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

Condensed Matter, Quantum Physics and Soft Matter M2 programs

exam 2016-2017

Statistical mechanics at the edge : Lee and Yang zeros

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.
The reasons to be afraid by the apparent length of the text are ill-founded. Spirits up... Spins up or down.
La rédaction pourra se faire en français pour ceux qui le souhaitent.

Introduction.

In the 1950s, soon after Onsager's work on Ising model, T.D. Lee and C.N. Yang had an idea that, as surprising as it may seem at first glance, has shed new light on the study of phase transitions. Their approach was initially couched for a lattice gas, but it holds equally well for a magnet in a fixed magnetic field. They realized that the partition function Z can fruitfully be viewed as a function of the external magnetic field B, not only when B is real (as is of course the experimentally relevant case), but more interestingly when B is a *complex number*. It soon appeared that the distribution of zeros of Z in the complex plane does reveal original information about the phase transition in the canonical ensemble.

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

$$H = -J \sum_{\langle i,j \rangle} S_i \, S_j \; - B \sum_{i=1}^{N} S_i, \tag{1}$$

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

1) We will here always consider ferromagnetic interactions. What does this mean ?

2) Is it possible for Z to vanish when B is a *real* magnetic field ? N is supposed fixed here.

3) We start with a system of $N = 2$ spins, with Hamiltonian $H = -J\, S_1 S_2 \, - B(S_1 + S_2)$.

- **a)** Introducing the inverse temperature $\beta = 1/(kT)$, write the partition function $Z_2(T, B)$.
- **b)** Show that $\exp(-2\beta B) Z_2$ is a polynomial of degree two in $z = \exp(-2\beta B)$.
- **c)** What are the two zeros of Z_2 ? Conclude that the two corresponding values of $z = \exp(-2\beta B)$ are on the unit circle (centered at the origin, and having radius 1).

The statement : unit circle phenomenon and real axis pinching

What is remarkable is that the above result is general, and is referred to as *Lee and Yang theorem :* 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 $B = i\, b$. Figure 1 illustrates the unit circle phenomenon, where each small disk denotes the location of a zero z of Z_N.

To make sense out of the Lee and Yang theorem, we need to remember a bit of complex analysis. Seen as a function of z, the partition function will be a smooth, non singular function (mathematicians would say "analytic"), for z in any region outside the Lee and Yang (LY) zeros. This holds in particular in the thermodynamic limit $N \to \infty$. Thus, one needs to have an accumulation of LY zeros in the z-plane, at a phase transition point where Z is by definition not analytic.

4) When B is real, is it possible to have a phase transition with N finite (i.e. non divergent) ?

5) In light of these results, what are the *real* values of B for which a phase transition can be observed ? Keep in mind that when B is real, z is real as well, and of course positive.

