ICFP M1 - Phase Transitions – TD n° 2 – Solution
Unidimensional Models

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1 Transfer matrix for unidimensional models

1.1 Ising spin chain

1. By definition of the partition function,

$$Z = \sum_{\underline{\sigma}} e^{-\beta H(\underline{\sigma})} = \sum_{\underline{\sigma}} \prod_{i=1}^{N} e^{\beta(J\sigma_i\sigma_{i+1} + \frac{h(\sigma_i+\sigma_{i+1})}{2})} = \sum_{\underline{\sigma}} \prod_{i=1}^{N} T(\sigma_i, \sigma_{i+1}) \ , \tag{1}$$

with the symmetric function $T(\sigma, \sigma') = e^{\beta(J\sigma\sigma' + \frac{h(\sigma+\sigma')}{2})}$.

This yields the matrix $\mathbb{T} = \begin{pmatrix} e^{\beta(J+h)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-h)} \end{pmatrix}$.

2. One has

$$Z = \sum_{\sigma_1,\dots,\sigma_N} \mathbb{T}_{\sigma_1,\sigma_2}\mathbb{T}_{\sigma_2,\sigma_3}\dots\mathbb{T}_{\sigma_N,\sigma_1} = \mathrm{Tr}(\mathbb{T}^N) \ ,$$

by recognizing the rules for matrix multiplication and the definition of the trace of a matrix.

3. The eigenvalues of $\mathbb{T}$ are the solutions of the characteristic equation $\det(\mathbb{T} - \lambda\mathbb{I}) = 0$, with $\mathbb{I}$ the identity matrix. This gives

$$0 = (e^{\beta(J+h)} - \lambda)(e^{\beta(J-h)} - \lambda) - e^{-2\beta J} = \lambda^2 - e^{\beta J}(e^{\beta h} + e^{-\beta h})\lambda + e^{2\beta J} - e^{-2\beta J} \ , \tag{2}$$

which is solved by

$$\lambda_\pm = e^{\beta J}\mathrm{ch}(\beta h) \pm \sqrt{e^{2\beta J}\mathrm{ch}^2(\beta h) - 2\,\mathrm{sh}(2\beta J)} \ . \tag{3}$$

4. One can use the expression of Z as a trace and the diagonalization of the matrix $\mathbb{T}$ to obtain $Z = \lambda_+^N + \lambda_-^N$. The free energy reads then:

$$f = -\frac{1}{\beta N}\ln(\lambda_+^N + \lambda_-^N) = -\frac{1}{\beta N}\left(\ln(\lambda_+^N) + \ln\left(1 + \frac{\lambda_-^N}{\lambda_+^N}\right)\right) = -\frac{1}{\beta}\ln(\lambda_+) - \frac{1}{N\beta}\ln\left(1 + \frac{\lambda_-^N}{\lambda_+^N}\right) \ .$$

As $|\lambda_-| < \lambda_+$ the second term is negligible in the thermodynamic limit, which yields

$$\lim_{N\to+\infty} f = -\frac{1}{\beta}\ln(\lambda_+) \ . \tag{4}$$

5. We can rewrite the average magnetization in terms of matrices as

$$\begin{aligned} m &= \frac{1}{Z}\sum_{\underline{\sigma}} \sigma_i\, e^{-\beta H(\underline{\sigma})} = \frac{1}{Z}\sum_{\sigma_1,\dots,\sigma_N} \mathbb{T}_{\sigma_1,\sigma_2}\mathbb{T}_{\sigma_2,\sigma_3}\dots\mathbb{T}_{\sigma_{i-1},\sigma_i}\sigma_i\mathbb{T}_{\sigma_i,\sigma_{i+1}}\dots\mathbb{T}_{\sigma_N,\sigma_1} \\ &= \frac{1}{Z}\sum_{\sigma_1,\dots,\sigma_N,\sigma_i'} \mathbb{T}_{\sigma_1,\sigma_2}\mathbb{T}_{\sigma_2,\sigma_3}\dots\mathbb{T}_{\sigma_{i-1},\sigma_i}\hat{\sigma}_{\sigma_i,\sigma_i'}\mathbb{T}_{\sigma_i',\sigma_{i+1}}\dots\mathbb{T}_{\sigma_N,\sigma_1} = \frac{\mathrm{Tr}(\mathbb{T}^{i-1}\hat{\sigma}\mathbb{T}^{N-i+1})}{\mathrm{Tr}(\mathbb{T}^N)} = \frac{\mathrm{Tr}(\hat{\sigma}\mathbb{T}^N)}{\mathrm{Tr}(\mathbb{T}^N)} \ . \end{aligned}$$

