ICFP M1 - Phase Transitions – TD n° 3 – Solution
The Critical Temperature of the Ising Model in 2D

Baptiste Coquinot, Guilhem Semerjian
baptiste.coquinot@ens.fr

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1 High temperature expansion

1. Each site has 4 neighbours. There are N sites. Therefore the sum over nearest neighbours with periodic boundary conditions consists of $4N/2 = 2N$ terms.

2. From TD 2, Question 2.1, we know that $\cosh(x)(1 + \epsilon \tanh(x)) = e^{\epsilon x}$, where $\epsilon = \pm 1$. Therefore $e^{\beta J \sigma_i \sigma_j} = c(1 + t\sigma_i\sigma_j)$, with $c = \cosh(\beta J)$ and $t = \tanh(\beta J)$.

3. We start from the definition of the partition function

$$\begin{aligned} Z_N(\beta) &= \sum_{\underline{\sigma}} e^{-\beta H(\underline{\sigma})} \\ &= \sum_{\underline{\sigma}} \prod_{\langle ij \rangle} e^{\beta J \sigma_i \sigma_j} \\ &= c^{2N} \sum_{\underline{\sigma}} \prod_{\langle ij \rangle} (1 + t\sigma_i\sigma_j). \end{aligned}$$

As before, the product over pairs of nearest neighbour sites consists of $2N$ factors, hence the expansion of the product contains 2^{2N} terms, as for each factor one takes either 1 or $t\sigma_i\sigma_j$.

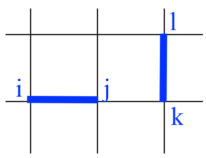
4. Blindly expanding the product gives

$$Z_N(\beta) = c^{2N} \sum_{\underline{\sigma}} \left(1 + t \sum_{\langle ij \rangle} \sigma_i\sigma_j + t^2 \sum_{\langle ij \rangle < \langle kl \rangle} \sigma_i\sigma_j\sigma_k\sigma_l + ... \right)$$

Let us represent this expansion graphically:

- a diagram is a 2d square lattice with N sites connected by thin or thick lines
- a thin line between site i and j carries value 1
- a thick line between sites i and j carries value $t\sigma_i\sigma_j$
- the value of a graph is the product of the values of all lines

For example:



$= t^2 \sigma_i\sigma_j\sigma_k\sigma_l$

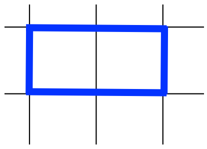
This means that

$$Z_N(\beta) = c^{2N} \sum_{\underline{\sigma}} (\text{sum of all possible distinct diagrams})\,.$$

Now note that

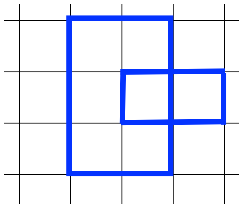
$$\sum_{\underline{\sigma}} \sigma_a\sigma_b...\sigma_n = \begin{cases} 2^N \text{ if each index } (a, ..., n) \text{ appears an even number of times} \\ 0 \text{ otherwise} \end{cases} \tag{1}$$

Therefore the only diagrams that will survive the sum $\sum_{\underline{\sigma}}$ are those where there is an even number of thick lines meeting at each site. This boils down to the condition that the *thick lines form closed curves* (including the case of no curve at all) and we call this a closed graph. An example is



$$= t^6. \tag{2}$$

In general, a closed graph can consist of several closed curves that are allowed to intersect (but not to overlap). A valid closed graph is for example



5. Keeping only closed graphs, the partition function becomes a power series in $t = \tanh(\beta J)$ with coefficients $a_{N,n}$ corresponding to the number of possible closed graphs on a lattice with N sites using exactly n thick lines:

$$Z_N(\beta) = (2c^2)^N \sum_{n=0}^{\infty} a_{N,n} t^n \tag{3}$$

The name "high temperature expansion" is justified since $\tanh(\beta J) \to 0$ as $T = 1/\beta \to \infty$. So we develop in a small parameter and can neglect higher order terms for which $a_{N,n}$ can be very difficult to calculate.

6.
   - $a_{N,0} = 1$ (empty diagram)
   - $a_{N,1} = a_{N,2} = a_{N,3} = 0$ (the square is the first possible closed graph)
   - $a_{N,4} = N$ (a unit square whose bottom left corner can be any of the N sites)
   - $a_{N,2n+1} = 0$ (uneven number of thick lines cannot form closed structures)
   - $a_{N,6} = 2N$ (one rectangle, as in (2), for each of the N sites, with horizontal or vertical orientation)

Let us make a side remark. The coefficients $a_{N,4}$ and $a_{N,6}$ are proportional to N; this is not the case for larger values of n. For instance $a_{N,8}$ contains both contributions of order N^2 (corresponding to diagrams containing two unit squares at arbitrary positions) and of order N (2×2 squares and 1×3 rectangles). In general the diagrams with k connected components will have degeneracies of order N^k. As a matter of fact the $a_{N,n}$ are the coefficients of the expansion for the partition function Z, which is not extensive: it is the free energy, proportional to $\ln Z$, which is extensive. It is a general feature in diagrammatic expansions that taking logarithms amounts to select only the connected diagrams.

2 Low temperature expansion

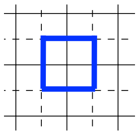
7. The order of magnitude that differentiates between "high" and "low" temperatures is fixed by J. If $\beta J \ll 1$ one is in the high temperature regime, for $\beta J \gg 1$ in the low temperature one.

