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

Lee and Yang zeros - short correction

1) With ferromagnetic interactions, $J > 0$, and spins tend to align to minimize energy.

2) The partition function is a sum of exponentials, and therefore strictly positive. It cannot vanish when B is a real magnetic field.

3) With Hamiltonian $H = -J\, S_1 S_2 - B(S_1 + S_2)$, we sum over the 4 configurations to get,

a) with $K = \beta J$,

$$\boxed{Z_2(T,B) = e^K e^{2\beta B} + 2e^{-K} + e^{K-2\beta B}}$$

b) $\exp(-2\beta B)\, Z_2 = e^K + 2e^{-K}\, z + e^K\, z^2$

c) The two zeros of Z_2 are complex conjugate :

$$z_\pm \;=\; -e^{-2K} \;\pm\; i\sqrt{1 - e^{-4K}}. \tag{1}$$

We have $z_+ z_- = 1$, as already visible on the polynomial itself (the coefficients of z^0 and z^2 terms are equal), and the two zeros are on the unit circle ($|z_+| = |z_-| = 1$)

4) With N fixed and finite, we see that all zeros are on the unit circle, but there can be no zero strictly on the real axis, which is the physical line associated to real magnetic fields. Thus, the partition function is analytic on the whole real axis, which is incompatible with a phase transition.

5) A phase transition point has to lie in the vicinity of a zero, and the only possibility for having a transition is when the real axis is pinched by the set of zeros, when $N \to \infty$. This can solely occur at $z = 1$, meaning that $\boxed{\text{a phase transition can take place at } B = 0 \text{ only}}$.

6) For all situations indicated with an arrow on the graphs, the non-closing gap "protects" the real axis : $\boxed{\text{no pinching of the real axis} \Longrightarrow \text{no phase transition}}$.

7) We know that Ising model exhibits a finite-temperature transition in $d = 2$, but not in $d = 1$.

a) Hence, $\boxed{\text{panel A}_1 \text{ is for 1d and panel A}_2 \text{ is for 2d}}$.

b) In panel A_2, the pinching occurs for $0.4 < K < 0.6$, i.e. $2/5 < K < 3/5$. The critical K is thus in this range. In terms of temperature, this means $\boxed{1.66 < kT_c/J < 2.5}$

c) Mean-field discards fluctuations, that have the tendency to destroy order. Hence, there is a temperature range where mean-field predicts order, while fluctuations have already washed it out, so that

$$\boxed{T_c^{\text{true}} < T_c^{mf}}$$

d) Within mean-field, we get $kT_c^{mf} = qJ$ where q is the number of neighbors of a given spin. Here, $q = 4$ and the mean-field critical temperature is larger than the true one. Its exact value was found by Onsager to be $kT_c/J = 2/\log(1+\sqrt{2}) \simeq 2.27$. The true critical K is close to 0.44.

8) The argument was seen in class... We consider an infinite system with $B \neq 0$ (and real). In the vicinity of the critical point, we assume a scaling relation between ξ, its value for $B = 0$ (i.e. $|t|^{-\nu}$ where $t = T - T_c$), B and the relevant scale for B, that reads m^δ. Remembering that $m \propto t^\beta$, we arrive at

$$\frac{\xi}{|t|^{-\nu}} \;=\; \psi\left(\frac{B}{t^{\beta\delta}}\right) \tag{2}$$

where ψ is some unknown scaling function. At the expense of introducing another such function $\widetilde{\psi}$, we can thus also write

$$\xi \,=\, B^{-\nu/(\beta\delta)}\ \widetilde{\psi}\left(\frac{B}{t^{\beta\delta}}\right). \tag{3}$$

At T_c but $B \neq 0$, ξ is expected to remain finite, which means that $\widetilde{\psi}(\infty)$ is finite. This in turn implies

$$\boxed{\xi \,\propto\, B^{-\nu/(\beta\delta)} \quad \text{at} \quad T = T_c}. \tag{4}$$

9) In our case, we seek for a scaling relation between $\xi(b=0)$, L, b_{min} and its relevant measure $t^{\beta\delta}$. We can thus essentially repeat the above argument :

$$\frac{L}{|t|^{-\nu}} \,=\, \psi\left(\frac{b_{\text{min}}}{t^{\beta\delta}}\right) \qquad \Longrightarrow \qquad L \,=\, b_{\text{min}}^{-\nu/(\beta\delta)}\ \widetilde{\psi}\left(\frac{b_{\text{min}}}{t^{\beta\delta}}\right) \qquad \text{and} \qquad \boxed{b_{\text{min}} \,\propto\, L^{-\beta\delta/\nu}} \tag{5}$$

where the last relation is found at $t = 0$. The exact values of the critical exponents yield $\beta\delta/\nu = 15/8 = 1.875$. This is compatible with the results of Figure 3...

