Mixed initial conditions to estimate the dynamic critical exponent in short-time Monte Carlo simulation

Roberto da Silva, Nelson A. Alves and J.R. Drugowich de Felício

Departamento de Física e Matemática, FFCLRP Universidade de São Paulo. Av. Bandeirantes 3900. CEP 01404-090 Ribeirão Preto, SP, Brazil

March 22, 2022

We explore the initial conditions in short-time critical dynamics to propose a new method to evaluate the dynamic exponent $z$. Estimates are obtained with high precision for 2D Ising model and 2D Potts model for three and four states by performing heat-bath Monte Carlo simulations.

Keywords: short-time dynamics, critical phenomena, dynamic exponent, Ising model, Potts model, Monte Carlo simulations.

PACS-No.: 64.60.Fr, 64.60.Ht, 02.70.Lq, 75.10.Hk

The description of static critical phenomena in terms of finite size scaling (FSS) relations, developed by Fisher et al. [1,2] has been extended by Halperin, Hohenberg, Ma and Suzuki [3,4] to include dynamical properties of the system. Later, Janssen et al. [5], and independently Huse [6] found evidence for an universal behavior far from equilibrium.

As discussed by Janssen et al. one finds an universal behavior already in the early stages of the relaxation process for systems prepared at an initial state characterized by non-equilibrium values of the order parameter. As a consequence, they could advance the existence of a new critical exponent $\theta$, independent of the known set of static exponents and of the dynamic critical exponent $z$. This new exponent characterizes the so called “critical initial slip”, the anomalous increasing of the magnetization when the system is quenched to the critical temperature $T_c$.

That new universal stage has been exhaustively investigated to confirm theoretical predictions and to enlarge our knowledge on phase transitions and critical phenomena. In this sense, several models and algorithms [6,7] have been used, as toy models, in order to check the ability of the new approach in obtaining dynamic and static critical exponents. Results are in good agreement with pertinent results for static exponents and seems to be confident even for the new critical exponent $\theta$. However, a reliable technique to obtain the dynamic exponent $z$ is lacking. A first proposal by Li et al. [10] using a time-dependent Binder’s cumulant yields estimates with low precision when compared with other techniques [11,12]. An alternative way which uses another kind of cumulant, proposed by Zheng [13], gives the right answer for the 2D Ising model but fails in determining the value of $z$ for the 3-state Potts model [14] and for the Ising model with multispin interactions [14].

In this letter, we introduce and check a new technique to obtain the exponent $z$, combining the behavior of the
order parameter and its second moment when the system is submitted to different initial conditions.

Before presenting our proposal, we shall review the main results in short time dynamics.

Although Halperin et al. [3] have studied systems with different dynamics, we consider only systems without conservation laws, the so called Model A [15] because our discussion aims dynamics generated by heat bath dynamics. Therefore, we consider a magnetic system prepared at high temperature ($T >> T_c$) with a small nonzero magnetization $m_0$, (this can be achieved with a small external magnetic field $h$) and quenched to the critical temperature $T_c$ without any external magnetic field. If the system is allowed to relax towards equilibrium with the dynamics of model A, the magnetization obeys the following scaling relation (generalized to $k$th moment),

$$M^{(k)}(t, \tau, L, m_0) = b^{-k\beta/\nu} M^{(k)}(b^{-z} t, b^{1/\nu} \tau, b^{-1} L, b^{x_0} m_0).$$  \hspace{1cm} (1)

Here $b$ is an arbitrary spatial scaling factor, $t$ is the time evolution and $\tau$ is the reduced temperature, $\tau = (T - T_c)/T_c$. The exponents $\beta$ and $\nu$ are the static critical exponents, while $z$ is the dynamic one. $M^{(k)} = \langle M^k \rangle$ are the $k$th moments of magnetization. This scaling relation depends on the initial magnetization $m_0$ and gives origin to a new, independent critical exponent $x_0$, the scaling dimension of the initial magnetization, which is related to $\theta$.

From Eq. (1) we can derive the power law increasing of the magnetization, observed in the initial stage of the dynamic relaxation. For this purpose, we consider large lattice sizes $L$ at $\tau = 0$ with $b = t^{1/z}$. This leads to the scaling relation

$$M(t, m_0) = t^{-\beta/\nu z} M(1, t^{x_0/z} m_0)$$  \hspace{1cm} (2)

for the first moment of the magnetization $M^{(1)} = M$. By expanding this equation for small $m_0$, we have the following power law,

$$M(t) \sim m_0^{t \theta},$$  \hspace{1cm} (3)

where, as anticipated, we identify $\theta = (x_0 - \beta/\nu)/z$. Here we also have the condition that $t^{x_0/z} m_0$ is small, which sets a time scale $t_0 \sim m_0^{-z/x_0}$ where that phenomena can be observed.

