Tutorial 7, Statistical Mechanics: Concepts and applications
2019/20 ICFP Master (first year)

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Tutorial exercises

I. WORKSHEET: THERMODYNAMIC QUANTITIES AND CORRELATION FUNCTIONS IN SERIES EXPANSIONS

1. **Ising model in 2D in magnetic field: high temperature expansion**

The model: Consider the high temperature expansion of the classical Ising model, defined on the square lattice with N sites and energy

$$E(\{\sigma\}) = -J \sum_{(i,j)} \sigma_i \sigma_j - H \sum_i \sigma_i \ , \tag{1}$$

where (i, j) signifies nearest neighbor pairs and J is assumed to be positive.

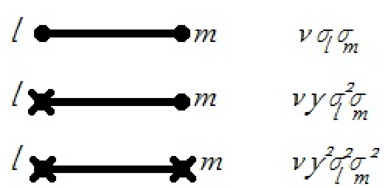
(a) Write down the partition function Z in the form that contains products of variables $v = \tanh \beta J$ and $y = \tanh \beta H$. The high temperature expansion derived in the steps to follow will be a series of powers of v and y.

:

$$Z = (\cosh \beta J)^{2N} (\cosh \beta H)^N \sum_{\{\sigma\}} \prod_{(i,j)} (1 + \sigma_i \sigma_j v) \prod_n (1 + \sigma_n y) \tag{2}$$

(b) Show that the terms in Z can be represented by graphs on the square lattice where each graph with l bonds and m odd vertices contributes a factor $2^N v^l y^m$ (here an odd vertex refers to there being an odd number of bonds connected to the vertex).

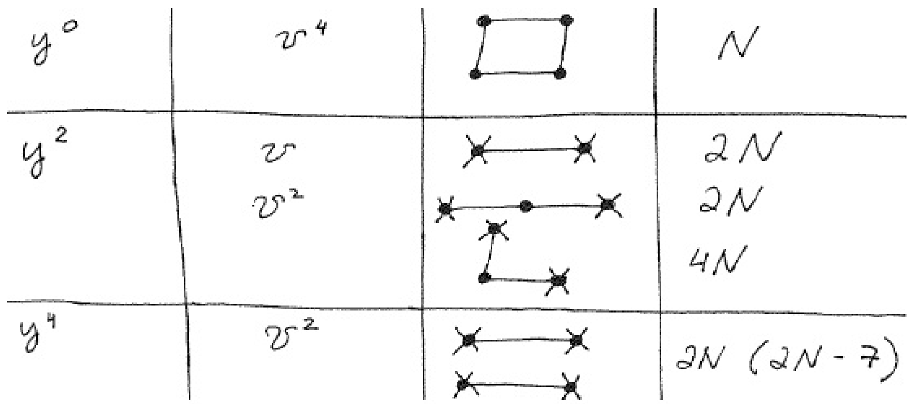
: *Each bond corresponds to one term $v\sigma_l\sigma_m$. Any odd vertices have to be "contracted" – multiplied by an appropriate term $\sigma_n y$ from $\prod_n (1 + \sigma_n y)$ (graphically we can denote this by a cross). Non-contracted odd vertices give rise to terms that cancel out in $\sum_{\{\sigma\}}$, whereas each non-zero diagram sums up to 2^N.*



The upper two diagrams give zero, the lowest one $2^N vy^2$.

(c) What diagrams contribute up to $O(y^4)$ and $O(v^2)$ (or the lowest order in v), and how many of them are there?

: *Since there can only be an even number of odd vertices in a graph, all odd orders of y give zero. The few lowest order graphs are listed below:*



(d) Write down Z to the fourth order in y.

:

$$Z = (\cosh \beta J)^{2N} (\cosh \beta H)^N \, 2^N \left(1 + S_0 + y^2 S_2 + y^4 S_4 + ...\right) \tag{3}$$

where $S_m(v, N)$ is the sum of all graphs with m odd vertices.

(e) Take the logarithm of Z to find the free energy F and expand for small v and y. What can you say about the contributions coming from disconnected graphs in the Z expansion? Use the linked cluster theorem below.

