Out-of-equilibrium finite-size method for critical behavior analyses

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We present a dynamic off-equilibrium method for the study of continuous transitions, which represents a dynamic generalization of the usual equilibrium cumulant method. Its main advantage is that critical parameters are derived from numerical data obtained much before equilibrium has been attained. Therefore, the method is particularly useful for systems with long equilibration times, like spin glasses. We apply it to the three-dimensional Ising spin-glass model, obtaining accurate estimates of the critical exponents and of the critical temperature with a limited computational effort.

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I. INTRODUCTION

Monte Carlo simulations combined with finite-size scaling (FSS) methods are, at present, the most successful tool for the identification of continuous transitions and the determination of the critical parameters. In this approach there are two main obstacles to a precise determination of the critical parameters. On one side, scaling corrections, related to the subleading irrelevant renormalization-group (RG) operators, may mask the asymptotic critical behavior, which shows up only when the system size L becomes large. On the other side, the Monte Carlo dynamics becomes increasingly slow as the critical point is approached, so that thermalization and equilibrium autocorrelation times become large as L increases, hampering large-L simulations. These problems are particularly serious in systems with quenched disorder. They occur, for instance, when studying the paramagnetic glassy transition in the $\pm J$ Ising model with random ferromagnetic and antiferromagnetic couplings, which represents a standard theoretical laboratory to understand the effects of quenched disorder and frustration. Its Hamiltonian is given by [1]

$$H = -\sum_{\langle xy\rangle} J_{xy}\sigma_x\sigma_y, \tag{1}$$

where the sum runs over all nearest neighbors $\langle xy\rangle$ of a cubic lattice, $\sigma_x = \pm 1$ are Ising spins, and J_{xy} are quenched random couplings that take the values ± 1 with equal probability. At the transition and, even worse, in the low-temperature phase, the standard Metropolis dynamics is very slow so that equilibration becomes very difficult, even for relatively small systems. Moreover, equilibration times depend strongly on the disorder realization, so that a sample-by-sample analysis is needed to guarantee that all measurements are obtained from well-equilibrated samples [2]. At present, even by using dedicated machines [3], it seems impossible to go much beyond sizes $L = 30 - 40$.

In this work we discuss a dynamic method to determine the critical temperature and the critical exponents. We will discuss it in the context of the $\pm J$ Ising model, but the method and the results are completely general, so it can be applied to the study of any continuous transition in pure or random systems. The method, which does not require the system to be in equilibrium, has two advantages. First, the difficult and time-consuming (at least in disordered systems) task of verifying equilibration is no longer needed. Second, we can stop the simulation much before equilibrium has been reached, saving a considerable amount of computing time. The method we discuss is somewhat different from previous off-equilibrium methods (see, e.g., Refs. [4–12] and references therein). Indeed, in most of those works it is generally assumed that L is so large that finite-size effects are negligible, a condition that is easily satisfied in pure systems but not in the disordered case. On the contrary, we will use the finite-size dependence of the physical observables to estimate the critical parameters. Our method is essentially an off-equilibrium generalization of the usual Binder crossing method [13].

The paper is organized as follows. In Sec. II we define the quantities that are measured in the Monte Carlo simulations. In Sec. III we describe the finite-size scaling method we use. In Sec. IV we present our numerical results for the spin-glass transition. Finally, we draw our conclusions in Sec. V.

II. OBSERVABLES

In our simulations we consider cubic lattices of linear size L and volume V with periodic boundary conditions. As usual in simulations of spin-glass systems, our basic observables are defined in terms of the overlap parameter. For each disorder realization, we consider n different replicas $\{\sigma_x^a(t)\}$, $a = 1,\ldots,n$, which are obtained by running the dynamics from different randomly chosen configurations of the spins at $t = 0$. For each pair of replicas we define the overlap local parameter ($a \neq b$)

$$q_x^{ab}(t) = \sigma_x^a(t)\,\sigma_x^b(t) \tag{2}$$

and

$$Q_k^{ab}(t) = \left(\sum_x q_x^{ab}(t)\right)^k. \tag{3}$$

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The dynamic overlap susceptibility is defined as

$$\chi(t) = \frac{1}{c_2 V} \sum_{a<b} \left[Q_2^{ab}(t) \right], \tag{4}$$

where the square brackets indicate the average over the disorder distribution and c_2 is the number of different replica pairs. In our simulations we take $n = 4$, so that $c_2 = 6$.

