Binder cumulants and phase transitions

The free energy of a finite system cannot be singular: a phase transition can only be observed in the thermodynamic limit, *i.e.* with infinitely large systems. 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. More often than naught, the computed observables are strongly system-size dependent, and thus quite different from their thermodynamic limit value. Interestingly, the proper treatment of finite-size effects turns this apparent drawback into a powerful and useful tool for the study of phase transitions, at a continuous but also a first order transition.

Here, we will focus on continuous phase transition. The rather general arguments below are illustrated on the example of Ising spin 1/2 model, on regular square lattices in dimension d (therefore cubic for $d = 3$ etc.). Couplings are restricted to nearest neighbors and there is no external field applied. The ferromagnetic coupling constant is denoted J and T is the temperature. The number of spins in the system is N. We define the instantaneous magnetization in the system from the spin configuration $\{s_i\}_{i=1\ldots N}$ by

$$s = \frac{1}{N}\sum_{i=1}^{N} s_i, \tag{1}$$

where 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.

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

2) 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) $\langle X^4 \rangle / \langle X^2 \rangle^2$.

3) Figure 1 displays the behaviour of the so-called Binder cumulant

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

Invoking the central limit theorem, explain the dominant small T and large T behaviours displayed by U_L. A thorough explanation goes through estimating the fluctuations of s, that obey the fluctuation-response connection

$$\langle s^2 \rangle_L - m_{\text{sp}}^2 = \frac{\chi\, kT}{N}, \tag{3}$$

where χ is the susceptibility per spin and m_{sp} is the spontaneous magnetization. Below the critical temperature, $m_{\text{sp}} > 0$.

4) It is observed on the right panel in Fig. 1 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?

5) It is seen in Fig. 1 that at small T, U_L departs from a constant by a small negative value. Using a combination of the central limit theorem and the fluctuation-response connection, show indeed that

$$U_L \simeq \frac{2}{3} - \frac{4\,\chi\, kT}{3\, N\, m_{\text{sp}}^2}. \tag{4}$$

References:

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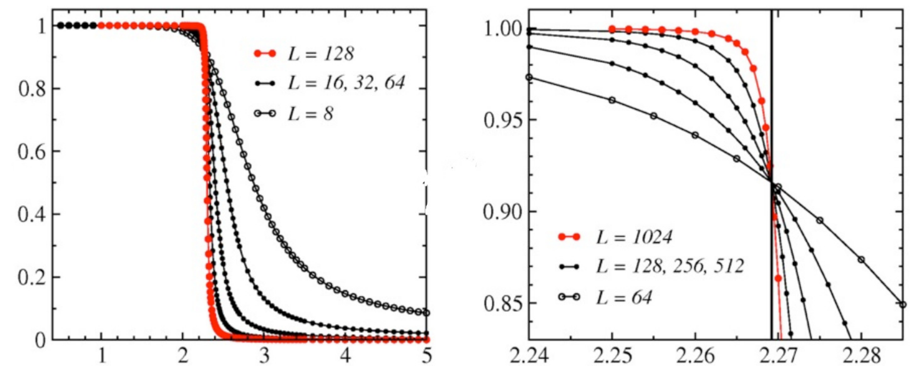

Figure 1: Binder cumulants. Plot of $3\,U_L/\,2$ as a function of kT/J, where k is the Boltzmann constant, for square lattices of growing sizes $N = L \times L$. The right panel is a zoom into the sector where the curves cross. From A. Sandvik (2015).