:

$$-\beta F = 2N \ln \cosh \beta J + N \ln \cosh \beta H + N \ln 2 + (S'_0 + y^2 S'_2 + y^4 S'_4 + ...) \tag{4}$$

where $S'_m(v, N)$ is the sum of all ***connected*** *graphs with m odd vertices. The disconnected graphs in Z cancel out from $\ln Z$ due to the* ***linked cluster theorem****.*

Linked cluster theorem Let

$$Z = Z_0 \left[1 + \sum \text{graphs}\right], \tag{5}$$

with Z_0 including the contribution of the "vacuum", *i.e.*, the weight associated to the configuration without any graphs in the lattice. The theorem states that

$$\log \frac{Z}{Z_0} = \sum \text{only connected graphs} \tag{6}$$

One way to show this is by the replica trick

$$\log \frac{Z}{Z_0} = \lim_{n \to 0} \frac{(Z/Z_0)^n - 1}{n} \tag{7}$$

Z^n can be written as a single partition function with n different Ising models. Each spin in one of the model is interacting with all other spins in the same model, but not with the ones inside the other replicas. Each connected graph in the perturbative expansion of Z^n can occur independently for each replica, therefore it can occur n times. Disconnected graphs of the perturbative expansion are instead at least of order n^2 (as each of them can occur independently for each replica). Any configuration containing m connected graphs comes with an additional multeplicity factor equal to n^m. In the limit (7), only the terms that are linear in n survive: those are the term with a number $m = 1$ of connected components.

(f) Compute the high temperature series for the zero-field susceptibility.

:

$$\chi = -\frac{1}{N}\frac{\partial^2 F}{\partial H^2}\Big|_{H=0} = \beta + 2\beta S_2'/N \tag{8}$$

Now we only need to consider the graphs with two odd vertices in order to derive the high temperature series expansion for χ:

$$\chi = \beta + 2\beta(2v + 6v^2 + 18v^3 + ...) \tag{9}$$

2. **Ising model in 2D: connected correlations functions**

Reminder: A connected correlation function is the joint cumulant of some random variables. For example, indicating the classical spins of a given statistical model by $\sigma_i \in \{-1, 1\}$, we have

$$\langle \sigma_{j_1}\sigma_{j_2}\cdots\sigma_{j_n}\rangle_c = \frac{\partial^n}{\partial J_1 \cdots \partial J_n} \log \langle e^{\sum_i J_i \sigma_{j_i}}\rangle\Big|_{J_1=\cdots=J_n=0}, \tag{10}$$

where the subscript c on the left hand side is used to indicate the connected correlation, while on the right hand side the brackets stand for the mean value.

The model: Consider a classical Ising model in a square lattice with energy

$$E(\{\sigma\}) = -J\sum_{(i,j)}\sigma_i\sigma_j - h\sum_i \sigma_i \ , \tag{11}$$

where (i, j) means that σ_j is adjacent to σ_i and periodic boundary conditions are imposed at the edges. As well known, for $J > 0$, the model is ferromagnetic below the critical temperature and paramagnetic at high temperature. Let then J be positive and N be the total number of spins.

(a) Assume $h = 0$ and consider the connected two-point function $\langle\sigma_1\sigma_{1+n}\rangle_c$ in the paramagnetic phase (let us assume that the spins σ_1 and σ_{1+n} belong to the same line). Perform a high-temperature expansion and list all the diagrams that give a contribution up to $O(\tanh^{n+4}(\beta J))$.

: *The expectation value can be written in the form*

$$\langle\sigma_1\sigma_{1+n}\rangle = \frac{Z_{\sigma_1\sigma_{1+n}}}{Z}\,, \tag{12}$$

where Z is the partition function and $Z_{\sigma_1\sigma_{1+n}}$ is the same as Z with an auxiliary $\sigma_1\sigma_{1+n}$ inside of the sum. The graphs contributing to the numerator and to the denominator are shown in fig. 2.

(b) Write down the correlator up to $O(\tanh^{n+2}(\beta J))$.