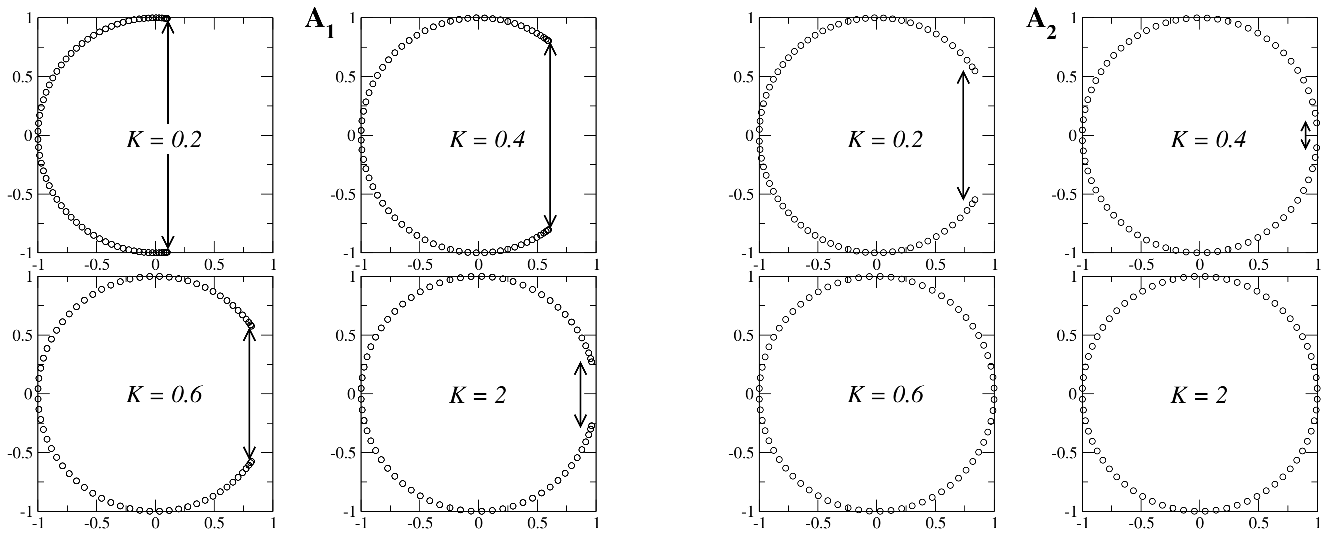


FIGURE 1 – Location of Lee and Yang zeros in the z-complex plane, for a system of $N = 68$ spins, where z is related to the magnetic field through $z = e^{-2\beta B}$. There are thus 68 zeros for each value of the coupling constant $K = J/(kT)$. The zeros go in conjugate pairs, so that the set of points shown enjoys reflection symmetry with respect to the x-axis. One panel (A_1 or A_2) if for a one-dimensional system, while the other (A_2 or A_1) is for a two-dimensional square lattice. You will have to find out which is which. For all numerical results shown in this paper, periodic boundary conditions have been enforced. The vertical arrows indicate a gap that does not close in the thermodynamic limit, see Fig. 2. Please, pay attention to the pinching [1] of the real axis, as K increases, in panel A_2.

In Fig. 1, some spacings between successive zeros along the unit circle are visible, and can be discriminated in two categories : either the spacing tends to 0 for large N, or it tends to a finite value. The latter case is represented by an arrow in Fig. 1. The fact that the arrow remains of finite size while $N \to \infty$, while other gaps do close, is shown in Fig. 2.

6) We focus on the situation reported in Fig. 2. For these parameters, is there a phase transition (for real B) ?

7) One of panels A_1 and A_2 in Fig. 1 is for $d = 1$ and the other for $d = 2$.

a) Which is which ? Explain.

b) From Fig. 1, estimate roughly the critical K and then the critical temperature, T_c, of the two dimensional model.

c) How should T_c compare to its mean-field counterpart T_c^{mf} ? Why ?

d) What is the value of T_c^{mf} on the 2d square lattice (no heavy calculation asked ; you can simply recall the result, or rederive it briefly) ? Check if the expected inequality holds.

Before studying the behavior of the system for b close to the "edge" $b_{\min}$, we investigate how the gap closes, at T_c, in the thermodynamic limit, assuming that the rather small systems addressed here provide indeed fair indication. The results are shown for $d = 2$ in Figs. 3 and 4, starting with N as small as 9.

8) For $T = T_c$, one can relate the divergence of the correlation length ξ to the magnetic field B (B is real here). Sketch the corresponding scaling argument, from which a power law involving the

1. pinching = *pincement*

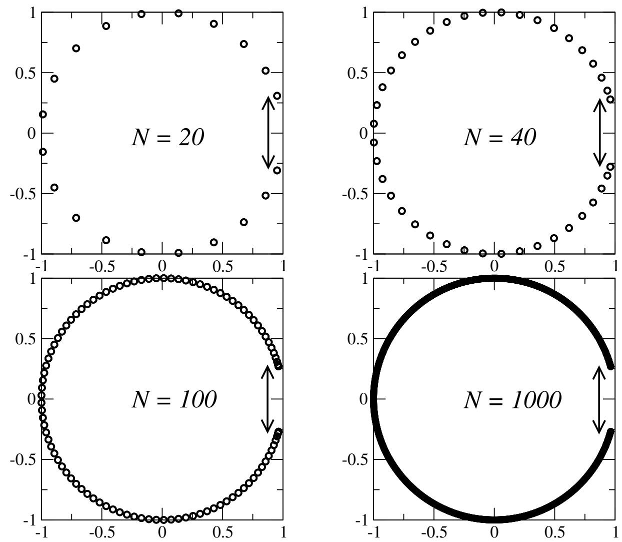


FIGURE 2 – LY zeros as in panel A_1 of Fig. 1, for $K = 2$, and different values of N. The gap shown by the arrow remains in the thermodynamic limit, while the other smaller gaps between consecutive zeros do vanish. Except for small N (results not shown), the size of the arrow (almost) does not depend on N. The arrow length can be written $2\sin(2\beta b_{\min})$ where $b_{\min} > 0$ is the smallest (positive) imaginary part of the LY zeros (in the B variable). Here, one has $b_{\min} \neq 0$ for all N.

standard exponents β, δ and ν does appear (as is customary, do not confuse this β with the inverse temperature). Given that Onsager's solution yields the exact results $\beta = 1/8$, $\delta = 15$, and $\nu = 1$, what is then the exponent in the relation $\xi \propto B^{\text{something}}$, where the symbol $\propto$ means "equal up to a constant" ?

