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Condensed Matter, Quantum Physics and Soft Matter M2 programs

exam 2020-2021

$\boxed{\textbf{Finite-size scaling - correction}}$

A. Introduction

1) In a finite system, the partition function is an analytic function of its parameters (T, $B\dots$). Its log inherits from this property : the free energy does not exhibit any singularity.

2) The critical temperature is bounded by $2.25\,J/k < T_c < 2.3\,J/K$

3) The mean-field critical temperature is $4J/k$ on a square lattice with four nearest neighbors. It has to be larger than the exact result : mean-field is blind to some fluctuations, and thus overestimates the extent of the ordered phase.

4) Since $\nu = 1$ in two dimensions, we have $\alpha = 0$, which hides a log divergence at T_c. This is special in the sense that other quantities like χ or ξ will diverge as a power law of t, and thus more "violently".

5) We generalize the vanishing field ansatz and write

$$\chi_{_L}(T,B) \;=\; |t|^{-\gamma} f\left(\frac{L}{\xi_\infty(t)}, \frac{B}{|t|^{\beta\delta}}\right) \tag{1}$$

where the field is "measured" in units of $M_{\text{sp}}^\delta \propto |t|^{\beta\delta}$, M_{sp} being the spontaneous magnetization. Strictly speaking, $M_{\text{sp}} \neq 0$ below T_c only ; yet, take take $|t|^{\beta\delta}$ as the relevant scaling variable also above T_c. Using that $\xi_\infty \propto |t|^{-\nu}$ and changing scaling function, we trade $|t|$ for $L^{-1/\nu}$ and arrive

$$\boxed{\chi_{_L}(T,B) \;=\; L^{\gamma/\nu} g\left(tL^{1/\nu}, BL^{\beta\delta/\nu}\right)}. \tag{2}$$

While f only depends on $|t|$, we chose for convenience to have g depend on t : we "glue" together the branches above and below T_c.

6) Then $\chi_{_L}(T_c,B) \;=\; L^{\gamma/\nu} g\left(0, BL^{\beta\delta/\nu}\right)$. This scaling behaviour explains the quantity plotted in the figure : $\gamma/\nu = 1.75$. This also tells us that the quantity shown on the x-axis is $\boxed{BL^{\beta\delta/\nu} = BL^{1.875}}$, or, more probably, $BL^{1.875}/J$ to have it dimensionless.

7) It is not possible to have a second order phase transition for $B \neq 0$: the susceptibility then does not diverge. Besides, one can observe a first order transition for $T < T_c$, when B changes, but this is again at $B = 0$.

8) In the language of the renormalization group, there are therefore two relevant scaling fields, associated to T and B, that need to be fine tuned to locate the critical point.

B. Finite-size scaling for the correlation length with $B = 0$

9) The spin-spin correlation length ξ is traditionally defined from the large distance asymptotics of the spin-spin correlation function. In a finite system, this may be a difficulty (large distance regime masked).

10) A very similar scaling argument as above leads to

$$\xi_{_L}(t) \;=\; |t|^{-\nu}\, \varphi(t\, L^{1/\nu}) \tag{3}$$

Thus $a = -\nu$ and $b = 1/\nu$.

11) Introducing $\phi(x) = x^{-\nu}\varphi(x)$, we get

$$\xi_L(t) \;=\; L\,\phi(t\,L^{1/\nu}). \tag{4}$$

12) In a very large system outside the critical point, ξ_L does not depend on L. Therefore, $\phi(x) \propto |x|^{-\nu}$ for large $|x|$. This is compatible with the expected behaviour for the correlation length at a given t for $L \to \infty$: it should behave like $|t|^{-\nu}$. In other words, $\varphi(x)$ goes to a constant for large x. We recover here $a = -\nu$.

13) At a given L when $t \to 0$, the correlation length cannot grow without bounds. When it "hits" the system size, L limits ξ, so that we expect in this regime $\xi_L \propto L$. As a consequence, we expect that for small x, $\phi(x)$ goes to a constant.

14) We expect the function ϕ to have a unique maximum since it is this maximum that will lead to the divergence of the corelation length when increasing L. We expect a unique critical point.

