Sorbonne Université, Université de Paris, Université Paris-Saclay, École normale supérieure, École Polytechnique

Condensed Matter, Quantum Physics and Soft Matter M2 programs

exam 2020-2021

Finite-size scaling

Pocket calculators and cell phones not allowed.
This part should be written on a separate paper. The different sections are mostly independent.
La rédaction pourra se faire en français pour ceux qui le souhaitent.

A number of relevant information is reminded in the annex, at the end of this text. The general arguments below are all illustrated on the example of Ising spin 1/2 model, on regular square or rectangle lattices in dimension d (therefore cubic for $d = 3$ etc.). Couplings are restricted to nearest neighbors. The ferromagnetic coupling constant is denoted J and T is the temperature. The "distance" to the critical temperature T_c will be $t = (T - T_c)/T_c$. The number of spins in the system is N and k is for the Boltzmann constant.

A. Introduction

The free energy of a finite system cannot be singular : a phase transition can only be observed in the thermodynamic limit.

1) Why is that so (brief answer expected) ?

While this limitation is of little practical relevance for experimental systems (finite but in general large enough to exhibit the hallmarks of phase transitions), it has important conceptual and practical consequences for computer simulations. It is our goal to tame finite-size effects and turn their treatment into a powerful tool for the study of phase transitions, at a continuous but also a first order transition. These two situations, that may have similar fingerprints in practice, can be discriminated by finite-size analysis. We will also see that finite-size effects are not only informative when coupled to numerical simulations, but also in conjunction with transfer matrix calculations. Figure 1 illustrates finite-size effects on the specific heat, with periodic boundary conditions.

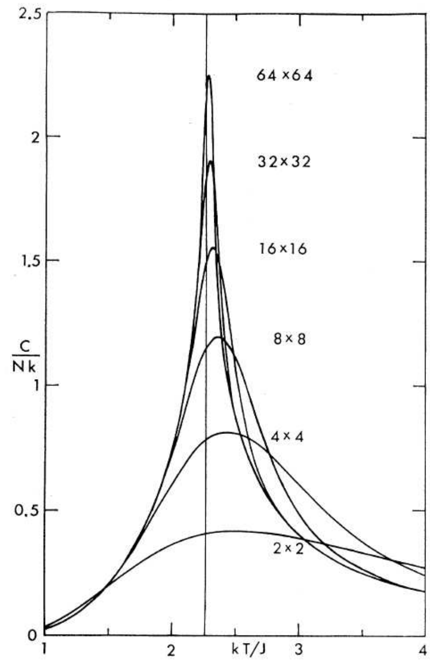

FIGURE 1 – Specific heat for $B = 0$ as a function of kT/J on various small square lattices, of size $L \times L$ in two dimensions (thus here, $N = L^2$). The vertical line indicates the location of the peak for $L \to \infty$. From Ferdinand and Fisher (1969).

2) What is the approximate critical temperature T_c revealed by Figure 1 ?

3) Is this critical temperature larger or smaller than its mean-field counterpart ? Why ? Give the value of the mean-field critical temperature.

4) What is the expected behavior here for the specific heat close to the critical point (use the annex) ? In which sense is this situation special ?

5) A classic finite-size scaling argument shows that with $\chi_L(T, B)$ the susceptibility of a finite system of $N = L^d$ spins at temperature T in an external magnetic field B, we have $\chi_L(T_c, 0) \propto L^{\gamma/\nu}$. How does this generalize to $\chi_L(T, B)$? Use here the reduced temperature $t = (T - T_c)/T_c$.

6) What is then $\chi_L(T_c, B)$? What should the quantity shown on the x-axis of Fig. 2 be ?

7) Is it possible to have a phase transition for $B \neq 0$?

8) In the language of the renormalization group, how many *relevant* scaling fields does our model exhibit ?

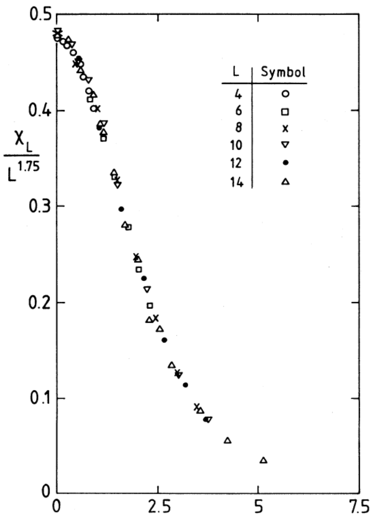

FIGURE 2 – Scaled susceptibility $\chi_L/L^{1.75}$ for $d = 2$ on square systems of sizes $L \times L$, at the critical temperature T_c, as a function of an unspecified variable involving the external field B and L. What is this variable ? From Binder and Landau (1984).

