Universités P. et M. Curie, Paris-Diderot, Paris-Sud, École normale supérieure, École Polytechnique

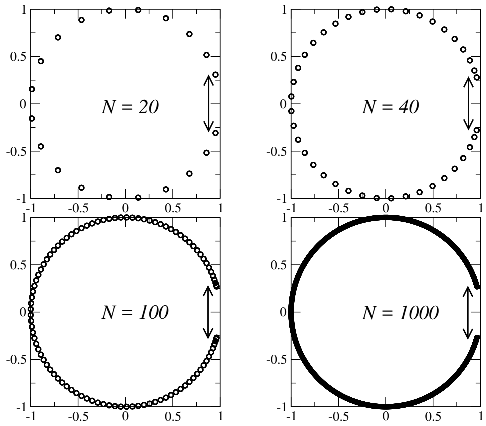
Condensed Matter, Quantum Physics and Soft Matter M2 programs

exam 2017-2018

Circling again with Lee and Yang

Should be written on a separate paper. It will be graded over 10 points.
One can often proceed with a given question without having answered the previous ones.
La rédaction pourra se faire en français pour ceux qui le souhaitent.

Previously, in the statistical mechanics course... we presented the perspective brought by T.D. Lee and C.N. Yang on Ising model phase transition. They studied the behaviour of the partition function Z as a function of a complex external magnetic field B, and realized that the distribution of its zeros does reveal original information about the phase transition in the canonical ensemble. More precisely, Lee and Yang showed that the partition function Z_N for an arbitrary ferromagnetic Ising model with N spins, vanishes for N values of $z = \exp(-2\beta B)$, that all lie on the unit circle. These zeros can be degenerate. The theorem holds on any lattice, any space dimension d, and is not restricted to nearest neighbor interactions. It implies that the zeros of Z_N, in the variable B, are purely imaginary quantities, and we shall thus introduce their imaginary part b such that $B = i\,b$. An interesting feature of Lee and Yang's idea (LY) is that it allows to extend the notion of phase transition and of criticality for temperatures T exceeding the critical one (T_c).



In the following, we are interested again in the spin 1/2 Ising model with ferromagnetic nearest neighbor interactions, on some d-dimensional lattice. The Hamiltonian reads

$$H = -J \sum_{\langle j,k \rangle} S_j\, S_k - B \sum_{j=1}^{N} S_j, \tag{1}$$

where the summation with brackets runs over pairs of nearest neighbors, and there are N distinct spins S_j, each taking two possible values $S_j = \pm 1$.

1) We start with an explicit check of LY result. Consider a system of $N = 3$ spins (and periodic boundary conditions), with Hamiltonian $H = -J\,(S_1S_2 + S_2S_3 + S_3S_1) - B(S_1 + S_2 + S_3)$.

- **a)** Introducing the inverse temperature $\beta = 1/(kT)$, write the partition function $Z_3(T, B)$.
- **b)** Show that $\exp(-3\beta B)Z_3$ is a polynomial of degree three in $z = \exp(-2\beta B)$.
- **c)** Z_3 admits a simple root; which one? Keeping in mind that the two other roots have to be complex conjugate, conclude that the values of $z = \exp(-2\beta B)$ for the three roots are on the unit circle (centered at the origin, and having radius 1).

2) The partition function $Z_N(T, B)$ exhibits terms of various power in z. What are the smallest, and largest powers? What is therefore the interest of considering, as in the following, the quantity $P_N(z) = Z_N \exp(-N\beta B)$? Pay attention to the fact that z is defined as $\exp(-2\beta B)$, and not as $\exp(-\beta B)$.

3) We denote as $z_j = \exp(-2\beta i b_j)$ the zeros of $P_N(z)$. Up to a function that does not depend on B, write P_N as a function of z and the $\{z_j\}_{1\leqslant j\leqslant N}$. No heavy calculation asked.

4) From P_N and its relation with Z_N, compute the magnetization per spin $m(T, B)$.

5) In the thermodynamic limit $N \to \infty$, we introduce the density of zeros, in the b-variable, as $\rho(b)$. This function is normalized to unity : $\int_{-\pi/2}^{\pi/2} \rho\, db = 1$. Show that

$$m(T, B) \;=\; \int \frac{\rho(b)}{\tanh[\beta(B - ib)]}\; db \tag{2}$$

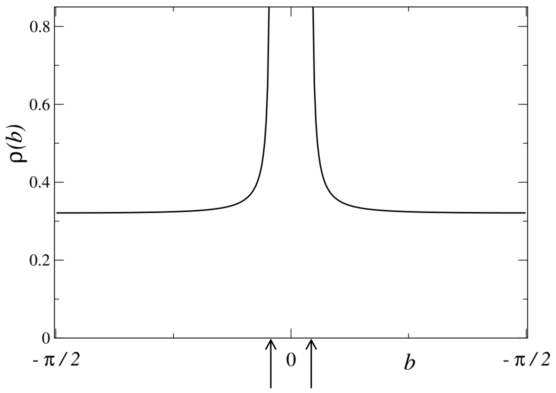


FIGURE 1 – Plot of $\rho(b)$.

The "angular" variable b is in $[-\pi/2, \pi/2]$; an important feature is that there may exist a gap in the distribution $\rho(b)$, for $b \in [-b_{\min}, b_{\min}]$, see an illustration in Fig. 1 for $K = 1$, $d = 1$, where the arrows indicate the values $\pm b_{\min}$ (the edges). For $T < T_c$, the gap closes and $b_{\min} = 0$. For $T > T_c$, $b_{\min}$ increases with T.

LY edge singularity : scaling relations

Our interest goes for a while to the behavior of the system for b close to the "edge" $b_{\min}$. For $B = i\, b_{\min}$ and at any $T > T_c$, it can be shown that the magnetic response is singular, associated to a new set of critical indices. This is the so-called LY edge singularity. In particular for $B \to ib_{\min}$, the (complex) magnetization behaves like

$$\delta m = m(T, B) - m(T, ib_{\min}) \;\propto\; (B - i\, b_{\min})^{1/\delta'} \tag{3}$$

and the correlation length, defined from the spin-spin correlation function, diverges like

$$\xi(T, B) \;\propto\; |B - i\, b_{\min}|^{-\nu'}. \tag{4}$$

On the other hand, for $|b| \to b_{\min}^{+}$ the density $\rho(b)$ behaves like

$$\rho(b) \propto (b - b_{\min})^{\sigma}, \tag{5}$$

while it vanishes for $|b| < b_{\min}$. At the "critical point" (meaning $B = i\, b_{\min}$ and $T > T_c$), the large-distance correlation function reads

$$\Gamma(r) \;\propto\; \frac{1}{r^{d-2+\eta'}}. \tag{6}$$

The exponents δ', ν', η' do not depend on the details of the lattice, but they do depend on space dimension d. They could *a priori* depend also on T, but it turns out that they do not ; their values are given in Figure 2. Whenever legitimate, we assume the system to be spatially homogeneous.

6) Invoking the fluctuation-response connection between the susceptibility χ and $\int \Gamma(r)\, d\mathbf{r}$, show that

$$1 - \frac{a_1}{\delta'} \;=\; \nu'(2 - \eta') \tag{7}$$

where a_1 is a constant to be given. To begin with, one may work out the dependence of χ on $B - i\, b_{\min}$.

7) We assume that the fluctuations of the intensive order parameter over a coherence volume (of measure ξ^d where d is space dimension), are of the same order of magnitude as its mean value

$$\delta m \;=\; m(T, B) - m(T, ib_{\min}). \tag{8}$$

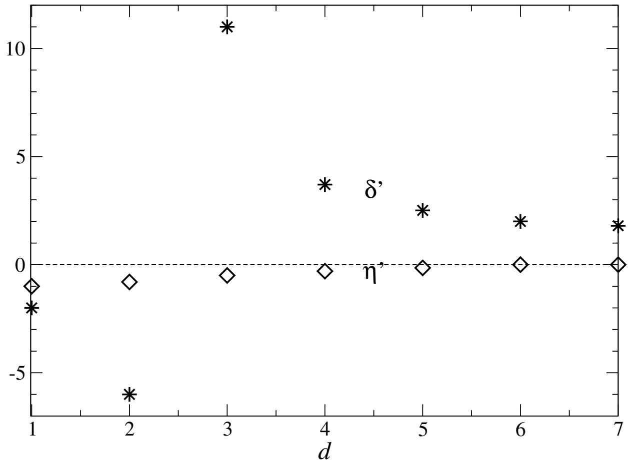


FIGURE 2 – Dependence of critical exponents η' (diamonds) and δ' (stars) on space dimension.

Show then that

$$\frac{1}{\delta'} = \frac{\nu'}{a_2}\left(d-2+\eta'\right) \tag{9}$$

where a_2 is a constant to be given. Can such a relation hold in all space dimensions ?

8) (*can be skipped, keeping the main result in mind*) The goal of this question is to show that $\sigma = 1/\delta'$. To this end, we consider B to be imaginary ($B = i\widetilde{b}$), with $|\widetilde{b}| < b_{\rm min}$. Making use of relation (2) to compute $m(T, i\widetilde{b}) - m(T, ib_{\rm min})$, and changing variables from b to $x = (b - b_{\rm min})/\delta b$ where $\delta b = b_{\rm min} - \widetilde{b}$, one can proceed expanding $1/\tanh(\alpha)$ into $1/\alpha + \mathcal{O}(\alpha)$ for small α, and conclude. Here, we do not pay specific attention to the values of σ that make the integrals convergent.