15) The idea is to plot ξ_L/L as a function of T. Remarkably, the curves at different sizes will cross exactly at T_c, if the scaling assumption is correct (and it is, provided T is not too far from T_c, and that the sizes are not too small). Fig. 1 provides a sketch of the expected behaviour for 3 system sizes. All curves cross at T_c, which offers a simple criterion for locating the critical temperature.

16) The localization of the maximum of ξ_L/L as a function of T will define a temperature

$$T_L^* = T_c + T_c x^* L^{-1/\nu}. \tag{5}$$

What matters here is $T_L^* - T_c \propto L^{-1/\nu}$. Thus, once T_c has been located by the crossing of curves, the behaviour of T_L^* as a function of L provides us with a measure of ν.

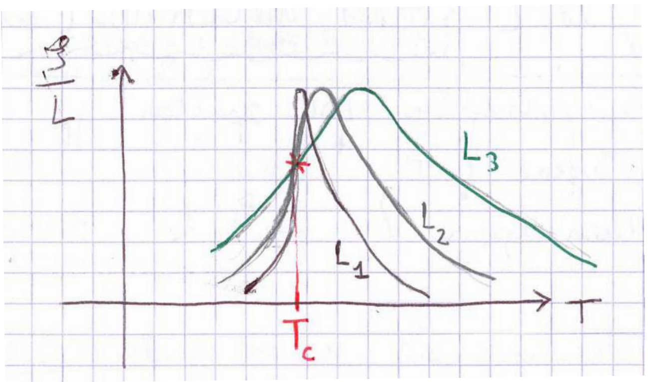

FIGURE 1 – Cartoon of rescaled correlation length ξ_L as a function of temperature, for three system sizes $L_1 > L_2 > L_3$. The maxima of ξ/L, reached at $T_c + T_c\, x^*\, L^{-1/\nu}$ where x^* is some constant, all coincide.

C. Finite-size scaling and transfer matrix calculations on strips : applications to two-dimensional Ising model

17) For a fixed M, the system is essentially one dimensional, especially seen from large distances. Hence, no phase transition.

18) The key is in the periodicity along the short dimension. The Hamiltonian reads

$$\beta H \;=\; -\beta J\left(s_1 s_2 + s_1^2 + s_2 s_3 + s_2^2 + s_3 s_4 + s_4^2 + \ldots\right) \tag{6}$$

A possible transfer matrix is $\mathbb{T}$ with elements $T(s_1, s_2) = \exp[\beta J(s_1 s_2 + 1)]$:

$$\mathbb{T} \;=\; \begin{pmatrix} e^{2\beta J} & 1 \\ 1 & e^{2\beta J}. \end{pmatrix} \tag{7}$$

19) The eigenvalues are $t_1 = 1 + x^2$ and $t_2 = x^2 - 1$ with $x = e^{\beta J}$.

20) No divergence at finite T, no critical point.

21) The size of the transfer matrix for $M = 2$ is 4×4.

22) For $M = 2$, we have two rows of interacting spins, as in Fig. 2. It is convenient to define a spin vector $\vec{s}_i$ for each column $i = 1, 2, \ldots$, with the two spin values associated to the two rows $j = 1$ and $j = 2$ $(s_i^{(1)}, s_i^{(2)})$, see the figure. It is because the $\vec{s}_i$ can take four different values,

$$\begin{pmatrix} s_i^{(1)} \\ s_i^{(2)} \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \begin{pmatrix} -1 \\ -1 \end{pmatrix} \tag{8}$$

that the transfer matrix is 4×4. For arbitrary M, the transfer matrix would be $2^M \times 2^M$. The Hamiltonian reads, remembering the boundary condition along the vertical direction

$$\beta H = -\beta J \sum_i \left(s_i^{(1)} s_{i+1}^{(1)} + 2\, s_i^{(1)} s_i^{(2)} + s_i^{(2)} s_{i+1}^{(2)} \right). \tag{9}$$

Therefore, the elements of the transfer matrix are

$$\mathbb{T}(\vec{s}_i, \vec{s}_{i+1}) \;=\; e^{\beta J \left[s_i^{(1)} s_{i+1}^{(1)} + 2\, s_i^{(1)} s_i^{(2)} + s_i^{(2)} s_{i+1}^{(2)} \right]}. \tag{10}$$

With the ordering convention as in Eq. (8) and with , we obtain

$$\mathbb{T} \;=\; \begin{pmatrix} x^4 & x^{-2} & x^{-2} & 1 \\ x^2 & 1 & x^{-4} & x^2 \\ x^2 & x^{-4} & 1 & x^{-2} \\ 1 & x^{-2} & x^{-2} & x^4 \end{pmatrix} \tag{11}$$

where $x = e^{\beta J}$. The two largest eigenvalues are

$$\left(x^4 + 2 + x^{-4} + \sqrt{x^8 + x^{-8} + 14} \right) /2 \;, \qquad x^4 - 1 \tag{12}$$

which is compatible with the result given for the correlation length in the main text.