10) $\ldots$ yet, one may argue that a power law with exponent -2 would be equally convincing. The goal of Fig. 4 is to help discriminating the two behaviors. Figure 4 shows on the right hand side a rather nice straight line at small $1/L$, which may indicate a relation like

$$b_{\text{min}} \propto L^{-1.875}\left(a - \frac{b}{L}\right) \tag{6}$$

where a and b are positive constants. There is a sort of "outlier" point at $1/L = 0.25$, that could not be spotted as such in Fig. 3. This indicates that the kind of plot provided on Fig. 4-left is a rather stringent test, magnifying numerical inaccuracies. On the other hand, the right hand side figure does not say much except that the power law -2 might be associated with a sub-leading correction that would differ from $1/L$. Anyway, it turns out that exponent 1.875 is the correct one, and it is well compatible with the data reported.

Note here the surprising fact that with small systems, having $3 \leqslant L \leqslant 10$, we already have a decent idea of thermodynamic limit behavior (even restricting to $3 \leqslant L \leqslant 5$).

11) The critical exponents reported have the same value for $d = 6$ and $d = 7$, which hints at $\boxed{d_u = 6}$. On the other hand, the "standard" ferromagnetic upper critical dimension is 4.

12) The data shown indicate that b_{min} decreases with K, and vanishes for $K > K_c$: $b_{\text{min}} = 0$ for $T < T_c$ and increases with T for $T > T_c$.

13) For $B = 0$, symmetry $m \to -m\ldots$, $a_4 > 0$, seen in class.

14) The condition $\mathcal{F}'(\mathcal{M}) = 0$ reads

$$\boxed{b \,-\, t\,\mathcal{M}^* \,+\, a_4\,\mathcal{M}^{*3} \,=\, 0}. \tag{7}$$

15) The relation $b(\mathcal{M}^*)$ is sketched in Figure C1. Note that b and $\mathcal{M}^*$ tend to "anti align" at large $|b|$, a consequence of having the field and the magnetization both complex ($i^2 = -1$).

It makes sense that the system's response is singular for the field where $\partial\mathcal{M}^*/\partial b$ diverges. This admits a simpler formulation : in addition to $\mathcal{F}'(\mathcal{M}) = 0$ that sets $\mathcal{M}^*$, b_{min} corresponds to $\mathcal{F}''(\mathcal{M}) = 0$. Thus, introducing $\mathcal{M}_{\text{min}}$ as in Fig. C1

$$\mathcal{F}''(\mathcal{M}_{\text{min}}) \,=\, 0 \quad \Longrightarrow \quad \mathcal{M}_{\text{min}}^2 \,=\, \frac{t}{3\,a_4}. \tag{8}$$

16) Going back to Eq. (7), this gives

$$b_{\text{min}} = t\,\mathcal{M}_{\text{min}} \,-\, a_4\,\mathcal{M}_{\text{min}}^3 \qquad \Longrightarrow \qquad \boxed{b_{\text{min}} \,\propto\, t^{3/2}} \tag{9}$$

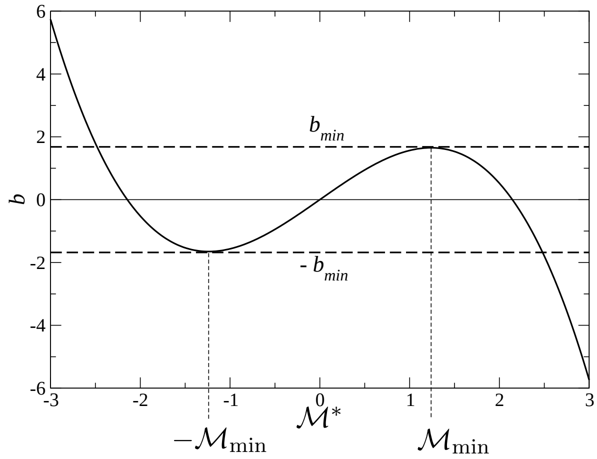

FIGURE C1 – Dependence of b with $\mathcal{M}^*$ as encoded in Eq. (7), and graphical meaning of $b_{\rm min}$.