: *From fig. 2 it follows*

$$\tanh^n(\beta J)[1 + n(n+1)\tanh^2(\beta J)]\,. \tag{13}$$

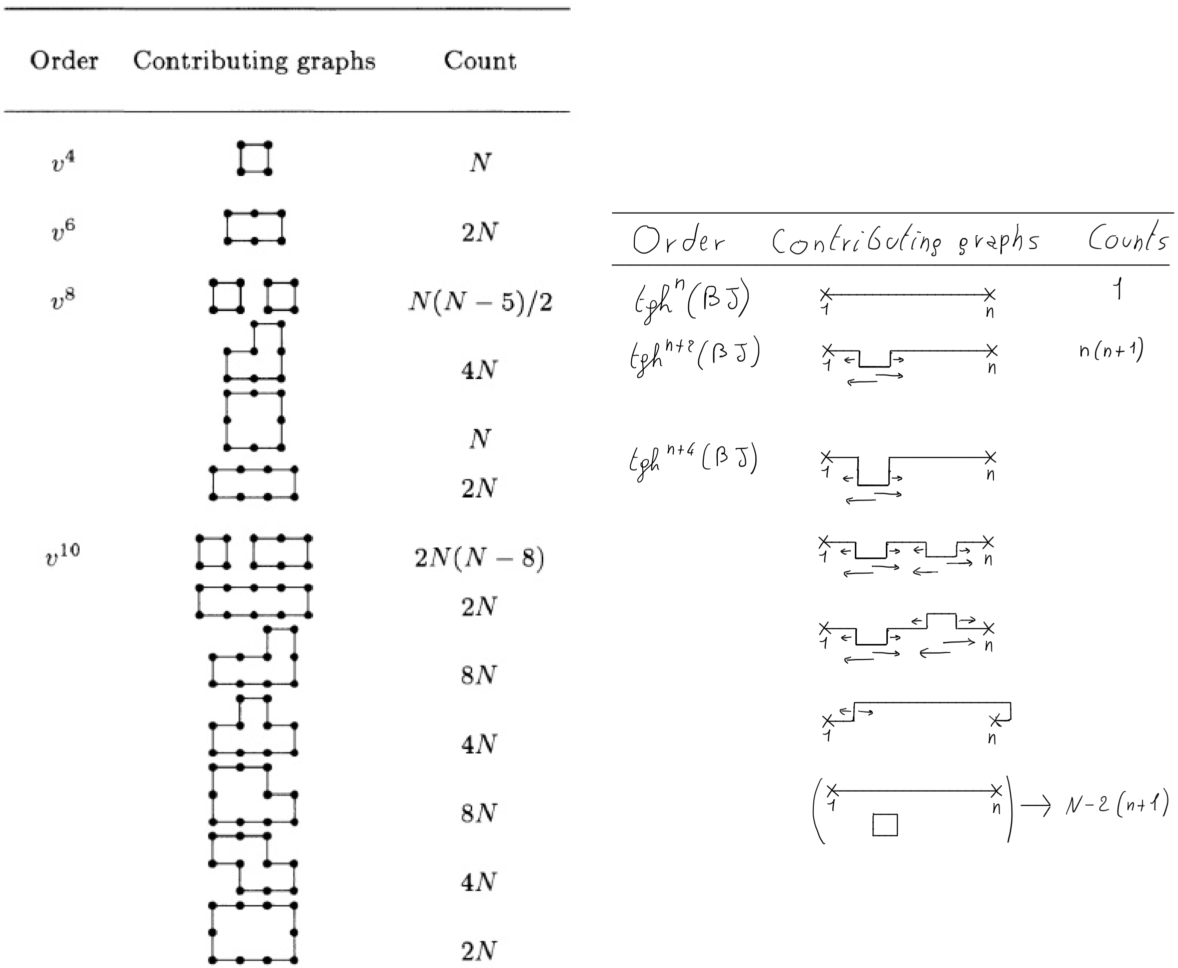


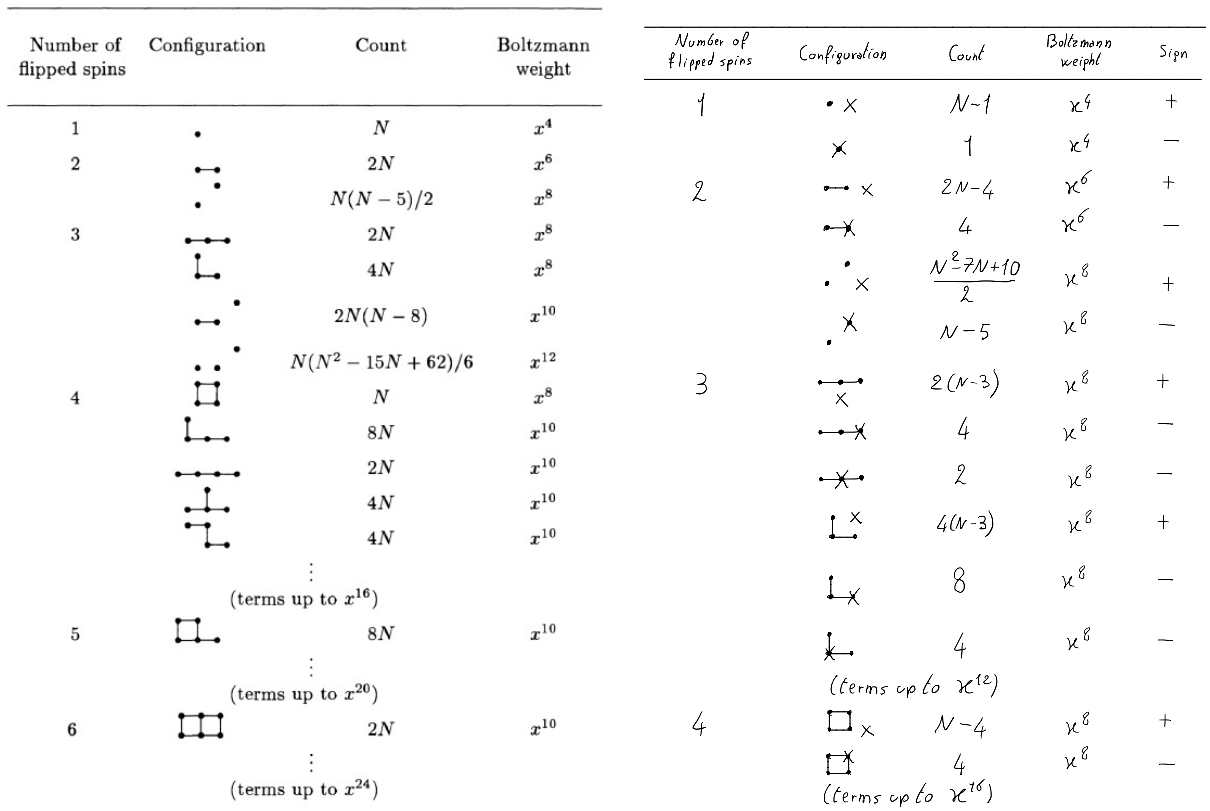
FIG. 1. Left: The configurations, together with their count, which contribute to the high temperature expansion of the partition function Z of the Ising model on a square lattice; $v = \tanh(\beta J)$ [From Yeomans.]. Right: The configurations for $Z_{\sigma_1\sigma_{1+n}}$, which appears in the two-point function (the crosses represent the spins σ_1 and σ_{1+n}).

(c) Can you draw some physical conclusion in the limit of large distance?

HINT: You can assume $n \ll \tanh^{-2}(\beta J)$ and $n \ll \tanh^{-1}(\beta J)$.

: *If n is large, but sufficiently smaller than $\tanh^{-2}(\beta J)$, the first terms of the series expansion show that the connected two-point function (which in this case is equal to the two-point function) approaches zero exponentially.*

(d) Assume again $h = 0^+$ and consider the (connected) one-point function $\langle\sigma_1\rangle$ in the ferromagnetic phase. Perform a low-temperature expansion and compute the correlator at $O(e^{-16\beta J})$.



Number of flipped spins	Configuration	Count	Boltzmann weight
1		N	x^4
2		$2N$	x^6
		$N(N-5)/2$	x^8
3		$2N$	x^8
		$4N$	x^8
		$2N(N-8)$	x^{10}
		$N(N^2-15N+62)/6$	x^{12}
4		N	x^8
		$8N$	x^{10}
		$2N$	x^{10}
		$4N$	x^{10}
		$4N$	x^{10}
	⋮ (terms up to x^{16})		
5		$8N$	x^{10}
	⋮ (terms up to x^{20})		
6		$2N$	x^{10}
	⋮ (terms up to x^{24})		