23) We have $kT_c \simeq J/0.435 \simeq 2.3\, J$. This compares well to the exact value in the figure.

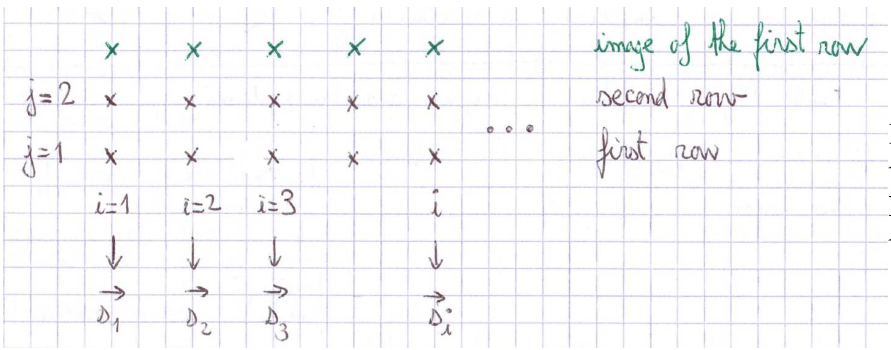

FIGURE 2 – Situation with $M = 2$ interacting spin chains. The two spin values for a given column i are lumped together to define the spin vector $\vec{s}_i$.

D. On the usefulness of Binder cumulants

24) For a Gaussian random variable X with mean 0, $\langle X^4 \rangle / \langle X^2 \rangle^2 = 3$.

25) Because σ is small compared to X^*, $\langle X^2 \rangle \simeq X^{*2}$, $\langle X^4 \rangle \simeq X^{*4}$. Thus, $\langle X^4 \rangle / \langle X^2 \rangle^2 \simeq 1$.

26) At large T, the system is not magnetized globally and the correlation length can be assumed significantly smaller than L. Thus, the global magnetization, which fluctuates around 0, results from the contribution of a large number of domains with size ξ^d. From the central limit theorem, the distribution is Gaussian, hence the vanishing of U_L. With $N = L^d$, we can compute the standard deviation from the fluctuation-response connection :

$$N\chi kT \;=\; \langle N^2 s_L^2\rangle \quad \Longrightarrow \langle s^2\rangle_L \;=\; \frac{\chi\, kT}{L^d}, \tag{13}$$

involving the susceptibility per spin, that is arguably quite close to its large size limit. Below the critical temperature, the right hand side of this relation still yields the standard deviation of magnetization fluctuations. This standard deviation becomes smaller and smaller as L grows, while the spontaneous magnetization will converge to a finite non-vanishing value. Hence, at small T, $U_L \to 1 - 1/3 = 2/3$.

27) The curves cross at the critical temperature (compatible with earlier estimates, more precise here). The reason is that at T_c precisely, the correlation length $\xi_\infty(t)$ diverges and no decomposition of the system in boxes of volume ξ^d is possible. On general grounds, we expect the distribution of magnetization $P_L(s)$ to exhibit a scaling form

$$P_L(s) \;=\; L^a \widetilde{P}(sL^b, L/\xi_\infty). \tag{14}$$

Normalization to unity imposes that $a = b$, but this is a detail. What matters is that at T_c, the dependence on L is lost : what is measured by U_L is the cumulant of a non-trivial function with zero mean. To summarize

$$\boxed{U_L \simeq 2/3 \text{ at small } T, \qquad U_L \text{ universal at } T_c, \qquad U_L \simeq 0 \quad \text{at large } T}. \tag{15}$$

The curves-crossing feature of the Binder cumulant, illustrated in the figure, is a widely used means to locate the critical point.