We will also define an out-of-equilibrium correlation (or coherence) length $\xi(t)$ as the second moment of the overlap two-point correlation function:

$$\xi(t) = \frac{1}{2\sin(k/2)} \sum_{m=1}^{3} \sqrt{\frac{\chi(t)}{\tilde{\chi}(t,k_m)} - 1}, \tag{5}$$

where $k_1 = (k,0,0)$, $k_2 = (0,k,0)$, $k_3 = (0,0,k)$, $k = 2\pi/L$, and

$$\tilde{\chi}(t,k) = \frac{1}{c_2 V} \sum_{a<b} \left[\left| \sum_x q_x^{ab}(t) e^{-ik\cdot x} \right|^2 \right]. \tag{6}$$

In order to apply the method we must define renormalized couplings, i.e., quantities that are invariant under renormalization-group transformations and are therefore universal at the critical point for $L \to \infty$. We consider all Binder cumulants that are at most quartic in the overlap parameter. They are defined as follows:

$$U_4(t) = \frac{\left[c_2^{-1} \sum_{a<b} Q_4^{ab}(t) \right]}{\left[c_2^{-1} \sum_{a<b} Q_2^{ab}(t) \right]^2}, \tag{7}$$

$$U_{22}(t) = \frac{\left[c_{22}^{-1} \sum_{a<b<c<d} Q_2^{ab}(t)\, Q_2^{cd}(t) \right]}{\left[c_2^{-1} \sum_{a<b} Q_2^{ab}(t) \right]^2} - 1, \tag{8}$$

$$U_{23}(t) = \frac{\left[c_{23}^{-1} \sum_{a<b<c} Q_2^{ab}(t)\, Q_2^{ac}(t) \right]}{\left[c_2^{-1} \sum_{a<b} Q_2^{ab}(t) \right]^2}, \tag{9}$$

$$U_{13}(t) = \frac{\left[c_{13}^{-1} \sum_{a<b<c} Q_1^{ab}(t)\, Q_1^{ac}(t)\, Q_1^{bc}(t) \right]}{\left[c_2^{-1} \sum_{a<b} Q_2^{ab}(t) \right]^{3/2}}, \tag{10}$$

$$U_{14}(t) = \frac{\left[c_{14}^{-1} \sum_{a<b<c<d} Q_1^{ab}(t)\, Q_1^{bc}(t)\, Q_1^{cd}(t)\, Q_1^{da}(t) \right]}{\left[c_2^{-1} \sum_{a<b} Q_2^{ab}(t) \right]^2}. \tag{11}$$

As before, the constants c_{ij} give the number of equivalent terms we are averaging over. For $n = 4$ we have $c_{22} = 3$, $c_{23} = 12$, $c_{13} = 4$, and $c_{14} = 3$. Note that $U_{14}(t)$ and $U_{22}(t)$ can only be defined if $n \geqslant 4$, explaining why we have chosen $n = 4$. Four cumulants defined here are directly related to those used in Ref. [3]. If $U_{4,J}$, $U_{22,J}$, $U_{111,J}$, and $U_{1111,J}$ are the quantities defined in Ref. [3], we have

$$\begin{aligned} U_{4,J} &= U_4, \\ U_{22,J} &= (U_{22} + 1)/U_4, \\ U_{111,J} &= U_{13}^{4/3}/U_4, \\ U_{1111,J} &= U_{14}/U_4. \end{aligned} \tag{12}$$

III. THE METHOD

As in FSS equilibrium computations, we begin by considering a RG invariant quantity $U(t,L,\beta)$ as a function of the Monte Carlo time t, inverse temperature β, and system size L. According to RG, for L and t large and close to the critical point β_c, $U(t,L,\beta)$ scales as [14–19]

$$U(t,L,\beta) = f_R(tL^{-z},\epsilon) + u_\omega(\beta) L^{-\omega} g_R(tL^{-z},\epsilon) + \cdots, \tag{13}$$

where next-to-leading scaling corrections have been neglected. Here ω is the leading correction-to-scaling exponent, $u_\omega(\beta)$ the associated nonlinear scaling field satisfying $u_\omega(\beta_c) \neq 0$, $\epsilon = u_\beta(\beta) L^{1/\nu}$, where $u_\beta \approx \beta - \beta_c$ is the temperature nonlinear scaling field which parameterizes the distance from the critical point. Equation (13) depends also on the dynamic critical exponent z, which represents an additional parameter to be determined. To avoid any reference to z, we now reparameterize the time evolution in terms of the correlation length ξ, or, better, in terms of the RG invariant ratio $R_\xi = \xi/L$. We will always start the simulations from disordered (random) configurations. Therefore, the correlation length ξ is an increasing function of t. Then, any function of tL^{-z} can be equivalently reexpressed in terms of R_ξ, so that we write