On the other hand, it has been realized the existence of another important dynamic process from an initial ordered state [18–20], which represents another fixed point in the context of renormalization group approach. This leads to a different universal behavior of the dynamic relaxation process also described by Eq. (1) with $m_0 = 1$. In particular, dealing with large enough lattice sizes at the critical temperature ($\tau = 0$), one obtains a power law decay of the magnetization

$$M(t) \sim t^{-\beta/\nu z},$$  \hspace{1cm} (4)

which follows from Eq. (1) when we choose $b^{-z} t = 1$ and shows the average magnetization is not zero as would be expected from a disordered initial state.

Equation (1) and their particular forms in (3) and (4) can be used to determine relations involving static critical exponents and the dynamic exponent $z$ [13,16].

The observables in short-time analysis are described by different scaling relations according to the initial magnetization. In particular, the second moment $M^{(2)}(t, L)$,
\[ M^{(2)} = \left( \frac{1}{L^d} \sum_{i=1}^{N} \sigma_i \right)^2 = \frac{1}{L^{2d}} \left( \sum_{i=1}^{N} \sigma_i^2 \right) + \frac{1}{L^{2d}} \sum_{i \neq j}^{N} \langle \sigma_i \sigma_j \rangle, \]  

behaves as \( L^{-d} \) since in the short-time evolution with initial condition \( m_0 = 0 \) the spatial correlation length is very small compared with the lattice size \( L \). Thus we have

\[ M^{(2)}(t, L) = t^{-2\beta/\nu z} M^{(2)}(1, t^{-1/z} L) \sim t^{(d-2\beta/\nu)/z}. \]  

(6)

Moreover, under this initial condition one can also define the time-dependent Binder’s cumulant at the critical temperature,

\[ U(t, L) = 1 - \frac{M^{(4)}(t, L)}{3(M^{(2)}(t, L))^2}, \]  

which leads at \( T = T_c \) to the FSS relation

\[ U(t, L) = U(b^{-z} t, b^{-1} L), \]  

(8)

and the exponent \( z \) can be independently evaluated through scaling collapses for different lattice sizes \([10,17]\).

In order to obtain more precise estimates for the dynamic exponent \( z \), another cumulant has been proposed \([13]\). It is given by

\[ U_2(t, L) = \frac{M^{(2)}(t, L)}{(M(t, L))^2} - 1 \]  

(9)

and should behave as

\[ U_2(t) \sim t^{d/z} \]  

(10)

when one starts from an ordered state. In this case, curves for all the lattices lay on the same straight line without any re-scaling in time and results in more precise estimates for \( z \). However, application of this procedure has not been successful in at least two well known models: the two-dimensional \( q = 3 \) Potts model \([13]\) and the Ising model with three spin interactions in just one direction \([14]\). The reason for the above disagreement could be related to the value of the second term of r.h.s in Eq. (5) when \( m_0 = 1 \).

A plausible way to circumvent this problem is to work with different initial conditions. For this we decided to follow the evolution of the ratio \( F_2 = M^{(2)}/M^2 \) but using different initial conditions to calculate each one of the mean values. The reason is we know the behavior of the second moment of the magnetization when samples are initially disordered (\( m_0 = 0 \)) and also the dependence on time of the magnetization of samples initially ordered (\( m_0 = 1 \)). Under the above mentioned conditions the ratio behaves as

\[ F_2(t, L) \bigg|_{m_0=0}^{m_0=1} \sim t^{(d-2\beta/\nu)/z} \sim t^{d/z}, \]  

(11)

which has the same potential law that the cumulant mentioned before but requires two independent simulations instead of one used for calculating \( U_2 \).

In short-time Monte Carlo (MC) simulations, the time scale \( t \) is settled in units of whole lattice updates, and does not depend on the initial conditions. However, the same dynamics (Metropolis, Glauber or heat-bath) should be used in both simulations \([8]\).
Now we present our estimates obtained for 2D Ising model, \( q = 3 \) and \( q = 4 \) Potts models.