In the last step we have used the invariance of the trace under cyclic permutations, which shows that $\langle\sigma_i\rangle$ is independent of i. This translates the invariance under translation of the model, thanks to the periodic boundary conditions.

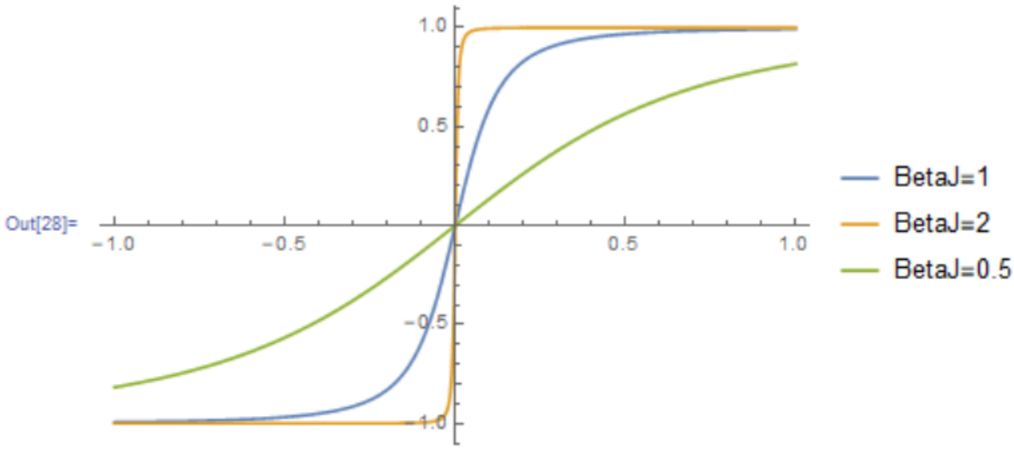


Figure 1: The magnetization as a function of h, for three different temperatures.

6. In general differentiating the free-energy with respect to a parameter of the Hamiltonian yields the average value of the conjugated observable. Here we have

$$\frac{\partial f}{\partial h} = \frac{\partial}{\partial h}\left(-\frac{1}{\beta N}\ln Z\right) = -\frac{1}{\beta N}\frac{1}{Z}\frac{\partial Z}{\partial h} = -\frac{1}{\beta N}\frac{1}{Z}\sum_{\underline{\sigma}} e^{-\beta H(\underline{\sigma})}\beta\sum_{i=1}^{N}\sigma_i = -\frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle = -m \ ,$$

using the invariance by translation.

For a finite value of N the derivative of f reads

$$\frac{\partial f}{\partial h} = -\frac{1}{\beta N}\frac{\partial}{\partial h}\ln(\lambda_+^N + \lambda_-^N) = -\frac{1}{\beta}\frac{\lambda_+^{N-1}\frac{\partial\lambda_+}{\partial h} + \lambda_-^{N-1}\frac{\partial\lambda_-}{\partial h}}{\lambda_+^N + \lambda_-^N} = -\frac{1}{\beta}\frac{\frac{\partial\lambda_+}{\partial h} + \left(\frac{\lambda_-}{\lambda_+}\right)^{N-1}\frac{\partial\lambda_-}{\partial h}}{\lambda_+ + \lambda_-\left(\frac{\lambda_-}{\lambda_+}\right)^{N-1}} \ .$$

As $|\lambda_-| < \lambda_+$ the second terms in the numerator and denumerator vanish in the thermodynamic limit, for which the magnetization reads $m = \frac{1}{\beta\lambda_+}\frac{\partial\lambda_+}{\partial h}$. This computation shows that, for this model, the differentiation and the thermodynamic limit commut; this is not true in general, the free energy might be non-differentiable in the $N \to \infty$ limit.