8. There are two configuration with a minimal energy of $E_0 = -2JN$: all spins up or all spins down.

9. The first excited state is the lowest energy state with one spin flipped. We can flip this spin at all N lattice sites and there are two lowest energy states. Therefore

$$\#(\text{states with } E_1) \equiv 2 \times N.$$

A single spin flip on a 2d lattice increases the energy by $\Delta E = 4 \times 2J$. Graphically this can be seen by drawing thick lines on the dual lattice (also called domain walls) to separate spins of different orientation and associating a factor $2J$ with each thick line.



10. The next higher energy state is built from the lowest energy state by flipping two neighbouring spins. Then $\Delta E = 6 \times 2J$. The corresponding graph is a rectangle. It has $2N$ possibilities to be placed on the dual lattice. Taking the degeneracy of the lowest energy states into account this gives

$$\#(\text{states with } E_2) = 2 \times 2N.$$

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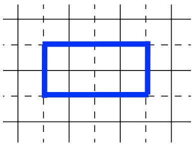

11. see next question

12. For low temperatures, only states with low energy will contribute to the partition function. Therefore we can expand it in terms of the energy levels E_0, $E_1 = E_0 + 4 \times 2J$, $E_2 = E_0 + 6 \times 2J$,... or more generally in terms of $E_0 + n2J$ for $n = 0, 1, 2, \ldots$. Surely, not all of these energy levels exist, so we have to weigh each term by a multiplicity factor $2b_{N,n}$ (the 2 accounts for the degeneracy of the ground state) which is zero if the energy level does not exist.

$$\begin{aligned} Z_N(\beta) &= \sum_{\underline{\sigma}} e^{-\beta H(\underline{\sigma})} \\ &= \sum_{n=0}^{\infty} 2b_{N,n} e^{-\beta(E_0 + n2J)} \\ &= 2e^{2N\beta J} \sum_{n=0}^{\infty} b_{N,n} (e^{-2\beta J})^n \end{aligned}$$

Comparing to our results above we find

- $b_{N,0} = 1$ (this corresponds to E_0)
- $b_{N,1} = b_{N,2} = b_{N,3} = 0$
- $b_{N,4} = N$ (this corresponds to E_1)
- $b_{N,5} = 0$
- $b_{N,6} = 2N$ (this corresponds to E_2)

In general, $b_{N,n}$ is the number of ways we can draw closed curves on the dual lattice with N sites using exactly n thick lines. Due to the periodic boundary conditions, the dual lattice is equal to the actual lattice, and so we have $b_{N,n} = a_{N,n}$.

3 Critical temperature

13. To compute the free energy per spin $f(\beta) = -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N} \log Z_N(\beta)$ we will be using the notation $A_N(x) := \sum_{n=0}^{\infty} a_{N,n} x^n$ and $g(x) := \lim_{N\to\infty} \frac{1}{N} \log A_N(x)$:

    - High temperature expansion: $Z_N(\beta) = (2\cosh^2(\beta J))^N A_N(\tanh(\beta J)$

    $$f_H(\beta) = -\frac{1}{\beta}\left(\log(2\cosh^2(\beta J)) + g(\tanh(\beta J)\right) \tag{4}$$

    - Low temperature expansion: $Z_N(\beta) = 2e^{2N\beta J} A_N(e^{-2\beta J})$

    $$f_L(\beta) = -\frac{1}{\beta}\left(2\beta J + g(e^{-2\beta J})\right) \tag{5}$$

14. If $f(\beta)$ is singular at a unique point β_c then there must be a singularity in the function g at a point where its arguments in the high and low temperature case are equal: $e^{-2\beta J} = \tanh(\beta J)$. One can solve this equation by noting that $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = \frac{e^{2x}-1}{e^{2x}+1}$. Denoting $X = e^{2\beta J}$ one has $\frac{1}{X} = \frac{X-1}{X+1}$, i.e. $X^2 - 2X - 1 = 0$, whose positive root is $1 + \sqrt{2}$. This yields

    $$\beta_c J = \frac{1}{2}\log(1+\sqrt{2}) \ . \tag{6}$$

    Note that the duality between the high and low temperature expansions gives further information on the free energy: suppose one knows $f(\beta)$ for some value β. Then from the high temperature expansion one knows the function $g(x)$ in $x = \tanh(\beta J)$, and thus from the low temperature expansion one knows f in $\beta^*(\beta)$ such that $e^{-2\beta^* J} = x = \tanh(\beta J)$. One can check that $\beta \mapsto \beta^*(\beta)$ is an involution mapping the high temperature regime $\beta \in [0, \beta_c]$ to the low temperature regime $\beta \in [\beta_c, \infty)$ and vice versa, admitting the critical temperature β_c as its unique fixed point.

4 Exact results

15. The singularity in this expression can only come from a vanishing argument of the logarithm. As $\cos(k_x) + \cos(k_y)$ is maximal in $k_x = k_y = 0$, where it is equal to 2, a singularity will appear if $(\cosh(2\beta J))^2 = 2\sinh(2\beta J)$. As $\cosh(x)^2 - 2\sinh(x) = 1 + \sinh(x)^2 - 2\sinh(x) = (1-\sinh(x))^2$ is ≥ 0 for all $x \geq 0$ and vanishes only in $x = \log(1+\sqrt{2})$, this confirms the determination of the critical temperature previously obtained by the simpler duality argument.

16. One has $\sinh(2\beta_c J) = 1$, hence $\sinh(2\beta J) \sim 1 + C(T_c - T)$ when $T \to T_c^-$, with C some positive constant. This gives $m_{sp}(T) \sim (1-(1-4C(T_c-T)))^{\frac{1}{8}} \propto (T_c - T)^{\frac{1}{8}}$, which shows that the critical exponent β is equal to $\frac{1}{8}$ for the Ising model in two dimensions.