9) We assume that a similar relation does hold in our case, between $b_{\min}$ and system size L. In light of Fig. 3, does this make sense ? Try to back up the argument.

10) *(subsidiary)* Fig. 4 actually yields a more refined, *plausible*, information, dealing also with the sub-leading correction in L of $b_{\min}$. How can this refined relation between $b_{\min}$ and L be written ?

Lee-Yang edge singularity

An interesting feature of Lee and Yang's idea applied to our spin model, is that it allows to extend the notion of criticality for temperatures larger than T_c. Indeed 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 Lee and Yang edge singularity. These indices are the focus of our interest in the remainder. In particular for $B \to ib_{\min}$, the (complex) magnetization behaves like

$$\delta m = m(T, B) - m(T, ib_{\min}) \;\propto\; (B - i\, b_{\min})^{1/\delta'} \tag{2}$$

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

$$\xi(T, B) \;\propto\; |B - i\, b_{\min}|^{-\nu'}. \tag{3}$$

At the "critical point" (meaning $B = i\, b_{\min}$ and $T > T_c$), the correlation function reads

$$\Gamma(r) \;\propto\; \frac{1}{r^{d-2+\eta'}}. \tag{4}$$

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 5.

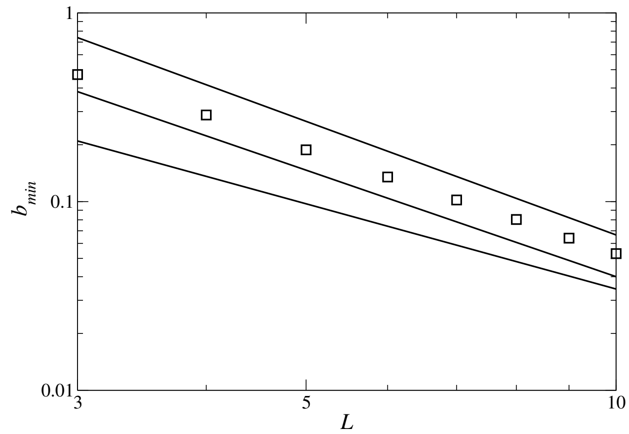


FIGURE 3 – Behavior of $b_{\rm min}$ at $T = T_c$, as a function of system size, for a $L \times L$ square lattice having $N = L^2$ spins. Note the log-log scale. The three lines are guides to the eye and to the brain, having slopes 1.5, 1.875 and 2. A more detailed information is available in Fig. 4.

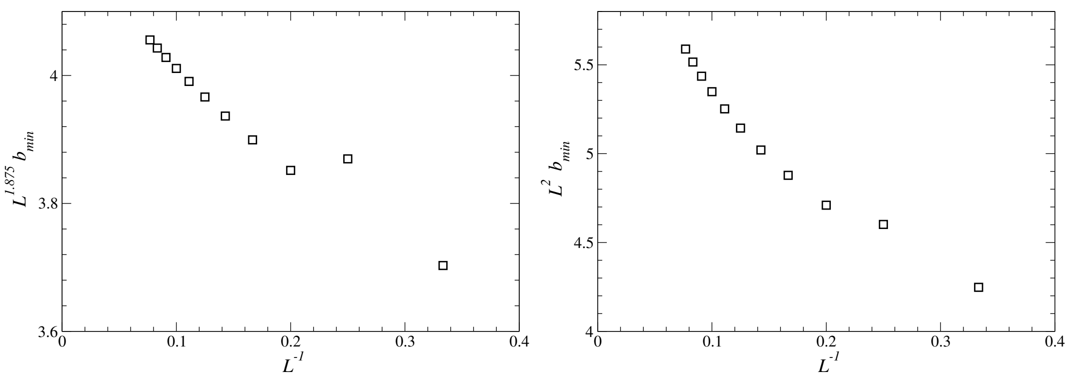


FIGURE 4 – Reprocessing of the same data as in Fig. 3, to test two slightly different scaling behaviors. As a function of $1/L$, we show $L^{1.875}\, b_{\rm min}$ (left) and $L^2\, b_{\rm min}$. The scale of the plots is now linear.

11) From Figure 5, what can you guess concerning the upper critical dimension d_u associated to this transition ? Do you remember what is the upper critical dimension of the standard Ising ferromagnetic transition ? (a simple "yes" will not be taken for an answer. . .)

12) How does $b_{\rm min}$ behave with T, both for $T < T_c$ and $T > T_c$? A rough and pictorial answer is sufficient : simply plot $b_{\rm min}$ as a function of T in a qualitative manner.

We will start by a mean-field treatment yielding the critical exponents, before analyzing the one-dimensional case. We will finally explicitly check that for $d > d_u$, fluctuations discarded at mean-field level are indeed irrelevant.

Landau approach to the edge

In Landau spirit, we write the free energy as a function of magnetization as

$$f(m, B, T) = \frac{t}{2} m^2 + \frac{a_4}{4} m^4 - B\, m. \tag{5}$$

where $t = T - T_c$ denotes the distance to the critical temperature, and will be positive. Strictly speaking, the prefactor of the quadratic term in the expansion is not exactly t, but some a_2 that behaves like t for small t.

13) Justify briefly the form chosen in Eq. (5). What is the sign of a_4 ?

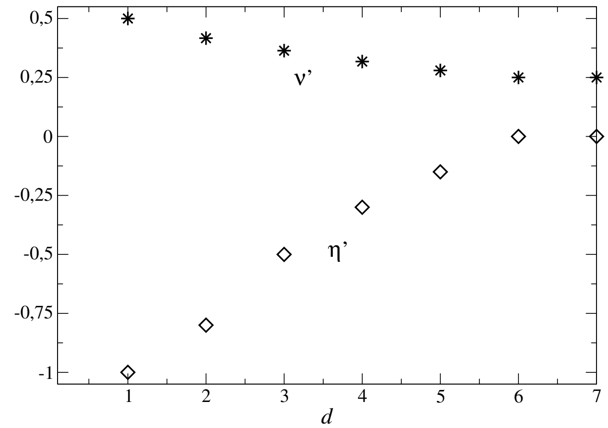


FIGURE 5 – Dependence of critical exponents η' and ν' on space dimension.

Considering complex fields $B = ib$ and anticipating that $m = i\mathcal{M}$ turns out complex as well, we focus on the free energy $\mathcal{F}$ as a function of the real quantity $\mathcal{M}$:

$$\mathcal{F}(\mathcal{M}) = -\frac{t}{2}\mathcal{M}^2 + \frac{a_4}{4}\mathcal{M}^4 + b\,\mathcal{M}. \tag{6}$$

14) For a given $t > 0$ and b, we denote by $\mathcal{M}^*$ the value adopted by the system. What is the equation encoding the dependence of the magnetization of the system on b, t and a_4 ?

15) Sketch graphically the connection between b and $\mathcal{M}^*$ (it may prove easier to plot b as a function of $\mathcal{M}^*$). Note that there exists a magnetic field such that $\partial\mathcal{M}^*/\partial b$ diverges. This singular behavior defines b_{min} and the associated $\mathcal{M}_{\text{min}}$. Indicate b_{min} and $\mathcal{M}_{\text{min}}$ on your graph (because of symmetry, this corresponds to two points). Note that $\pm\mathcal{M}_{\text{min}}$ stand for two specific values of $\mathcal{M}^*$, but to avoid cumbersome notation, the * index is dropped in $\mathcal{M}_{\text{min}}$.

16) Show that $b_{\text{min}} \propto t^{\Omega}$. What is the exponent Ω ?

17) Knowing b_{min}, compute the value of exponent δ'.
Hint : For all calculations of this type, it is convenient to work with $\mathcal{F}(\mathcal{M})$, keeping in mind the vanishing of the first and second derivatives : $\mathcal{F}'(\mathcal{M}_{\text{min}}) = 0$ and $\mathcal{F}''(\mathcal{M}_{\text{min}}) = 0$, where $m(T, ib_{\text{min}}) = i\mathcal{M}_{\text{min}}$. Then, introducing $\delta\mathcal{M}^* = \mathcal{M}^* - \mathcal{M}_{\text{min}}$ and $\delta b = b - b_{\text{min}}$ is useful.

18) From Eq. (6), how should one proceed to compute the correlation function $\Gamma(r)$, from which exponents ν' and η' follow ? No calculation asked, just a roadmap and a functional.

19) Show the correlation function to be given by

$$\Gamma(r) \propto \int d\mathbf{q}\, \frac{e^{-i\,\mathbf{q}\cdot\mathbf{r}}}{\xi^{-2} + q^2} \tag{7}$$

where $\xi^{-2} \propto -t + 3a_4\mathcal{M}^{*2}$. Relate ξ^{-2} to $\delta\mathcal{M}$. What is the value of exponent ν' appearing in Eq. (3) ?

20) Show that for $b \to b_{\text{min}}$, $\delta\mathcal{F}_{\text{mf}} = \mathcal{F}(\mathcal{M}^*) - \mathcal{F}(\mathcal{M}_{\text{min}})$ behaves like some power law of $\delta b = b - b_{\text{min}}$.

21) In view of computing the upper critical dimension d_u, we estimate the fluctuation-induced correction to the mean-field prediction $\delta\mathcal{F}_{\text{mf}}$, as being proportional to ξ^{-d}, in terms of scaling with respect to δb. Why ? *(subsidiary)* How could one perform a calculation of the free energy "beyond the saddle point" ?

22) Using the results of the two previous questions, compute the upper critical dimension. Is your result compatible with the data in Fig. 5 ?

The one dimensional case

The edge singularity occurs in $d = 1$ as well, where its study, together with its mean-field counterpart, provides "bounds" for intermediate dimensions. We therefore address the regular 1d lattice where each of the N spins has two neighbors, with periodic boundary conditions ($S_{N+1} = S_1$).

23) Briefly explain why the partition function can be put in the form $Z_N(T, h) = \lambda_+^N + \lambda_-^N$ with

$$\lambda_\pm = e^K \operatorname{ch} \beta B \pm \sqrt{e^{2K} \operatorname{sh}(\beta B)^2 + e^{-2K}} \tag{8}$$

24) Noting that λ_+ and λ_- do not vanish, prove the zeros of Z_N to be imaginary magnetic fields. It can be used that if $|a - b| = |a + b|$ where a and b are complex numbers, then $a\bar{b}$ is purely imaginary ($\bar{b}$ being the complex conjugate of b). Prove that

$$\sin(\beta b_{\min}) = e^{-2K}, \tag{9}$$

which leads to the vanishing of the square root in Eq. (8).

25) By a technique akin to that leading to Z_N through (8), it can be shown that the correlation length is given by $\exp(-1/\xi) = \lambda_-/\lambda_+$. From this, compute exponent ν'.

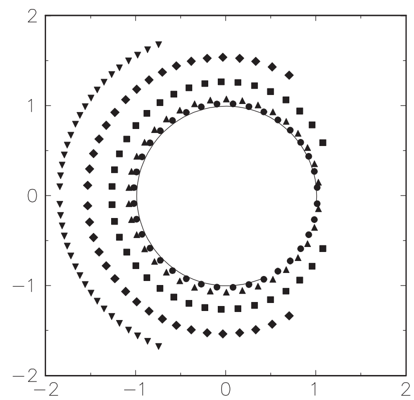
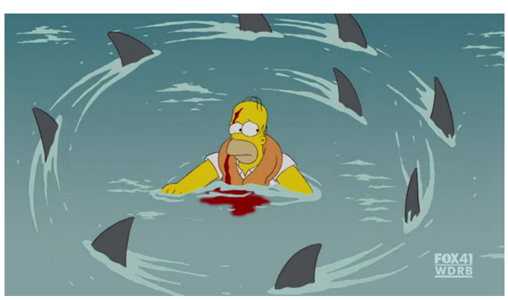


FIGURE 6 – Location of LY zeros, for a magnetic model where 6^2 spin variables no longer take two values as within spin 1/2 Ising, but three (this is the so-called three-state Potts model). The different symbols correspond to different temperatures. The discs, triangles up, squares, diamonds and triangles down are for $x = 2x_c$, x_c, $2x_c/3$, $x_c/2$ and $x_c/4$ respectively, where $x = e^{\beta J}$ and the subscript c denotes the critical value. From Kim and Creswick, Phys. Rev. Lett. **81**, 2000 (1998).

26) Going beyond Ising modelology, what do you conclude from Fig. 6 ?



Epilogue. Our zheroes got the Nobel prize in 1957, a couple of years after this work, but this was for another achievement (parity violation in particle physics). Recently, imaginary magnetic fields have been produced in the real world, which allowed to study Lee-Yang phenomenology in the lab, hitherto viewed as unphysical [Peng et al. *Phys. Rev. Lett.* **114**, 010601 (2015)].