$$U(t,L,\beta) = \hat{f}_U(R_\xi,\epsilon) + u_\omega(\beta) L^{-\omega} \hat{g}_U(R_\xi,\epsilon) + \cdots, \tag{14}$$

which is defined for $R_\xi \leqslant R_{\xi,\mathrm{eq}}(\epsilon)$, where $R_{\xi,\mathrm{eq}}(\epsilon)$ is the equilibrium value of R_ξ for the given ϵ. Equation (14) is the basic relation we use to compute critical temperature and exponents. Indeed, ignoring scaling corrections close to the critical point Eq. (14) can be expanded in ϵ, obtaining

$$U(t,L,\beta) = \hat{f}_U(R_\xi,0) + (\beta - \beta_c) L^{1/\nu} \hat{f}'_U(R_\xi,0) + \cdots. \tag{15}$$

At fixed R_ξ, the quantity $U(t,L,\beta)$ behaves exactly as in the equilibrium case: β_c is determined as the crossing point and ν is obtained by computing the slope at β_c. However, in this formulation, equilibration is not needed.

Equation (14) is valid for any value of R_ξ, so one might think of choosing a small value for such a parameter, reducing significantly the length of the runs. However, one must not forget that the method is intrinsically a finite-size method; hence, it can only work if finite-size effects are not too tiny, and this, in turn, requires R_ξ to be not too small. Mathematically, these considerations can be understood by considering Eq. (15). The method is expected to be precise if the coefficient $\hat{f}'_U(R_\xi,0)$ is not too small. Such a coefficient depends on R_ξ and it is expected to increase with R_ξ. In particular, it is expected to be very small for small R_ξ, so that if one chooses a small value of R_ξ, the crossing becomes undetectable, unless statistical errors are very tiny. Hence, R_ξ should be chosen small but still large enough to have a reasonable sensitivity of the results on system sizes.

IV. NUMERICAL RESULTS

We perform large-scale simulations on cubic lattices of volume $V = L^3$ with $8 \leqslant L \leqslant 64$, considering five values of β between 0.880 and 0.910. Statistics is a crucial factor

in the analysis and hence we consider a very large number N_s of samples for each L and β. Typically, N_s varies between 3×10^5 and a few million. Only for $L = 48,64$ is N_s smaller: $N_s = 6 \times 10^4, 10^4$ in these cases. Essentially all runs end when the system is still out of equilibrium. In most of the cases, data extend only up $R_\xi \approx 0.5$, in some cases even less (at equilibrium [3] $R_\xi = 0.652(3)$ at the critical point). Simulations were performed on a small graphics processing unit (GPU) cluster using a very efficient asynchronous multispin coding technique [20]. In each run we simulate together $32k$ different disorder realizations with four replicas for each disorder realization. The value of k is tuned for each L to have the best performance of the GPUs. As a result, one spin flip takes 2.9 ps (essentially for all sizes) on the GTX Titan, the fastest GPU we have. The simulations presented here took approximately 3.1 CPU years of the GTX Titan GPU.

Moreover, we must somehow parameterize the scaling functions $\hat{f}_U(R_\xi,\epsilon)$ and $\hat{g}_U(R_\xi,\epsilon)$. Since the data belong to a small temperature interval, we use the expansion (15) to first order in ϵ. We have also performed some analyses using a second-order approximation, without observing significant differences. As for the correction-to-scaling function, we have verified that we can assume it to be independent of temperature. Finally, we should make approximations for the nonlinear scaling fields. Relying on the analysis of Refs. [21] and [22], we set $u_\beta(\beta) = \beta - \beta_c$ and $u_\omega(\beta) = 1$, neglecting the additional corrections. Given the small temperature interval we consider, these approximations should hold quite precisely. Hence, each $U(t,L,\beta)$ was fitted to

$$U(t,L,\beta) = P_1(R_\xi) + P_2(R_\xi)(\beta - \beta_c)L^{1/\nu} + P_3(R_\xi)L^{-\omega}, \tag{16}$$

with $P_1(R_\xi)$, $P_1(R_\xi)$, and $P_3(R_\xi)$ polynomials of degree 6, 3, and 3, respectively. The fit of the five renormalized couplings is quite complex, as we take ω, β_c, ν, and the coefficients of the polynomials as free parameters. As a whole, there are 78 free parameters that must be optimized. In the fits we have not taken into account the time correlations among data at the same β and L, so that statistical errors (computed using the jackknife method) are not *a priori* optimal.

To verify that such neglect is not relevant for the final estimates, we have performed some fits of a single cumulant taking time correlations into account. The corresponding estimates and error bars are essentially equal to those obtained without including statistical correlations.

As usual in this type of analyses, the most difficult issue is the estimation of the systematic errors due to the neglected correction terms. This is very important here, since the attainable values of L are not very large. We have thus performed fits with several types of cuts. We perform fits including each time only data satisfying $L \geqslant L_{\min}$, $\xi \geqslant \xi_{\min}$, and $R_\xi \geqslant R_{\xi,\min}$, considering several values for $L_{\min}$, $\xi_{\min}$, and $R_{\xi,\min}$. Results obtained by taking $3 \leqslant \xi_{\min} \leqslant 5$, $8 \leqslant L_{\min} \leqslant 12$, and $0 \leqslant R_{\xi,\min} \leqslant 0.4$ show some scatter, which is somewhat larger than statistical errors, indicating that the neglected systematic effects may be as important as the statistical ones. The most crucial parameter is $\xi_{\min}$. When such a parameter is increased from 3 to 4, the exponent

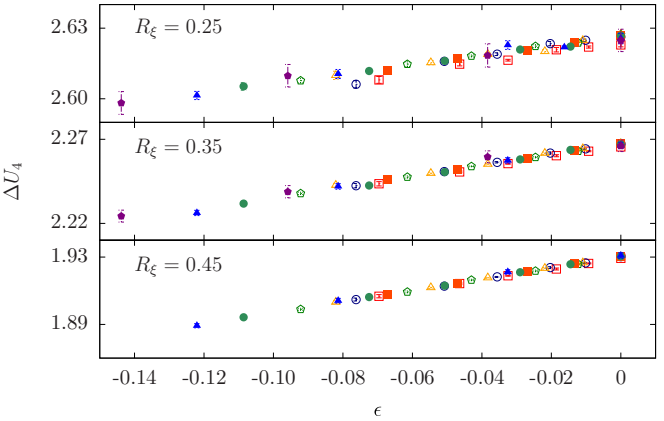

FIG. 1. Plot of ΔU_4 versus $\epsilon = (\beta - \beta_c)L^{1/\nu}$ for $R_\xi = 0.25$ (top), $R_\xi = 0.35$ (middle), and $R_\xi = 0.45$ (bottom). We set $\beta_c = 0.910$, $\omega = 1.3$, and $\nu = 2.47$. Symbols: empty square ($L = 8$), empty circles ($L = 10$), empty triangles ($L = 12$), empty pentagons ($L = 16$), filled squares ($L = 20$), filled circles ($L = 24$), filled triangle ($L = 32$), filled pentagon ($L = 48$).

ω decreases sharply, by more than one error bar, while β_c increases. Such a systematic drift occurs also when $\xi_{\min}$ is further increased to 5, but now the change is much less than one error bar. Therefore, the results we quote correspond to fits with $\xi_{\min} = 4$. For such a value of $\xi_{\min}$ we obtain $\beta_c = 0.911(2)$, 0.916(4), 0.909(4) for $L_{\min} = 8, 10, 12$ and $R_{\xi,\min} = 0$, and $\beta_c = 0.911(2)$, 0.909(2), 0.909(3) for $R_{\xi,\min} = 0$, 0.2, 0.4 and $L_{\min} = 8$. No systematic trends can be observed, all estimates being consistent within errors. Except for one estimate, all results (with their errors) we are quoting here lie in the interval $0.906 \leqslant \beta_c \leqslant 0.913$. Therefore, we take $\beta_c = 0.910(4)$ as our final estimate. The error, which is twice the error affecting the results with $L_{\min} = 8$, is somewhat subjective and should take into account the effect of the neglected next-to-leading scaling corrections. Analogously, we can estimate ω and ν obtaining

$$\omega = 1.3(2), \qquad \nu = 2.47(10). \tag{17}$$

The estimates of ω are strongly correlated with those of β_c: the larger β_c, the smaller ω is. If $\beta_c = 0.906$, fits keeping β_c fixed give $\omega \approx 1.5$, while $\omega \approx 1.1$ is obtained by fixing $\beta_c = 0.914$. The exponent ν is instead much less correlated with β_c, changing at most by ± 0.03 when β_c varies by ± 0.004.

To show the quality of the results, in Fig. 1, we report ΔU_4, defined by

$$\Delta U_4(\beta,L,R_\xi) = U_4(\beta,L,R_\xi) - P_3(R_\xi)L^{-\omega} \tag{18}$$

versus ϵ. We consider $R_\xi = 0.25$, 0.35, and 0.45. Very good scaling is observed, confirming the correctness of the scaling ansatz and the accuracy of the estimates of the critical exponents. Note also that the data lie on an essentially straight line, validating our choice of expanding $f_U(R_\xi,\epsilon)$ to first order in ϵ. From the figure, we can also clarify why a large number of samples, of order 10^6, is needed to estimate the critical parameters. For instance, U_4 at $R_\xi = 0.35$ varies by 0.04 within our temperature interval. Therefore, the temperature dependence of the data can be observed only if the errors on U_4 are significantly less than 10^{-2}, for instance, if they are equal to 10^{-3}. Since errors scale as $a/\sqrt{N_s}$ with $a \approx 1$ for

all values of L, a 10^{-3} error is obtained by taking $N_s \approx 10^6$. Note that this requirement is not specific of the off-equilibrium method we use. Also, equilibrium analyses require N_s to be large [3,21,22].

The analysis we have performed for the renormalized couplings can be extended to the susceptibility. The finite-time scaling behavior can now be written as

$$\ln \chi = (2-\eta)\ln L + P_1(R_\xi) + (\beta-\beta_c)L^{1/\nu}P_2(R_\xi) + L^{-\omega}P_3(R_\xi) + P_4(\beta), \quad (19)$$

where the last term $P_4(\beta)$ is the contribution of the nonlinear scaling field associated with the magnetic field; see Refs. [21] and [22] for a discussion. A good parametrization is obtained by taking $P_1(R_\xi)$, $P_2(R_\xi)$, $P_3(R_\xi)$ as polynomials of degree 6, 3, 3, respectively, as before. For $P_4(\beta)$, we set $P_4 = a_4\beta$. We obtain the final estimate

$$\eta = -0.39(1), \quad (20)$$

which is fully consistent with those of Refs. [22] and [3].

Finally, we estimate z by requiring data to satisfy the general scaling form (13). We obtain

$$z = 6.80(15), \quad (21)$$

where the error should be quite conservative. The scaling behavior of R_ξ and U_4 is shown in Fig. 2. Scaling corrections are clearly visible, but large L data appear to fall onto a single universal curve as L increases. The value we obtain is in agreement with the estimate of Refs. [8] and [11] at $T = 1.1$. Instead, it is larger than those of Refs. [5,6,12]. However, note that in all these works no scaling corrections, crucial to control possible systematic errors, were included in the analyses. (They play a fundamental role in the derivation of our result.)

It is interesting to compare these results with previous ones, see Table I. (Older estimates are summarized in Ref. [24].) For the critical-point position, our estimate $T_c = 1/\beta_c = 1.099(5)$ agrees within errors with the estimates $T_c = 1.102(3)$ and $T_c = 1.109(10)$ of Refs. [3] and [22], obtained from the analysis of equilibrium results. Our error is larger than that reported in Ref. [3], but note that our final error includes a subjective estimate of the systematic error. Had we reported only the statistical error for $L_{\min} = 8$, we would have obtained the same accuracy. The estimates of ν are also consistent, while our final estimate of ω is slightly larger than previous estimates, though still consistent with them within errors. The off-equilibrium estimates of Ref. [11] are consistent with ours but less precise. Previous dynamic estimates of T_c are instead not consistent. It is now clear that the reported errors are underestimated as a consequence of the neglect of the subleading scaling corrections in the analyses.

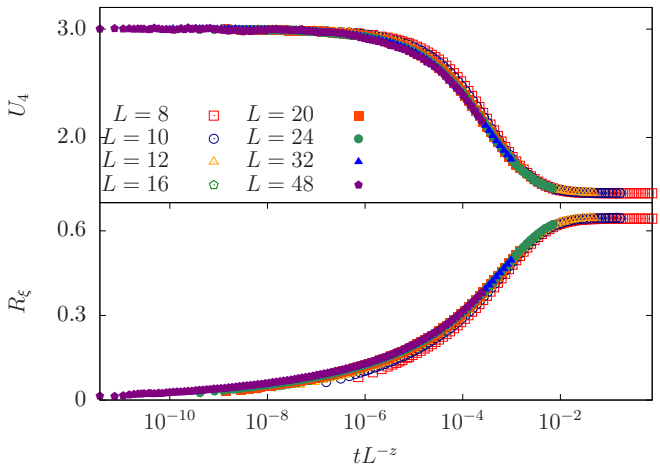

FIG. 2. Plot of U_4 and R_ξ versus tL^{-z} for $\beta = 0.910$. We set $z = 6.80$.