17) We are looking for the relation between $\delta\mathcal{M}^* = \mathcal{M}^* - \mathcal{M}_{\rm min}$ and $\delta b = b - b_{\rm min}$. To this end, we can Taylor expand $\mathcal{F}'(\mathcal{M}^*) = 0$ in the vicinity of $\mathcal{M}_{\rm min}$:

$$0 \;=\; \delta b \,+\, \mathcal{F}'(\mathcal{M}_{\rm min}) \,+\, \mathcal{F}''(\mathcal{M}_{\rm min})\,\delta\mathcal{M}^* \,+\, \frac{1}{2}\,\mathcal{F}'''(\mathcal{M}_{\rm min})\,\delta\mathcal{M}^{*2} \;=\; \delta b + 3\,a_4\,\mathcal{M}_{\rm min}\,\delta\mathcal{M}^{*2}. \qquad (10)$$

This is indeed the parabolic behavior expected in the vicinity of the point $(\mathcal{M}_{\rm min}, b_{\rm min})$ (with proper signs, see Fig. C1). We conclude that $\boxed{\delta\mathcal{M}^* \,\propto\, \delta b^{\,1/2}}$, or $\boxed{\delta' = 2}$.

18) Proceed as in class, upgrading Landau free energy into a Ginzburg-Landau functional

$$\mathcal{F}\{\mathcal{M}\} \;=\; \int d\mathbf{r}\left[-\frac{t}{2}\,\mathcal{M}^2(\mathbf{r}) \,+\, \frac{a_4}{4}\,\mathcal{M}^4(\mathbf{r}) \,+ b\,\mathcal{M}(\mathbf{r}) \,+\, \lambda(\nabla\mathcal{M})^2\right] \qquad (11)$$

where λ is a positive rigidity term.

19) Same story. Consider b to be position dependent as well ; the correlation function is then $\Gamma(\mathbf{r},\mathbf{r}') = \delta\mathcal{M}(\mathbf{r})/\delta b(\mathbf{r}')$ where

$$0 \;=\; b(\mathbf{r}) \,-\, t\,\mathcal{M}(\mathbf{r}) + a_4\,\mathcal{M}^3(\mathbf{r}) \,-\, \lambda\,\nabla^2\mathcal{M}. \qquad (12)$$

We get

$$0 \;=\; \delta(\mathbf{r}-\mathbf{r}') \,+\, (-t + 3a_4\mathcal{M}^{*2} - \lambda\nabla^2)\Gamma(\mathbf{r}-\mathbf{r}'), \qquad (13)$$

that has been written for a homogeneous system where $\mathcal{M}$ is no longer position dependent, and has value $\mathcal{M}^*$. This is familiar looking, and can be solved by Fourier transform to yield the formula of the text.

We have $\xi^{-2} = (-t+3a_4\mathcal{M}^{*2})/\lambda$. This can be computed explicitly, introducing $\mathcal{M}^* = \mathcal{M}_{\rm min} + \delta\mathcal{M}^*$ but it is more convenient to note that ξ^{-2} is proportional to $\mathcal{F}''(\mathcal{M}^*)$, and therefore of order $\delta\mathcal{M}^*$: $\mathcal{F}''(\mathcal{M}^*) = \mathcal{F}''(\mathcal{M}_{\rm min}) + (...)\delta\mathcal{M}^* \propto \delta\mathcal{M}^*$. Hence,

$$\xi^{-2} \,\propto\, \delta\mathcal{M}^* \quad\Longrightarrow\quad \xi \,\propto\, (\delta\mathcal{M}^*)^{-1/2} \qquad\Longrightarrow\qquad \boxed{\xi \,\propto\, (\delta b)^{-1/4} \quad \text{and} \quad \nu' = \frac{1}{4}.} \qquad (14)$$

This indeed is what can be read in Fig. 5 of the main text. The correlation length diverges when $b \to b_{\rm min}$.

20) Another Taylor expansion in the vicinity of $\mathcal{M}_{\rm min}$ yields

$$\begin{aligned} \delta\mathcal{F}_{\rm mf} = \mathcal{F}(\mathcal{M}^*) - \mathcal{F}(\mathcal{M}_{\rm min}) \;&=\; 0 + 0 + \frac{1}{6}\mathcal{F}'''(\mathcal{M}_{\rm min})(\delta\mathcal{M}^*)^3 \propto (\delta\mathcal{M}^*)^3 \\ &\propto\; (\delta b)^{3/2}, \end{aligned} \qquad (15)$$

making use of $\delta\mathcal{M}^* \,\propto\, \delta b^{\,1/2}$.