28) (bonus) Another central limit argument points to the Gaussianity of s fluctuations below T_c. Attention should be paid to the fact that the definition of U_L involves $\langle s^4\rangle_L$ which is not the cumulant. Denoting by M_{sp} the spontaneous magnetization, we have

$$\langle (s - M_{\text{sp}})^4\rangle \;=\; 3\,\sigma^4 \qquad \text{with} \qquad \sigma^2 = \frac{\chi\, kT}{L^d}. \tag{16}$$

After a bit of algebra, one finds that at small T,

$$U_L \;\simeq\; \frac{2}{3} - \frac{4\,\chi\, kT}{3\,L^d\,M_{\text{sp}}^2}. \tag{17}$$

The deviation from 2/3 is negative, as expected from the figure, and provides us with a measure of χ.

E. Finite-size scaling for the order parameter

29) We start with the scaling assumption

$$\langle |s|\rangle_L \;=\; |t|^\beta\, h_1\left(\frac{L}{\xi_\infty}\right) \;=\; |t|^\beta\, h_2\left(L|t|^{1/\nu}\right) \;=\; L^{-\beta/\nu}\, \widetilde{h}\left(L|t|^{1/\nu}\right) \tag{18}$$

where c is some coefficient while h_1, h_2, $\widetilde{h}$ are scaling functions.

30) In light of our scaling ansatz, the "rescaled magnetization" defined, as plotted in the figure, should be

$$\boxed{|t|^{\beta/\nu}\,\langle |s|\rangle_L, \quad \text{plotted as a function of} \quad L\,|t|^{1/\nu}}. \tag{19}$$

The two branches in the figure correspond to $T < T_c$ and $T > T_c$. The behaviours for large $x = L\,|t|^{1/\nu}$ appear power-law.

— Take $T < T_c$ fixed, and L increases ; we expect $\langle |s| \rangle_L \propto |t|^\beta$, meaning $\widetilde{h}(x) \propto x^\beta$ for large x.

— Take $T > T_c$, T fixed, and L again increases : $\langle |s| \rangle_L$ is the sum of uncorrelated random variables with 0 mean and variance in $1/N$ (always the same argument of partitioning space in cells of volume $\xi_\infty^d \ll L^d$), hence $\langle |s| \rangle_L \propto 1/\sqrt{N} = 1/L$. Thus, $\widetilde{h}(x) \propto x^c$ for large x with exponent c determined from the condition

$$\frac{1}{L} = L^{-\beta/\nu} L^{c/\nu} \quad \Longrightarrow \quad c = \beta - \nu. \tag{20}$$

We conclude that the two slopes in Figure 3 are

$$\boxed{\beta = \frac{1}{8} \text{ for the upper branch } (T < T_c) \qquad \text{and} \qquad \beta - \nu = -\frac{7}{8} \text{ for the lower branch } (T > T_c).} \tag{21}$$

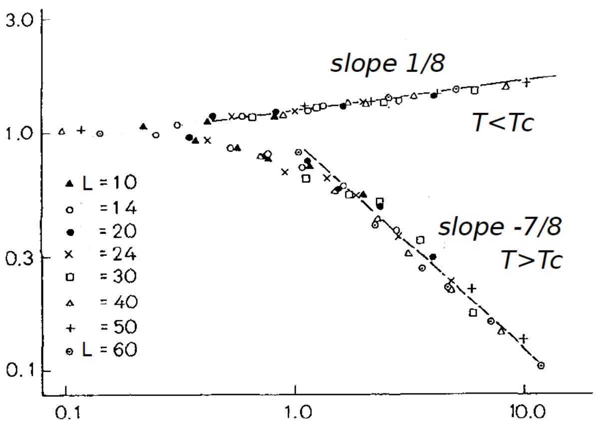

FIGURE 3 – Slopes of the two branches of the order parameter plot, that correspond to $T > T_c$ and $T < T_c$ as indicated

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F. How to distinguish first-order from second-order phase transitions ?

31) Weakly first-order means that the discininuity of the order parameter at T_c is small, which may confuse and lead to believe that the transition is continuous.