B. Finite-size scaling for the correlation length

It is assumed in this section that $B = 0$.

9) How is the spin-spin correlation length ξ traditionally defined ? What is the problem raised by this definition in a finite system ?

There are actually several ways to circumvent this difficulty (bonus question : propose one such solution), and we take for granted that we can define ξ here. It is a function of temperature through t and L, that we denote $\xi_L(t)$.

10) Propose a scaling ansatz for $\xi_L(t)$ in the form $\xi_L(t) = |t|^a \varphi(|t|L^b)$. What are the exponents a and b ? Allowing φ to have also negative arguments, this can be rewritten $\xi_L(t) = |t|^a \varphi(tL^b)$. Such a form makes sense close to T_c only, i.e. for $|t|$ small enough.

11) Rewrite this relation in the form

$$\xi_L(t) = L\,\phi(tL^b). \tag{1}$$

How are the two scaling functions φ and ϕ related ?

12) In a very large system outside the critical point, does ξ_L depend on L ? Therefore, how do you expect $\phi(x)$ to behave for large $|x|$? Do you recover the expected behaviour for the correlation length as a function of t ? Note that if you have not found a in previous questions, this is an occasion to fill the gap and relate this quantity to a critical exponent.

13) How do you expect $\phi(x)$ to behave for small x ?

14) Why do we expect the function ϕ to have a unique maximum ?

15) It turns out that the maximum of $\phi(x)$ is at $x^* \neq 0$. Sketch a graph of ξ_L/L as a function of T for three sizes $L_1 > L_2 > L_3$. In practice of course, T_c is not *a priori* known. Propose a simple procedure for locating T_c by comparing the graphs of $\xi_L(T)$ at different sizes.

16) We define T_L^* as the temperature for which ξ_L/L versus T is maximal. Explain how the measure of T_L^* allows to complete our previous graphical localization of the critical temperature, since it gives access to a critical exponent.

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

We consider next the model in a rectangular domain of size $M \times N$, where M is small, and $N \to \infty$. We will see that comparing the cases $M = 1$ to $M = 2$, as small as these values may seem, yields an original estimation of the critical temperature for the bulk $d = 2$ system. We enforce periodic boundary conditions in both directions. We need here the explicit expression of the Hamiltonian :

$$H = -J \sum_{\langle i,j \rangle} s_i \, s_j \tag{2}$$

where the summation runs over pairs of nearest neighbors, and the spins take values $s_i = \pm 1$.

17) Do you expect that for a fixed M, a phase transition may arise. Why ?

18) We start with the case $M = 1$. The spins can be numbered s_1, $s_2 \ldots s_N$. Yet, the resulting one dimensional chain slightly differs from the traditional situation, since every spin s_i is not only coupled to its neighbors s_{i-1} and s_{1+1}, but also to itself due to the periodicity along the short edge of the rectangle. Write explicitly the corresponding transfer matrix.

19) What are the eigenvalues ? t_1 will denote the largest, t_2 the second largest.

20) It is a general result that the inverse log of the ratio of eigenvalues t_1/t_2 yields the correlation length. Here, we get

$$\xi_{M=1} = \left(-\log \tanh \frac{J}{kT} \right)^{-1} \tag{3}$$

Is there a critical point ?

21) What is the size of the transfer matrix for $M = 2$?

22) (bonus question) Write the transfer matrix for $M = 2$.

23) From the transfer matrix with $M = 2$ and its two largest eigenvalues, we obtain the correlation length

$$\xi_{M=2} = \left[\log \left(\frac{x^4 + 2 + x^{-4} + \sqrt{x^8 + x^{-8} + 14}}{2(x^4 - 1)} \right) \right]^{-1}, \tag{4}$$

where $x = \exp[J/(kT)]$. We then adapt the conclusion of section B. It leads to a simple criterion for the critical coupling constant J_c : it should be that for which

$$\frac{1}{2} \xi_{M=2} = \xi_{M=1}, \tag{5}$$

which gives $x_c \simeq 1.546$ and so $J \simeq 0.435 \, kT_c$. How does this compare to the exact value appearing in Fig. 1 ?