We have performed independent heat-bath (HB) MC simulations for a large lattice \((L = 144)\) according to the required initial conditions and the evolutions have been done until the maximum time \( t = 200 \) MC sweeps with \( N = 10000 \) samples. This gives averages for the magnetization and its second moment. We have performed this kind of simulation 20 times to obtain our final estimates for each moment in function of \( t \). Since all runs are independent due to the choice of random numbers, we have a total of 400 time series for Eq. (11).

Our results are shown on a log-log scale for the time interval \([10, 100]\) in Fig.1 and Fig.2, respectively for three and four-state Potts model (a similar figure is obtained for 2D Ising model) and they appear to be clearly consistent with a power law in that time interval. The error bars are also presented in those figures but they are hardly seen in that scale.

Our estimates for \( z \) comes from a least square fitting in the time interval \([t_i, t_f]\). Due to our small statistical errors, we can make a systematic study for the range in \( t \) where we find acceptable goodness-of-fit \( Q \) \([21]\). As examples, we obtain for 2D Ising model, \( z = 2.1435(2) \) in the time interval \([10, 200]\) with \( Q = 10^{-250} \), \( z = 2.1359(3) \) in \([50, 200]\), with \( Q = 10^{-41} \), and the most acceptable \( Q = 0.99 \) in \([30, 90]\), which yields \( z = 2.1565(7) \). This value is presented in Table 1, where we also include some estimates for comparison. Here we observe that our result is in agreement with more recent estimates within two standard-deviations. This indicates our statistical errors are presumably underestimated possibly due to corrections to scaling.

We complete the overview in Table 1 with data from \([23]\). Estimates have been obtained from the long time behavior of the magnetization for the square lattice (sq), \( z = 2.168(5) \), for the triangle (TP), \( z = 2.180(9) \), and for the honeycomb (hc) lattice, \( z = 2.167(8) \), while from damage spreading in short-time the authors quote 2.166(7), 2.164(7) and 2.170(10) for sq, TP and hc lattices.

For \( q = 3 \) Potts model, our study monitoring \( Q \) gives \( z = 2.198(2) \) in the interval \([50, 90]\) with \( Q = 0.82 \). This result agrees with \( z = 2.203(11) \) (Ref. \([13]\)) obtained from the Binder cumulant in Eq. (9), and with the estimate obtained in \([8]\) with HB algorithm from the second moment \( M^{(2)}(t) \) in short-time analysis.

The value in \([8]\) refers to TP lattice, presenting further numerical evidence (comparing \([8]\) and \([9]\)) to the dynamic universality. Reference \([13]\) also presents the value 2.14(3), obtained from Eq. (9), in clear disagreement with 2.203(11) as commented in \([8]\). On the other hand, our estimate from Eq. (11) gives a value in full agreement with the Binder cumulant and collapse data analysis in short time.

The case \( q = 4 \) has been less studied. Our analysis gives \( z = 2.290(3) \) in the interval \([60, 90]\) with \( Q = 0.72 \). Here, we stress the importance of monitoring \( Q \), since we may find values for \( z \) as large as \( z = 2.3483(2) \) in \([10, 200]\) but with unacceptable value, \( Q = 10^{-269} \) or \( z = 2.3532(3)(2) \) in \([10, 100]\) with \( Q = 10^{-202} \).

As a final comment, the suspected \( z \) as been weakly \([28]\) or even independent on \( q \) \([27]\) is not supported by the most recently results presented in Table 1.
Acknowledgements

R. da Silva gratefully acknowledges support by FAPESP (Brazil), and N. Alves by CNPq (Brazil). Thanks are also due to DFMA for computer facilities at IFUSP.

[1] M.E. Fisher and M.N. Barber, Phys. Rev. Lett. 28 (1972) 1516; M.E. Fisher and A.N. Berker, Phys. Rev. B26 (1982) 2507; V. Privman and M.E. Fisher, J. Stat. Phys. 33 (1983) 385; V. Privman and M.E. Fisher, Phys. Rev. B30 (1984) 322.
[2] M.N. Barber, in Phase Transitions and Critical phenomena, v.8. Edited by C. Domb and J.L. Lebowitz, 1973 (Academic Press).
[3] B.I. Halperin, P.C. Hohenberg and S-K. Ma, Phys. Rev. B10 (1974) 139.
[4] M. Suzuki, Prog. Theor. Phys. 58 (1977) 1142.
[5] H.K. Janssen, B. Schaub and B. Schmittmann, Z. Phys. B 73 (1989) 539.
[6] D. Huse, Phys. Rev. B40 (1989) 304.
[7] U. Ritschel and P. Czerner, Phys. Rev. E 55 (1997) 3958.
[8] K. