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Phase transition in 2D and 3D Ising model by time-series analysis

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Abstract

The critical temperatures for 2D and 3D ferromagnetic Ising model are well-known using several methods. In the present paper we introduce a new technique: to study the time-series of different order parameters established by means of a single-spin Monte Carlo evolution of the system in a prefixed thermal bath. Temperature of the simulations is changed as to include a broad range around the critical temperature. We will show that the autocorrelation functions for different sizes of square and cubic lattices intersect in a way similar to the Binder cumulant of the same parameter. This opens new possibilities to study phase transitions by locating the order parameter and the time window leading to the best resolution. Moreover, we will also discuss initial applications of this technique to the Edwards–Anderson model in 2D.

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For any given order parameter Q ascribed to a system of N spins, over M random distribution of mixed bonds in contact with a thermal bath at a temperature T, the Binder cumulant is defined as [1]

$$\psi_N(T) = 1 - \frac{|\langle Q^4 \rangle_T|_M}{3|\langle Q^2 \rangle_T|_M^2} \tag{1}$$

which requires a fairly good knowledge of the distribution of Q values after a large number of measurements. Function ψ goes abruptly to zero over a critical temperature T_C for a system of infinite dimensions [1] in the so-called thermodynamic limit. For finite systems this function rounds off going smoothly to zero over T_C. However, ψ curves for different finite sizes they all cross at T_C. Thus, the crossing of Binder cumulants is a powerful technique to recognize the critical temperature and it has been used in many applications to a variety of systems. On the other hand, we can examine the time evolution of the same parameter Q, namely $Q(t)$. This allows to define time autocorrelation functions. In this work we show that autocorrelation functions also cross at T_C thus providing an alternative method to recognize phase transitions.

In the applications below we consider the Ising model for three different cases: the three-dimensional (3D) ferromagnetic cubic lattice; the two-dimensional (2D) ferromagnetic square lattice; and the 2D Edwards–Anderson (EA) model on a square lattice. Let us briefly describe this last system in some detail defining the symbols to be used later on. The EA model considers random distributions of both ferromagnetic (F) and antiferromagnetic (AF) interactions, which we assume of the same magnitude. Let the concentration of AF interactions be denoted by x. A state $\alpha(S_1, S_2, \ldots, S_i, \ldots, S_N)$ is a collection of ordered spin orientations. We begin at an arbitrary state and let the system evolve over 1000 Monte Carlo (MC) steps by means of a single spin flip Metropolis dynamics. At this "moment" we record the reached state as the initial state α_0 or just α, for time $t = 0$. We let the system evolve. At any time t the system is at state β, then we can calculate any order parameter $Q(t)$. For the EA model, the order parameter $q(t)$ can be calculated as

$$q(t) = q_{\alpha,\beta} = \frac{1}{N}\sum_{i=1}^{N} S_i^{\alpha} S_i^{\beta}. \tag{2}$$

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The time-series evolution of $q(t)$ was calculated and stored, for 2D and 3D systems of different sizes N and different concentrations x.

The autocorrelation function $C_N(T,\tau)$ for any given function $Q(t)$ compares all the values of $Q(t)$ separated by an interval τ that can be formed for the stored time-series of the parameter. Namely,

$$C_N(T,\tau) = \frac{v}{v-\tau}\,\frac{\sum_{t'=0}^{v-\tau} Q(t')Q(t'+\tau)}{\sum_{t'=0}^{v} Q(t')Q(t')}. \tag{3}$$

Obviously, $C_N(T,0) = 1.0$ which marks the initial value of the autocorrelation function. As the events become more and more separated in time (namely, as τ grows) the behavior of $C_N(T,\tau)$ depends strongly on the way the associated order parameter $Q(t)$ behaves. If $Q(t)$ changes only very slightly, meaning that states β are genetically connected to initial state α, $C_N(T,\tau) \approx 1.0$ and rather constant as illustrated in Fig. 1a for parameter $q(t)$ corresponding to the purely ferromagnetic sample ($x = 0.0$) of size $N = 2500$, below the critical temperature T_C. A different behavior is found in the same sample for temperatures close to T_C, then $q(t)$ may change abruptly from one regime to another at a certain time, which is recognized by a decrease of $C_N(T,\tau)$ as can be seen in Fig. 1b. Way over $T_C q(t)$ does not show any stable value varying essentially in a random way over a wide range; then, $C_N(T,\tau)$ goes quickly to zero as shown by Fig. 1c.