D. On the usefulness of Binder cumulants

We present here a classical method for locating a critical point at a continuous phase transition.

24) For a Gaussian random variable X with mean 0 and standard deviation $\sqrt{\langle X^2 \rangle} = \sigma$, what is the value of $\langle X^4 \rangle / \langle X^2 \rangle^2$?.

25) For a random variable X that would be sharply peaked around $X^* \neq 0$ (meaning that X^* is much larger than the standard deviation), what is the approximate value of $\langle X^2 \rangle$? Same question for $\langle X^4 \rangle$ (or actually for the mean of any power of X). What is then (approximately) $\langle X^4 \rangle / \langle X^2 \rangle^2$.

We define the instantaneous magnetization in the system from the spin configuration $\{s_i\}_{i=1 \ldots N}$ by

$$s = \frac{1}{N} \sum_i s_i. \tag{6}$$

It is reminded that every spin takes value ± 1. By averaging over a number of equilibrium configurations in a finite-size $L \times L$ system, we thereby define the moments $\langle s^2 \rangle_L$, $\langle s^4 \rangle_L$ etc.

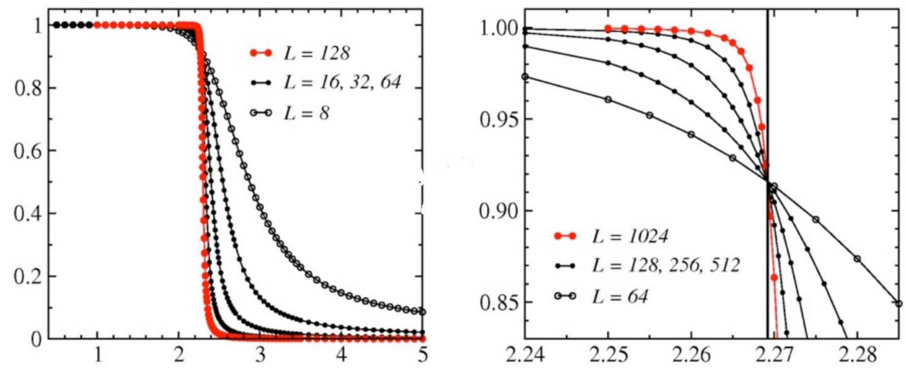

FIGURE 3 – Binder cumulants. Plot of $3\,U_L/\,2$ as a function of kT/J for square lattices of growing sizes. The right panel is a zoom into the sector where the curves cross. From A. Sandvik (2015).

26) Figure 3 displays the behaviour of the so-called Binder cumulant

$$U_L \;=\; 1 - \frac{1}{3}\,\frac{\langle s^4\rangle_L}{\langle s^2\rangle_L^2}\,. \tag{7}$$

Explain the small T and the large T behaviour displayed by U_L, for the left panel. It is possible to answer at various levels of depth. A thorough explanation goes through estimating the fluctuations of s, which can be done invoking the fluctuation-response connection.

27) It is observed on the right panel in Fig. 3 that the curves at different sizes do cross at a special point. What is this point, and why is there crossing ? How can this feature be used to study the phase transition ?

28) (bonus) It is seen in Fig. 3 that at small T, U_L departs from a constant by a small negative value. Compute this contribution. What thermodynamic quantity does this give access to ?

E. Finite-size scaling for the order parameter

29) Propose a concise finite-size scaling analysis of the order parameter (mean magnetization taken here as $\langle |s|\rangle_L$) as a function of T and L at $B = 0$, assuming that T_c is known.

30) How is the “rescaled magnetization” defined, as plotted in Fig. 4 ? Why are there two branches in the figure ? What are the two slopes displayed by the straight lines (the graph is log-log) ? Note that for $T > T_c$, a central-limit-theorem argument is useful to find the dependence of the order parameter on the number of spins $N = L^2$.