We finish the computation from the expression of λ_+ obtained previously:

$$\lambda_+ = e^{\beta J}\left(\mathrm{ch}(\beta h) + \sqrt{\mathrm{sh}^2(\beta h) + e^{-4\beta J}}\right)$$

$$\frac{1}{\beta}\frac{\partial\lambda_+}{\partial h} = e^{\beta J}\left(\mathrm{sh}(\beta h) + \frac{\mathrm{ch}(\beta h)\mathrm{sh}(\beta h)}{\sqrt{\mathrm{sh}^2(\beta h) + e^{-4\beta J}}}\right)$$

$$= \frac{e^{\beta J}\mathrm{sh}(\beta h)}{\sqrt{\mathrm{sh}^2(\beta h) + e^{-4\beta J}}}\left(\mathrm{ch}(\beta h) + \sqrt{\mathrm{sh}^2(\beta h) + e^{-4\beta J}}\right)$$

$$m = \frac{1}{\beta\lambda_+}\frac{\partial\lambda_+}{\partial h} = \frac{\mathrm{sh}(\beta h)}{\sqrt{\mathrm{sh}^2(\beta h) + e^{-4\beta J}}} \tag{5}$$

The curves of the magnetization as a function of h can be found in Figure 1. The function $m(h)$ is odd and increasing; its limit as $h \to 0$ vanishes for all positive temperatures, there is never any spontaneous magnetization, and no phase transition as the thermodynamic potential is always a smooth function. The slope of m in $h = 0$ increases when the temperature decreases, and the zero temperature limit is singular: if it is taken with $h > 0$ then the unique groundstate is $\underline{\sigma} = (+1, \dots, +1)$, hence the limit of m is 1, whereas if $T \to 0$ with $h < 0$ the goundstate is $\underline{\sigma} = (-1, \dots, -1)$ and m goes to -1.

7. Reasoning as in question 5 we write

$$C_N(k) = \frac{1}{Z}\sum_{\underline{\sigma}} \sigma_i \sigma_{i+k}\, e^{-\beta H(\underline{\sigma})} = \frac{\mathrm{Tr}(\mathbb{T}^{i-1}\hat{\sigma}\mathbb{T}^k\hat{\sigma}\mathbb{T}^{N-k-i+1})}{\mathrm{Tr}(\mathbb{T}^N)} = \frac{\mathrm{Tr}(\hat{\sigma}\mathbb{T}^k\hat{\sigma}\mathbb{T}^{N-k})}{\mathrm{Tr}(\mathbb{T}^N)} \ .$$

8. Let us denote $\{|+\rangle, |-\rangle\}$ the orthonormal basis of eigenvectors of the symmetric matrix $\mathbb{T}$, associated to the eigenvalues λ_+ and λ_- respectively. For any matrix $\mathbb{O}$ one has

$$\frac{\mathrm{Tr}(\mathbb{O}\mathbb{T}^N)}{\mathrm{Tr}(\mathbb{T}^N)} = \frac{\lambda_+^N \langle +|\mathbb{O}|+\rangle + \lambda_-^N \langle -|\mathbb{O}|-\rangle}{\lambda_+^N + \lambda_-^N} \underset{N\to\infty}{\longrightarrow} \langle +|\mathbb{O}|+\rangle \ ,$$

as $|\lambda_-| < \lambda_+$. Applying this formula with $\mathbb{O} = \hat{\sigma}\mathbb{T}^k\hat{\sigma}\mathbb{T}^{-k}$ yields a simplified form of the correlation function in the thermodynamic limit,

$$\lim_{N\to+\infty} C_N(k) = \langle +|\hat{\sigma}\mathbb{T}^k\hat{\sigma}\mathbb{T}^{-k}|+\rangle = \lambda_+^{-k}\langle +|\hat{\sigma}\mathbb{T}^k\hat{\sigma}|+\rangle = \left(\frac{\lambda_-}{\lambda_+}\right)^k \langle +|\hat{\sigma}|-\rangle\langle -|\hat{\sigma}|+\rangle + \langle +|\hat{\sigma}|+\rangle\langle +|\hat{\sigma}|+\rangle \ .$$

The explicit diagonalization of $\mathbb{T}$ yields $|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $|-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$, in such a way that $\hat{\sigma}|+\rangle = |-\rangle$ and $\hat{\sigma}|-\rangle = |+\rangle$. We thus obtain finally

$$\lim_{N\to+\infty} C_N(k) = \left(\frac{\lambda_-}{\lambda_+}\right)^k = e^{-\frac{k}{\xi}} \ ,$$

with the correlation length $\xi = -\frac{1}{\ln(\mathrm{th}(\beta J))}$. The correlation length is finite for all positive temperature, no phase transition is seen on this quantity. It grows monotonously when the temperature is decreased, and diverges as $T \to 0$, confirming that the zero-temperature limit is singular.

1.2 Ising spin chain with second neighbours interaction

9. We break the N spins into $N/2$ blocks of 2 consecutive spins and regroup the interactions inside and between succesive blocks. There are different possible ways to distribute the interactions in order to count all of them exactly once, one of them is

$$Z = \sum_{\underline{\sigma}} \prod_{i=0}^{(N/2)-1} e^{\beta(J_1(\sigma_{2i+1}\sigma_{2i+2}+\sigma_{2i+2}\sigma_{2i+3})+J_2(\sigma_{2i+1}\sigma_{2i+3}+\sigma_{2i+2}\sigma_{2i+4}))} \ , \tag{6}$$

which is indeed of the form given in the text, with $T((\sigma_1,\sigma_2),(\sigma_3,\sigma_4)) = e^{\beta(J_1(\sigma_1\sigma_2+\sigma_2\sigma_3)+J_2(\sigma_1\sigma_3+\sigma_2\sigma_4))}$.

10. We can consider the values of $T((\sigma_1,\sigma_2),(\sigma_3,\sigma_4))$ as the matrix elements of a 4×4 matrix $\mathbb{T}$ whose rows are indexed by (σ_1,σ_2) and the columns by (σ_3,σ_4). Choosing an arbitrary order for the four possible values of the row and column indices, for instance $(1,1),(-1,1),(1,-1),(-1,-1)$, this yields the matrix:

$$\mathbb{T} = \begin{pmatrix} T((1,1),(1,1)) & T((1,1),(-1,1)) & T((1,1),(1,-1)) & T((1,1),(-1,-1)) \\ T((-1,1),(1,1)) & T((-1,1),(-1,1)) & T((-1,1),(1,-1)) & T((-1,1),(-1,-1)) \\ T((1,-1),(1,1)) & T((1,-1),(-1,1)) & T((1,-1),(1,-1)) & T((1,-1),(-1,-1)) \\ T((-1,-1),(1,1)) & T((-1,-1),(-1,1)) & T((-1,-1),(1,-1)) & T((-1,-1),(-1,-1)) \end{pmatrix} .$$

We can now interpret the summation over $\underline{\sigma}$ in equation (6) as a sum over the row and column indices in a product of matrices, which yields the expression $Z = \mathrm{Tr}\,\mathbb{T}^{(N/2)}$. At the price of considering "block spins" (σ,σ') which can take 4 values instead of 2 for the original ones we transformed the interactions of range 2 on the original spins into a nearest neighbor interaction for the block spins, which allows to apply the transfer matrix method.

11. We want to show that the thermodynamic limit of the free energy is an analytic function of the temperature, for any positive temperature, which implies the absence of phase transition in such unidimensional models.

For any unidimensional model with degrees of freedom taking a finite number of values, and with finite range interactions, we can write the partition function as $Z = \mathrm{Tr}\, \mathbb{T}^{(N/b)}$, by considering blocks of b successive spins. The size of the transfer matrix $\mathbb{T}$ depends on the range of the interactions and on the number of possible values for the variables, but it is independent of N. The matrix elements of $\mathbb{T}$ are of the form $e^{-\beta E}$ for some finite energy E, and hence are strictly positive for any finite β. According to the Perron-Frobenius theorem the transfer matrix $\mathbb{T}$ thus admits a strictly positive eigenvalue $\lambda_0(\beta)$, strictly larger than the modulus of all other eigenvalues, hence the free-energy density reads in the thermodynamic limit :

$$f(\beta) = \lim_{N\to\infty} -\frac{1}{N\beta} \ln \mathrm{Tr}\, \mathbb{T}^{(N/b)} = -\frac{1}{b\beta} \ln \lambda_0(\beta) \ .$$

The eigenvalues λ of $\mathbb{T}$ are the roots of the characteristic polynomial $\det(\lambda \mathbb{I} - \mathbb{T}) = P(\lambda, \beta)$. The coefficients of the monomials λ^n in P are products of matrix elements of $\mathbb{T}$, and hence depends analytically on β. As $\lambda_0(\beta)$ is a simple root of the characteristic polynomial (thanks to the Perron-Frobenius theorem), the second result of the text (which is based on the implicit function theorem) shows that $\lambda_0(\beta)$ is analytic in a neighborhood of any β_0, and hence is analytic for all positive temperatures. As it is moreover strictly positive its logarithm is well-defined and analytic, and hence finally $f(\beta)$ is analytic.

2 The correlation functions of the unidimensional Ising model via diagrammatic expansions

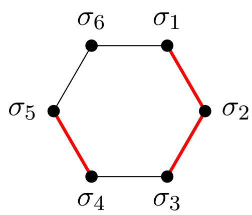
1.

$$\begin{aligned} \mathrm{ch}(x)(1 \pm \mathrm{th}(x)) = \mathrm{ch}(x) \pm \mathrm{sh}(x) &= \frac{e^x + e^{-x} \pm (e^x - e^{-x})}{2} \\ &= \frac{(1\pm 1)e^x + (1\mp 1)e^{-x}}{2} = e^{\pm x} \ . \end{aligned} \tag{7}$$

2.

$$\begin{aligned} Z &= \sum_{\underline{\sigma}} \prod_{i=1}^{N} e^{\beta(J\sigma_i\sigma_{i+1})} = \sum_{\underline{\sigma}} \prod_{i=1}^{N} [(\mathrm{ch}\beta J)(1 + \sigma_i\sigma_{i+1}(\mathrm{th}\beta J))] \\ &= (\mathrm{ch}\,\beta J)^N \sum_{\underline{\sigma}} \prod_{i=1}^{N} [1 + \sigma_i\sigma_{i+1}(\mathrm{th}\,\beta J)] \end{aligned}$$

3. We give an example of diagram on the following figure, drawing in thick red the edges of the diagram, and in black the other edges :



This diagram corresponds to the term $\sigma_1\sigma_2(\mathrm{th}\beta J)\sigma_2\sigma_3(\mathrm{th}\beta J)\sigma_4\sigma_5(\mathrm{th}\beta J)$ of the product.

As $\sigma_i = \pm 1$ it is easy to see that

$$\sum_{\underline{\sigma}} \sigma_1^{n_1}\sigma_2^{n_2}\dots\sigma_N^{n_N} = \begin{cases} 2^N & \text{if all the } n_i \text{ are even} \\ 0 & \text{otherwise} \end{cases} \ .$$

Therefore only the empty diagram (corresponding to $n_1 = \cdots = n_N = 0$) and the diagram with all the edges present ($n_1 = \cdots = n_N = 2$) contribute, if some spin σ_i is present once (or for later an odd number of times), the term cancels with σ_i taking value 1 and -1.

4. Summing the contributions of the two diagrams yields

$$Z = (\text{ch}\,\beta J)^N 2^N (1 + (\text{th}\,\beta J)^N) = (2\text{ch}\,\beta J)^N + (2\text{sh}\,\beta J)^N \ ,$$

which coincides with the expression found in the first exercise as $\lambda_+ = 2\text{ch}\,\beta J$ and $\lambda_- = 2\text{sh}\,\beta J$ when $h = 0$. The free energy density in the thermodynamic limit is then $f = -\frac{1}{\beta}\ln(2\text{ch}\,\beta J)$.

