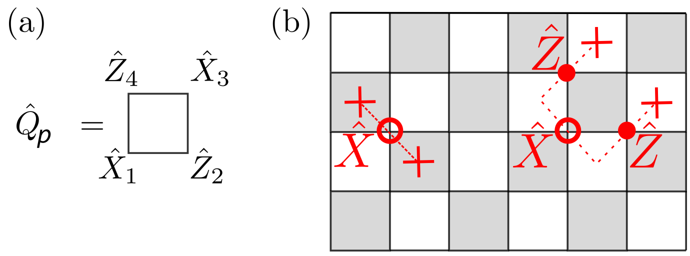

FIG. 2: Wen's plaquette model. $\hat{X}$ and $\hat{Z}$ in the Fig. correspond to σ^x and σ^z, respectively. (a) Building blocks of the Hamiltonian (8) are plaquette operators $\hat{Q}_p$. The form of $\hat{Q}_p$ is the same for all of the square plaquettes. (b) Excitations (indicated by red crosses) are located at the ends of string operators consisting of successive $\hat{X}$ and $\hat{Z}$, shown as dotted lines connecting the centers of diagonal plaquettes.

In Wen's plaquette model, spins live on the *sites* of a square lattice. This model is equivalent to the toric code, in which spins are located at the *bonds* of a square lattice. The Hamiltonian is a sum of plaquette operators, taken over all squares making up the lattice:

$$H = -\sum_p \hat{Q}_p, \quad \hat{Q}_p = \sigma_1^x \sigma_2^z \sigma_3^x \sigma_4^z, \tag{8}$$

where all operators $\hat{Q}_p$ have the form shown in Fig. 2(a).

1. Show that all operators $\hat{Q}_p$ commute (Hint: Avoid lengthy calculations and simply use the properties of σ^x and σ^z). Show that this implies that eigenstates of eq. (8) are characterized by one eigenvalue of $\hat{Q}_p$ per square.

   - When squares do not share any spins, their $\hat{Q}_p$ commute trivially.

- When squares share one spin, that spin contributes to the two $\hat{Q}_p$ with the same component, so they commute.
- When squares share two spins, their two sigmas anti-commute, $(-1) \times (-1) = 1$, so the two $\hat{Q}_p$ still commute.

2. What are the possible eigenvalues of $\hat{Q}_p$? (Hint: There are only two. No need to diagonalize the matrix $\hat{Q}_p$, just use the properties of Pauli matrices).

   $Q_p^2 = 1$ so $Q_p = \pm 1$

3. What are the values of $\hat{Q}_p$ that minimize the energy? (These are the quantum numbers of the system's ground state)

   In the ground state, all $Q_p = +1$

4. If your system is initially in a ground state, what does a single spin flip do? Consider both the action of σ_i^z on an arbitrary spin i, and the action of σ_i^x on an arbitrary spin i. Describe verbally and/or pictorially the new state(s) of the system using Q_p quantum numbers.

   See Fig. 2(b), single X flip produces a pair of excitations on two diagonal plaquettes. A single Z flip would create excitations on two diagonal plaquettes in the other possible direction.

5. You now know how to create excitations in this system. After flipping a single spin, excitations are located at two square plaquettes sharing a corner. Show that the two excited squares can be separated in space and can be thought of as being located at the endpoints of a string operator (Hint: consider Fig. 2(b)).

   Flip a spin, create two excitations. Flip another spin to flip one of these two squares again, and the excitation gets "shifted".

6. Just as in the original toric code, there are two types of excitations in Wen's model. Both look like squares with $Q_p = -1$. What allows us to distinguish the two? (Hint: Think about question (5) and consider Fig. 2(b)).

   Strings connect diagonal plaquettes $\rightarrow$ strings come in two colors, just like the checkerboard $\rightarrow$ excitations come in two flavors.

7. The two types of excitations are both bosons. When two bosons are exchanged, nothing happens to the wavefunction. When two fermions are exchanged, the wavefunction picks up a minus sign. If we exchange two identical particles, and then exchange them again, nothing happens to the wavefunction because for bosons we have $(+1) \times (+1) = 1$ and similarly for fermions we have $(-1) \times (-1) = 1$. If we perform a double exchange of two particles and get something other than the identity $(+1)$, these particles are *anyons*: neither bosons nor fermions.

   If you attach yourself to one of the two particles, and exchange them twice, to you it will look as if the second particle went around you in a circle. In Wen's plaquette model, just as in the toric code, moving particles involves extending strings, and closed strings are not observable (only the strings' endpoints are). Thus, exchanging two particles twice is equivalent to have one go around the other in a closed string – a circle. Use this and the properties of Pauli matrix operators to show that the two types of excitations in Wen's plaquette model are anyons with respect to one another.

   Strings of different flavors anti-commute when they cross.