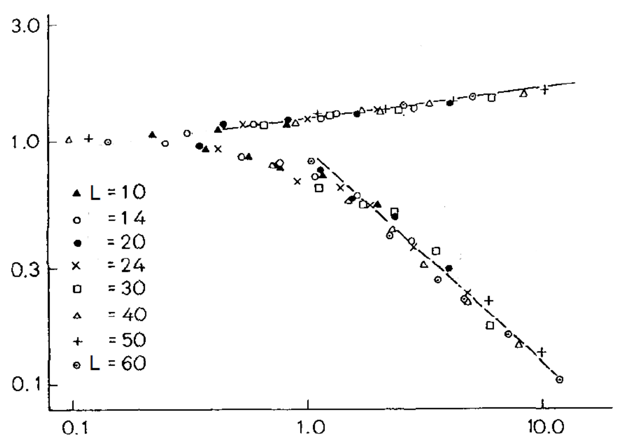

FIGURE 4 – Ising models on square lattices of various sizes $L \times L$. Plot of the rescaled order parameter as a function of $|t|L^{1/\nu}$. The scales are logarithmic on both axis. From Binder (1986).

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

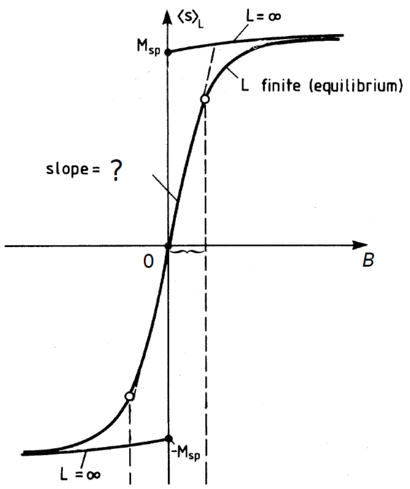

FIGURE 5 – Variation of the mean magnetization in a finite-size Ising cubic ferromagnet of linear size L, as a function of the magnetic field B. As expected, the curves are odd with respect to B. Here, we have $T < T_c$ so that in an infinite system, the magnetization $\langle s \rangle$ would jump from $-M_{\rm sp}$ to $+M_{\rm sp}$ when B goes from 0^- to 0^+. The smallness of L washes out this discontinuity. The two vertical dashed lines indicate the region where finite size effects are most pronounced, i.e. where the finite-L and thermodynamic limit curves largely differ. The extension of this region along the B-axis is denoted ΔB. A goal here is to compute ΔB and to infer the resulting slope at the origin, defined in Eq. (8). From Binder and Landau (1984).

31) It is in practice not always a simple task to discriminate a second order from a weakly first-order phase transition. Can you guess what “weakly first-order” means ?

Figure 5 illustrates the problem with a B-field scan. When $T < T_c$ and if the system is small enough (or left enough time) so that thermal fluctuations ensure an ergodic behaviour, a continuous magnetization will be measured as a function of B, while the thermodynamic limit would yield a discontinuous order parameter. Besides, the susceptibility defined as

$$\chi_L \; = \; \frac{\partial \langle s \rangle_L}{\partial B} \; , \tag{8}$$

as would be measured in a computer simulation for instance, is not immediately related to the thermodynamic susceptibility χ. The slope χ_L near the origin in Fig. 5 becomes system-size dependent, which may mimick a second-order phase transition, lead to $\chi_L \gg \chi$, and mislead us. It can be kept in mind that χ_∞ (defined from χ_L for $L \to \infty$) and χ are distinct quantities, since the first one is infinite while the second is not. It therefore seems that finite-size effects are detrimental here. We shall see though that they offer a way out, and bear a distinct first-order signature. The idea is to construct a phenomenological probability distribution $P_L(s, B)$ for the magnetization defined in Eq. (6). Although s takes discrete values in a finite system, we will treat this variable as continuous, which allows to write normalization and the various moments as

$$\int_{-1}^{1} P_L(s,B)\, ds = 1 \quad , \qquad \langle s^2 \rangle_L \; = \; \int_{-1}^{1} s^2\, P_L(s,B)\, ds \quad \ldots \tag{9}$$

It is a fair approximation here (except in very small systems) that $P_L(s, B)$ vs. s is double-peaked at $s = \pm M_{\rm sp} + \chi B$, that each peak is Gaussian with standard deviation σ (unspecified for the moment, but rather small), and that the weights $p_\pm$ of each peak are B-dependent, with $p_+ + p_- = 1$.

32) To find $p_\pm$, we can consider that we have a simpler two-states problem, with all L^d spins either taking value $+M_{\rm sp}$, or $-M_{\rm sp}$. This system is in an external field B. What are then the weights $p_\pm$? When $B = 0$, check that $p_+ = p_- = 1/2$.

33) Compute the corresponding mean value $\langle s \rangle_L$. When $B = 0$, check that $\langle s \rangle_L = 0$ (see Fig. 5).