In the simulations below, a wide range of temperatures was used as to include the expected critical temperature. Size of the systems was varied up to a point allowed by our present computer facilities. The emphasis is on the validation of the method based on the autocorrelation function rather than presenting simulations on large systems. In each case, we present results based on the two methods. On one side, the crossing of the Binder cumulant discussed in the introduction. On the other side, the crossing of the autocorrelation functions leading to exactly the same results, which validates this method at least from an empiric point of view.

As a first application let us consider the cubic (3D) ferromagnetic lattice for three different sizes: 8 × 8 × 8, 12 × 12 × 12, and 16 × 16 × 16. The procedure was the same for the other simulations so we describe it here in detail. A lattice size is chosen and a temperature is defined. The system is allowed to equilibrate for 1000 MC steps, then the time evolution begins evolving over 2 400 000 MC steps while time-series for $q(t)$ is obtained for $v = 120\,000$ "instants", separated at intervals of 20 MC steps. Then, the Binder cumulant $\psi_N(T)$ is calculated . Once the vector $q(t)$ is obtained, the autocorrelation function $C_N(T,\tau)$ for the absolute value of $q(t)$ (namely $|q(t)|$) is also calculated for a maximum span of $v/3 = 40\,000$ instants. Notice that for simplicity we will omit N and T in the figures. In the upper part of Fig. 2a we present the curves $\psi_{512}(T)$, $\psi_{1728}(T)$, and $\psi_{4096}(T)$ showing that they cross at about $T \approx 4.51$ which is in excellent agreement with reported values for the crossing of Binder cumulant for the 3D ferromagnetic cubic lattice at 4.515 [2], 4.5103 [3], and 4.5115 [4]. In the lower part of Fig. 2a we present the curves $C_{512}(T)$, $C_{1728}(T)$, and $C_{4096}(T)$, where a crossing at about 4.51 is again observed. This is a first evidence that the autocorrelation function for $|q(t)|$ leads to crossing of the curves for different sizes at the expected transition temperature.

We now do the same procedure for 2D square Ising lattice of sizes 16 × 16, 20 × 20, 28 × 28, 40 × 40, 50 × 50, and 100 × 100. In the upper part of Fig. 2b we present the curves $\psi(256,T)$, $\psi(400,T)$, $\psi(784,T)$, $\psi(1600,T)$, $\psi(2500,T)$, and $\psi(10\,000,T)$ showing that the crossing occurs at about $T \approx 2.27$ which is in excellent agreement with values expected for the crossing of Binder cumulants for the 2D ferromagnetic square lattice at 2.27 [2], and 2.269185 [5]. The same samples were used to obtain the crossing of the autocorrelation functions $C_{256}(T)$, $C_{400}(T)$, $C_{784}(T)$, $C_{1600}(T)$, $C_{2500}(T)$, and $C_{10\,000}(T)$ which are plotted in the lower part of Fig. 2b; as it can be seen the crossing of the autocorrelation functions for the absolute value of q also coincides with the crossing of the Binder cumulants.

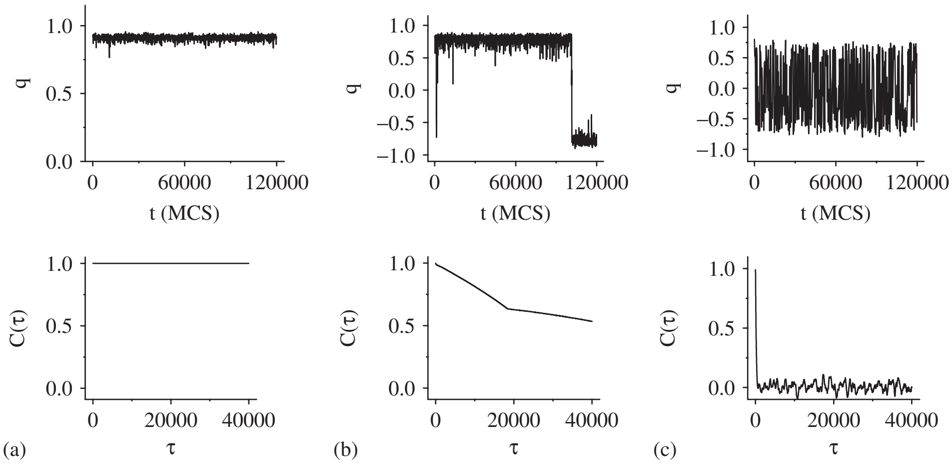

Fig. 1. Upper parts show the time-series associated to E—a parameter q for a ferromagnetic sample of size $N = 2500$. Lower parts represent the corresponding autocorrelation function for the $|q(t)|$ series on top: (a) is for a temperature $T < T_C$; (b) is for $T \approx T_C$ and (c) is for $T > T_C$.