Number of flipped spins	Configuration	Count	Boltzmann weight	Sign
1		$N-1$	x^4	+
		1	x^4	−
2		$2N-4$	x^6	+
		4	x^6	−
		$\frac{N^2-7N+10}{2}$	x^8	+
		$N-5$	x^8	−
3		$2(N-3)$	x^8	+
		4	x^8	−
		2	x^8	−
		$4(N-3)$	x^8	+
		8	x^8	−
		4	x^8	−
	(terms up to x^{12})			
4		$N-4$	x^8	+
		4	x^8	−
	(terms up to x^{16})			

FIG. 2. Left: The configurations, together with their count, which contribute to the low temperature expansion of the partition function Z of the Ising model on a square lattice; $x = e^{-2\beta J}$ [From Yeomans.] Right: The configurations for Z_{σ_1}, which appears in the two-point function (the cross represents the spin σ_1).The sign is the value of σ_1 in the configuration considered.

: *The expectation value can be written in the form*

$$\langle \sigma_1 \rangle = \frac{Z_{\sigma_1}}{Z}\,, \tag{14}$$

where Z is the partition function and Z_{σ_1} is the same as Z with an auxiliary σ_1 inside of the sum. Fig. 2 shows the configurations that give the leading contribution at low temperature. We find (in principle, this expansion is meaningful only for $\beta \gg \log N$)

$$\begin{aligned} Z_{\sigma_1} &= 1 + (N-2)e^{-8\beta J} + (2N-8)e^{-12\beta J} + \frac{N^2+5N-52}{2}e^{-16\beta J} + O(e^{-20\beta J}) \\ Z &= 1 + Ne^{-8\beta J} + 2Ne^{-12\beta J} + \frac{N^2+9N}{2}e^{-16\beta J} + O(e^{-20\beta J})\,. \end{aligned} \tag{15}$$

The inverse of the partition function is

$$Z^{-1} = 1 - Ne^{-8\beta J} - 2Ne^{-12\beta J} + \frac{N^2 - 9N}{2} e^{-16\beta J} + O(e^{-20\beta J})\,. \tag{16}$$

Thus

$$\langle \sigma_1 \rangle = 1 - 2e^{-8\beta J} - 8e^{-12\beta J} - 26e^{-16\beta J} + O(e^{-20\beta J})\,. \tag{17}$$

In fact, we can avoid computing the inverse of the denominator, indeed this will be a function of the volume with the leading term equal to 1. As a consequence, it can only modify the term that depend explicitly on N. Since the correlation function is an intensive quantity, the denominator does not affect the contributions independent of N and simply cancels all the terms that grow with N in the numerator. This also suggests that such perturbative result is correct even in the thermodynamic limit.

(e) Compute the connected two-point function $\langle \sigma_1 \sigma_{1+n} \rangle_c$ up to $O(e^{-12\beta J})$. What happens in the limit of large distance?

: *Since we already computed the one-point function, we can focus on the two-point function. The configurations are similar to the ones shown for the one-point function - fig. 2, but now there are two crosses. For the distance $n > 1$ we find*

$$Z_{\sigma_1 \sigma_{1+n}} = 1 + (N-4)e^{-8\beta J} + (2N - 16)e^{-12\beta J} + O(e^{-16\beta J})\,. \tag{18}$$

As before, the partition function results in the cancellation of all the terms proportional to N. Thus we find

$$\langle \sigma_1 \sigma_{1+n} \rangle \sim 1 + (N-4)e^{-8\beta J} + (2N-16)e^{-12\beta J} \sim (1 - 2e^{-8\beta J} - 8e^{-12\beta J})^2 \sim \langle \sigma_1 \rangle^2\,. \tag{19}$$

For $n = 1$ we obtain

$$\langle \sigma_1 \sigma_{1+n} \rangle \sim 1 + (N-4)e^{-8\beta J} + (2N-12)e^{-12\beta J} \sim (1 - 2e^{-8\beta J} - 8e^{-12\beta J})^2 + 4e^{-12\beta J}\,. \tag{20}$$

In conclusion, the connected correlation is given by

$$\langle \sigma_1 \sigma_{1+n} \rangle_c = 4\delta_{n1} e^{-12\beta J} + O(e^{-16\beta J})\,. \tag{21}$$

In the limit of large distance, we find again that the connected two-point function approaches zero (at the order considered, it is exactly zero).