34) Assuming χ to be independent from B, show then that

$$\chi_L \; = \; \chi \; + \; M_{\rm sp}^2 \, \frac{L^d}{kT} \left[1 - \tanh^2 \left(\frac{L^d M_{\rm sp} B}{kT} \right) \right] . \tag{10}$$

35) From expression (10), what is the width ΔB of the transition region, as defined in Fig. 5 ? What is the resulting slope at the origin ?

36) Use relation (10) to make sense of Fig. 6 ; explain. One notices a small lack of scaling (data collapse) in Fig. 6 in the vicinity of the origin. Why is that so ? Why is Fig. 7 more useful in this respect ? What is the limiting value shown by the arrows in both Figs. 6 and 7 ?

37) We compare these results to those obtained in section A. How can finite size effects discriminate between first and second order transitions ? Hint : compare Fig. 2 and Figs. 6/7.

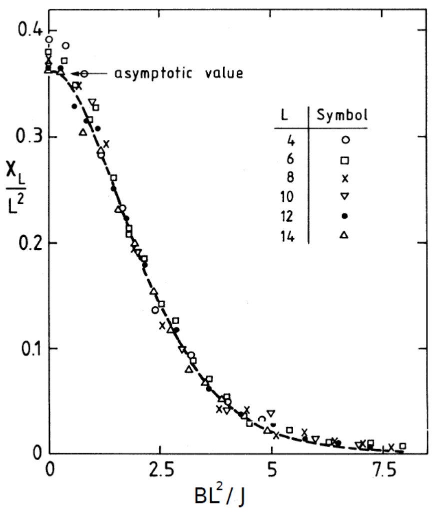

FIGURE 6 – Scaled susceptibility χ_L/L^2 for $d = 2$ on square lattices of sizes $L \times L$, at temperature $kT = 2.1\,J$, as a function of BL^2/J. From Binder and Landau (1984).

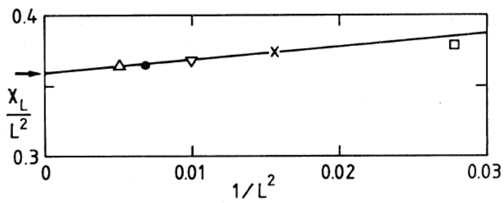

FIGURE 7 – Scaled susceptibility χ_L/L^2 for $d = 2$ on square lattices of sizes $L \times L$, at temperature $kT = 2.1\,J$ and $B = 0$, plotted versus $1/L^2$. The horizontal arrow indicates the same limiting value as that in Fig. 6. From Binder and Landau (1984).

G. Slab geometry

38) In an infinite three-dimensional Ising ferromagnet, we consider a finite slab of size $L_\parallel \times L_\parallel \times L_\perp$. We assume that $L_\parallel \to \infty$. We fix $L_\perp$ large enough, but finite. We take for granted that this finite system features a critical point. Sketch the expected behavior of the susceptibility per spin χ vs $|t| = |T - T_c|/T_c$ in a log-log graph. In which sense does this quantity exhibit a *cross-over* phenomenon ?

39) Same question for the two-dimensional version, in a strip $L_\parallel \times L_\perp$.

40) (bonus) Remembering that the spin-spin correlation function asymptotically obeys $G(r) \propto r^{-d+2-\eta}$ at T_c, write a scaling form for χ for the $d = 2$ system. Show then the scaling relation $2 - \eta = \gamma/\nu$.

41) (harder) The situation is different in a fully finite system, meaning, not some subpart of an otherwise infinite system. Then, at T_c and $d = 2$, the correlation function takes a different form : $G(r) \propto L_\perp^{-\eta} \exp(-a|x|/L_\perp)$ in the regime $L_\perp \ll x \ll L_\parallel$, where a is some constant and x is the coordinate along $L_\parallel$. Why is this plausible ? The precise choice of boundary conditions is not essential. Show next that the susceptibility per spin becomes independent of $L_\parallel$. How does it depend on $L_\perp$?

Annex. We denote critical exponents by a subscript referring to space dimension
• In two dimensions, we have $\nu_2 = 1$, $\beta_2 = 1/8$ and $\gamma_2 = 7/4$, $\delta_2 = 15$, associated to the correlation length, the order parameter, the susceptibility and the equation of state respectively
• In three dimensions : $\nu_3 \simeq 1.25$.
• For $d \leq 4$, we have $\nu d = 2 - \alpha$ where α is the critical exponent associated to the specific heat.

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