9) From the previous questions, prove that

$$\sigma = \frac{1}{\delta'} = \frac{d-2+\eta'}{d+2-\eta'} \qquad \text{and} \qquad \nu' = \frac{2}{d+2-\eta'}. \tag{10}$$

Are these results compatible with the data reported in Fig. 2 ?

In the remainder, we will perform a mean-field treatment yielding the critical exponents, before studying the one-dimensional case. We will finally establish that the spontaneous magnetization of the system, for $T < T_c$, is nothing but $\rho(0)$ up to a prefactor.

Mean-field analysis

We denote c the number of nearest neighbors of a given site on the lattice. We perform here a mean-field treatment.

10) Write the magnetization is a self-consistent fashion, as $m = \tanh(\ldots)$. What is the critical temperature T_c of the paramagnetic/ferromagnetic transition taking place at $B = 0$?

11) Show that the susceptibility can be written

$$\chi = \frac{\cdots}{1 - \beta J\, c\,(1-m^2)}. \tag{11}$$

12) The above expressions for m and χ remain valid for complex fields B, and in particular at the edge. Explain why one has

$$1 - m(T, ib_{\rm min})^2 = \frac{T}{T_c}. \tag{12}$$

Making use of $\tanh(x) = x - x^3/3 + \mathcal{O}(x^5)$, find how $b_{\rm min}$ depends on $t = T - T_c$, for small t.

13) Compute δ'.

14) Are we working here at $T < T_c$ or $T > T_c$?

15) How should one proceed to get the (mean-field) correlation function Γ (including its short scale features, which precludes a Landau-like approach) ? Which value of ν' would ensue ? No calculation asked.

The one dimensional case

For a one-dimensional regular lattice, standard techniques allow for the full solution of the problem.

16) Briefly sketch the ideas behind one such technique.

17) Having computed exactly the zeros of Z_N, one can establish that their density reads

$$\rho(b) \;=\; \frac{1}{\pi\, kT}\, \frac{|\sin(\beta b)|}{\sqrt{\sin^2(\beta b) - e^{-4K}}}. \tag{13}$$

What is then the expression for $b_{\min}$? Can it vanish ? Why ?

18) From Eq. (13), what is the value of σ ?

19) We define Δb as the spacing between consecutive zeros ; this quantity is b-dependent, and computed at finite but large N. How does $\rho(b)$ relate to Δb ? A scaling argument only is required here.

20) How can one recover the value of σ from Fig. 3 ?

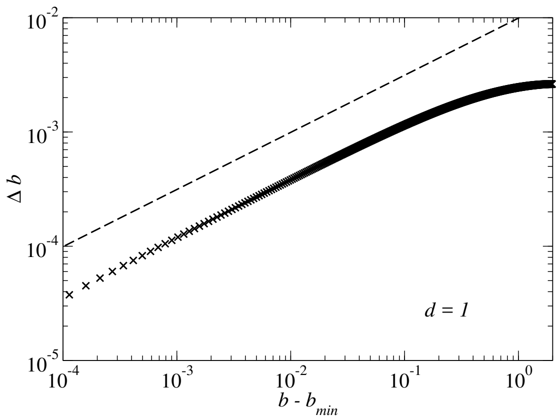


FIGURE 3 – Spacing between consecutive zeros ($N = 2000$, $K = 0.6$, $d = 1$). The line is a guide to the eye.

Back to reality

For $T < T_c$, the density of complex zeros, $\rho(b)$, encodes an interesting information for real magnetic fields B : the spontaneous magnetization $m_s(T)$, chosen to be positive.

21) Why should one pay attention when taking the limit $B \to 0$, to obtain $m_s(T)$?

22) Show that for $T < T_c$,

$$m_s(T) \;=\; \pi\, kT\, \rho(0). \tag{14}$$

To this end, invoking the parity of $\rho(b)$, we write Eq. (2) as

$$m(T, B) \;=\; \int_0^{\pi/2} \rho(b) \left\{ \frac{1}{\tanh[\beta(B - ib)]} + \frac{1}{\tanh[\beta(B + ib)]} \right\} db. \tag{15}$$

For $B \to 0$ (and real), explain first why the integral is dominated by small b contributions, and compute $m_s(T)$. It is useful here to use that

$$\int_0^{\infty} \frac{1}{1 + x^2}\, dx \;=\; \frac{\pi}{2}. \tag{16}$$