V. CONCLUSIONS

The method we have discussed represents a significant improvement with respect to equilibrium analyses. Indeed, since the scaling variable is tL^{-z}, the time needed to extend Metropolis runs from any value of R_ξ to equilibrium scales as L^z, i.e., as L^7 given that $z \approx 7$ for the Ising spin glass. Therefore, the advantage is very large and increases rapidly with L. To make a fair comparison with equilibrium studies, we should, however, take into account that in those studies one combines the parallel-tempering method [25] with the Metropolis or heat-bath algorithm. It is not clear how equilibration times

TABLE I. Estimates of T_c and of the critical exponents by off-equilibrium methods. Results of Refs. [22] and [3] are obtained in equilibrium simulations. The exponents β and γ are related to ν and η by $\beta = \nu(1+\eta)/2$, $\gamma = \nu(2-\eta)$.

	T_c	ν	η	ω	z	β	γ	$z\nu$
Ref. [4]	1.12(12)							5.7(5)
Ref. [5]	1.17(4)	1.5(3)			6.2(2)		3.6(6)	
Ref. [6]	1.19(1)		−0.22(2)		5.7(2)			
Ref. [7]	1.154(3)					0.52(9)		
Ref. [8]					6.86(16)			
Ref. [9]	1.135(5)							
Ref. [10]	1.18(1)	1.40(5)	−0.20(1)					
Refs. [11,23]	1.115(15)	2.2(3)	−0.380(7)		6.79(6)			
Ref. [12]					5.85(9)			
This work	1.099(5)	2.47(10)	−0.39(1)	1.3(2)	6.80(15)			
Ref. [22]	1.109(10)	2.45(15)	−0.375(10)	1.0(1)				
Ref. [3]	1.1019(29)	2.562(42)	−0.3900(36)	1.12(10)				

scale for this combined algorithm, and in particular, how long it takes to thermalize the hard samples. However, the results reported in Ref. [3] are consistent with a sample-dependent time that scales as L^2 for the samples that equilibrate fast and as L^7 for those that are slower. The off-equilibrium method is still significantly faster. A more direct comparison can be obtained by using the results published in Ref. [3]. In our simulations at the critical point, runs extending up to $R_\xi \approx 0.5$ require 2.5×10^6, 16×10^6 Metropolis sweeps for $L = 24$ and 32, respectively. In the parallel-tempering simulations for $L = 32$ of Ref. [3], the number of iterations discarded for thermalization varies between 8×10^6 and 500×10^6 (on average 13×10^6) sweeps. Taking into account that 22 systems at different temperatures are simulated together, our simulations are shorter by a factor of 10 at least. If one were stopping the off-equilibrium runs at $R_\xi = 0.40$, one would gain an additional factor of 3 for this value of L.

In spite of the significant improvement with respect to equilibrium studies, the computing time needed for a simulation scales as L^z even in the off-equilibrium case, since we need to collect data at fixed R_ξ for all values of L. This requirement makes our method not suitable to investigate large system sizes. Since errors are independent of system size as a consequence of the absence of self-averaging, the Monte Carlo time needed to obtain the same statistical errors scales also as L^z. This explains why we have not considered lattices with $L > 64$. If we increase L, we should increase t at the same time, making simulations far too long.

Let us now summarize our results. We have presented a dynamic off-equilibrium method suitable for the determination of the critical temperature and of the critical exponents. Such a method represents a significant improvement with respect to previous ones. In particular, there is no need for L to be large enough to avoid finite-size effects—thus, a source of systematic errors is absent—nor does it require an *a priori* knowledge of the critical temperature. We have used the method to determine critical exponents and temperature for the $\pm J$ Ising model. With a relatively modest investment of computing time, thanks also to a very efficient GPU multispin code, we obtain results that have a comparable precision with that of the estimates of Ref. [3], which are the most precise equilibrium estimates available today. The method is completely general and can be applied to any pure or disordered system.

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