32) We have

$$p_\pm = \frac{e^{\pm\beta B L^d M_{\rm sp}}}{e^{\beta B L^d M_{\rm sp}} + e^{-\beta B L^d M_{\rm sp}}} \tag{22}$$

33) The corresponding mean value reads

$$\langle s \rangle_L = p_+ \left[M_{\rm sp} + \chi B\right] + p_- \left[-M_{\rm sp} + \chi B\right] = \boxed{M_{\rm sp} \tanh\left(\beta L^d M_{\rm sp} B\right) + \chi B}. \tag{23}$$

34) It then follows that that

$$\boxed{\chi_L = \chi + M_{\rm sp}^2 \frac{L^d}{kT}\left[1 - \tanh^2\left(\frac{L^d M_{\rm sp} B}{kT}\right)\right]}. \tag{24}$$

35) From expression (24), the width ΔB is

$$\boxed{\Delta B = \frac{kT}{M_{\rm sp} L^d}}. \tag{25}$$

The resulting slope at the origin is $M_{\rm sp}^2 L^d/(kT)$, and diverges with system size. The key feature is that this divergence is not of the same type as that which holds at the critical point.

36) Relation (24) fully explains the two figures... The limiting value shown by the arrows in both Figures is χ.

37) The divergence of the susceptibility is not the same : simply L^2 at a first order transition, for a more subtle $L^{\gamma/\nu}$ at the critical point. Besides, the scaling variable for B is not the same in the two situations : BL^2 in the first case, $BL^{\beta\delta/\nu}$ in the second.

G. Slab geometry

38) Getting closer to the critical point, the correlation length will grow, and the system will behave as fully 3D, with thus $\chi \propto |t|^{-1.25}$. Then, close enough to T_c, the correlation length will hit $L_\perp$, and decreasing further $|t|$, the system will more and more behave like a two-dimensional one, with $\chi \propto |t|^{-1.75}$. In this sense, the susceptibility features a crossover behaviour.

39) For the two-dimensional system in a strip $L_\parallel \times L_\perp$, we may observe first $\chi \propto |t|^{-1.75}$ until the correlation length reaches $L_\perp$. Closer to T_c, χ will saturate and stop to grow (one-dimensional behaviour).

40) (bonus) We use the fluctuation-response connection and the fact that $G(r) \propto r^{-\eta}$ at T_c with $d = 2$:

$$NkT\chi \;=\; \sum_{i,j} G_{i,j} \simeq \int d\mathbf{r}d\mathbf{r}'\, G(\mathbf{r}-\mathbf{r}') \tag{26}$$

and since $N = L_\parallel L_\perp$:

$$\chi kT \;=\; \frac{1}{L_\parallel L_\perp} \int_O^{L_\parallel} dx_1 \int_O^{L_\perp} dy_1 \int_O^{L_\parallel} dx_2 \int_O^{L_\perp} dy_2 \; \frac{1}{[(x_1-x_2)^2+(y_1-y_2)^2]^{\eta/2}}. \tag{27}$$

It is safe to make use of the large r behaviour of G only, since we are interested in how χ diverges at T_c. The above means that

$$\boxed{\chi \;=\; L_\parallel^{1-\eta}\, L_\perp\, \widetilde{\psi}\left(\frac{L_\parallel}{L_\perp}\right)} \tag{28}$$

where $\widetilde{\psi}$ is a scaling function. If we take $L_\parallel L_\perp = L$, we get $\chi \propto L^{2-\eta}$, to be compared with the law $L^{\gamma/\nu}$ obtained earlier. This shows that $\boxed{2-\eta = \gamma/\nu}$.

41) The situation is different if the system is not some subpart of an otherwise infinite system, but finite with some boundary conditions (periodic or free do not make a real difference). The correlation function takes then a one dimensional form, exponential, in the regime $L_\perp \ll x \ll L_\parallel$. We next go back to the fluctuation -response connection :

$$\chi kT \;=\; \frac{1}{L_\parallel L_\perp} \int_O^{L_\parallel} dx_1 \int_O^{L_\perp} dy_1 \int_O^{L_\parallel} dx_2 \int_O^{L_\perp} dy_2 \; L_\perp^{-\eta} e^{-a|x_1-x_2|/L_\perp}. \tag{29}$$

This results in

$$\boxed{\chi kT \;\propto\; L_\perp^{2-\eta}}, \tag{30}$$

which does not depend on $L_\parallel$. There is a transition only for $L_\perp \to \infty$ (keep in mind that $L_\perp$ is the smallest dimension of the slab).