5. One has $\langle \sigma_i \rangle = 0$. Indeed, in absence of a magnetic field, $H(\underline{\sigma}) = H(-\underline{\sigma})$ (the system is invariant by flipping all spins), one can then make a change of variable $\underline{\sigma} \to -\underline{\sigma}$ in the sum defining $\langle \sigma_i \rangle$:

$$\langle \sigma_i \rangle = \frac{1}{Z}\sum_{\underline{\sigma}} \sigma_i e^{-\beta H(\underline{\sigma})} = \frac{1}{Z}\sum_{\underline{\sigma}} \sigma_i e^{-\beta H(-\underline{\sigma})} = \frac{1}{Z}\sum_{\underline{\sigma}} (-\sigma_i) e^{-\beta H(\underline{\sigma})} = -\langle \sigma_i \rangle \ .$$

One can also use the diagrammatic expansion

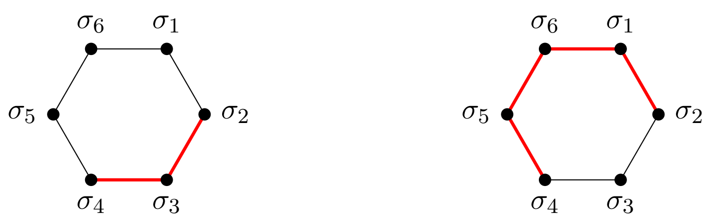
$$\langle \sigma_i \rangle = \frac{1}{Z}(\text{ch}\,\beta J)^N \sum_{\underline{\sigma}} \sigma_i \prod_{j=1}^{N} (1 + \sigma_j \sigma_{j+1} (\text{th}\,\beta J)) \ ,$$

and see that for all diagrams σ_i is always present as an odd power (σ_i or σ_i^3), hence the sum vanishes and $\langle \sigma_i \rangle = 0$.

6. In the diagrammatic expansion of the correlation function,

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z}(\text{ch}\,\beta J)^N \sum_{\underline{\sigma}} \sigma_i \sigma_j \prod_{k=1}^{N} (1 + \sigma_k \sigma_{k+1} (\text{th}\,\beta J)) \ ,$$

the terms that will contribute are thus in which σ_i and σ_j appears once, and all other spins zero or twice. There are two such diagrams that link i and j, as represented on the following figure for $N = 6$, $i = 2$ and $j = 4$:



The number of edges in the diagram is $j - i$ in the first one, $N - (j - i)$ in the second, which yields

$$\langle \sigma_i \sigma_j \rangle = \frac{(\text{th}\,\beta J)^{j-i} + (\text{th}\,\beta J)^{N-(j-i)}}{1 + (\text{th}\,\beta J)^N} \ .$$

In the thermodynamic limit, as $(\text{th}\,\beta J) < 1$, this simplifies in $\langle \sigma_i \sigma_j \rangle = (\text{th}\,\beta J)^{j-i}$, which coincides with the result of the first exercise, in particular $\xi = -\frac{1}{\ln(\text{th}(\beta J))}$.

7. The symmetry argument of question 5 shows that $\langle g(\underline{\sigma}) \rangle = 0$ for any function that is antisymmetric with respect to the reversal of all the spins, i.e. such that $g(-\underline{\sigma}) = -g(\underline{\sigma})$. This is the case for the product of an odd number of spins, in particular $\langle \sigma_i \sigma_j \sigma_k \rangle = \langle \sigma_i \sigma_j \sigma_k \sigma_l \sigma_m \rangle = 0$.

8. As in question 6 we have to retain the diagrams in which σ_i, σ_j, σ_k and σ_l appears once, and all other spins zero or twice. There are two such diagrams, one containing $(j - i) + (l - k)$ edges, the other $N - (j - i) - (l - k)$ edges, hence

$$\langle \sigma_i \sigma_j \rangle = \frac{(\text{th}\,\beta J)^{j-i+l-k} + (\text{th}\,\beta J)^{N-(j-i+l-k)}}{1 + (\text{th}\,\beta J)^N} \underset{N\to\infty}{\longrightarrow} (\text{th}\,\beta J)^{j-i+l-k} \ .$$