21) The scaling argument seen in class applies, allowing to write the fluctuation-induced correction $\mathcal{F}_{\text{fluct}}$ as kTV/ξ^d where V is the volume of the system, and plays no role here. Alternatively, one can proceed more technically, and compute explicitly the fluctuation correction to the saddle point. It takes the form

$$\frac{kT}{2} V \int \frac{d\mathbf{q}}{(2\pi)^d} \log\left(\xi^{-2} + \lambda q^2\right), \tag{16}$$

leading again to the ξ^{-d} dependence on δb.

22) Given that $\xi \propto (\delta b)^{-1/4}$, we can see when the fluctuation correction indeed is a correction :

$$\mathcal{F}_{\text{fluct}} \ll \delta\mathcal{F}_{\text{mf}} \iff \xi^{-d} \ll (\delta b)^{3/2} \iff (\delta b)^{d/4} \ll (\delta b)^{3/2} \iff \boxed{d > 6} \tag{17}$$

We recover $\boxed{d_u = 6}$. All this is compatible with Fig. 5 : mean-field is trustworthy for $d > 6$.

23) Done in class. Define the transfer matrix T

$$T = \begin{pmatrix} e^{K+\beta B} & e^{-K+\beta B} \\ e^{-K-\beta B} & e^{K-\beta B} \end{pmatrix} \quad \text{or} \quad T = \begin{pmatrix} e^{K+\beta B} & e^{-K} \\ e^{-K} & e^{K-\beta B} \end{pmatrix} \tag{18}$$

or yet another equivalent choice (there are infinitely many, all having the same trace and determinant, and thus the same eigenvalues in the present 2×2 case). The partition function follows

$$Z_N = \text{Tr}\left[T^N\right] = \lambda_+^N + \lambda_-^N. \tag{19}$$

24) When does Z_N vanish ?

$$Z_N = 0 \implies 1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N = 0 \implies \left|\frac{\lambda_-}{\lambda_+}\right| = 1 \tag{20}$$

Without finding explicitly the zeros, we can see that the latter relation forces B to be imaginary. Indeed,

$$\frac{\lambda_-}{\lambda_+} = \frac{e^K \,\text{ch}\,\beta B - \sqrt{e^{2K}\,\text{sh}^2(\beta B) + e^{-2K}}}{e^K \,\text{ch}\,\beta B + \sqrt{e^{2K}\,\text{sh}^2(\beta B)^2 + e^{-2K}}} \tag{21}$$

and we make use of the $|a+b| = |a-b| \implies a\overline{b} \in i\mathbb{R}$ property [1], to write that

$$\text{ch}^2(\beta\overline{B})\left[e^{4K}\,\text{sh}^2(\beta B) + 1\right] \leqslant 0. \tag{22}$$

Since $\text{ch}^2 = 1 + \text{sh}^2$, it follows that $\text{sh}^2(\beta\overline{B}) = \text{sh}^2(\beta B)$. The inequality (22) is polynomial in sh^2 ; the expression on the left hand side is negative when sh^2 lies between the two roots -1 and $-e^{-4K}$. From $\text{sh}(ib) = i\sin(b)$, it follows that B is purely imaginary. Thus, $z = e^{-2\beta B}$ lies on the unit circle. Next, having a LY zero requires $B = ib$ with $e^{-2K} < \sin(\beta b) < 1$. The smallest value of b admissible is b_{min} with

$$\boxed{\sin(\beta b_{\text{min}}) = e^{-2K}}. \tag{23}$$

It might be objected that we have proceeded through necessary conditions, so that we only get a lower bound for b_{min}. This is a fair point. The complete calculation of all zeros nevertheless corroborates our finding.

25) We expand λ_-/λ_+ in powers of $\delta b = b - b_{\text{min}}$ in the vicinity of b_{min}. For $b = b_{\text{min}}$, the square root term in $\lambda_\pm$ vanishes, meaning that $\sqrt{\ldots} = \mathcal{O}(\delta b)^{1/2}$. Thus, $\lambda_-/\lambda_+ - 1 = \mathcal{O}(\delta b)^{1/2}$ meaning that ξ^{-1} is of order $(\delta b)^{1/2}$, and finally that $\boxed{\nu' = 1/2}$.

26) At each temperature, a circle remains, but it is no longer of unit radius. Ising model thus appears as somewhat specific with respect to LY zeros. Pinching of the real axis at the critical temperature is also visible. This has to happen, but teaches us that phase transitions, again, are only possible at zero field for the Potts model under study.

1. in other words, a equals ib times a real number ; this simply means that going from complex numbers to vectors, $\vec{a}$ and $\vec{b}$ have to be perpendicular ; a and b define the hypotenuse of a right triangle having right angle at the origin.