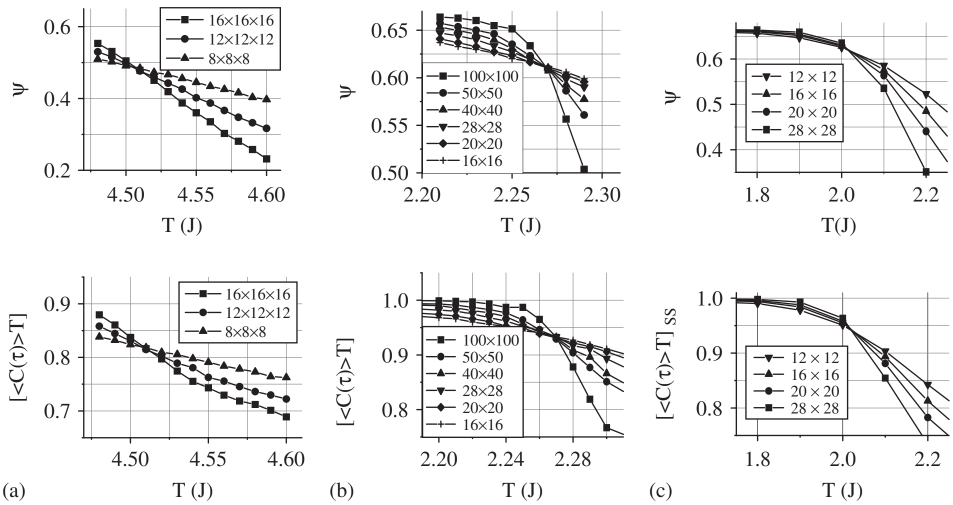

Fig. 2. Upper parts plot Binder cumulants Ψ as functions of temperature showing the crossing of the curves obtained for the sizes indicated in the insets. Lower parts plot the average values of the autocorrelation functions $[\langle C_N(T)\rangle]_\tau$ for different sizes showing that they cross at the same values where the Binder cumulants cross: (a) corresponds to the ferromagnetic case in 3D; (b) corresponds to the ferromagnetic case in 2D; (c) corresponds to the case with $x = 0.03125$ where 100 samples were used to do the configurational averages.

Finally, we go to the EA model for the particular case of $x = 0.03125 = \frac{1}{32}$. For such disordered systems, there is a large number of possible ways to distribute this concentration of AF bonds for each size. To consider this dispersion we consider average values for $\psi_N(T)$ and $C_N(T)$ over 100 samples ($[C(\tau)]_{\text{ss}}$) at each temperature for each size (the number of samples per size was $M = 100$). Sizes here are 12×12, 16×16, 20×20, 28×28. In the upper part of Fig. 2c we represent the crossing of Binder cumulants, while in the lower part of Fig. 2c we obtain the crossing of autocorrelation functions at exactly the same temperature $T_C \approx 2.0$. These results are in good agreements with previous calculations for Binder cumulants: 2.0 [6] Actually, the reason to use this particular concentration is the possibility to compare with previous results for Binder cumulants.

We can conclude that the curves $C_N(T,\tau)$ for the absolute value of the EA order parameter $q(t)$, for different sizes, cross at the same point where the crossing of equivalent Binder cumulants occur. Thus, the study of crossing of autocorrelation functions also leads to the finding of critical temperatures.

The advantage of the use of the method of autocorrelation function is two-fold. On one hand, the time-series needed for the study can be obtained as a by-product of usual studies of evolution of these systems to establish genetic characteristics of the visited portion of the configuration space (aging is an example of this). On the other hand, the physical interpretation of the variations of $C_N(T,\tau)$ outlined previously in the definition of q above. In contrast, the Binder cumulant arises as a mathematical artifact which is not so easy to interpret.

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References

[1] K. Binder, Z. Phys. B 43 (1981) 119.
[2] P. Meyer, Computational studies of pure and dilute spin models, School of Mathematics and Computing, University of Derby, 2000, ⟨http://www.hermetic.ch/compsci/thesis/contents.htm⟩.
[3] M.E. Fisher, Rep. Prog. Phys. 30 (1967) 615.
[4] H.-O. Heuer, J. Phys. A 26 (1993) L333.
[5] L. Onsager, Phys. Rev. 65 (1944) 117.
[6] F. Romá, Master Thesis, Universidad Nacional de San Luis, San Luis, Argentina, 2004.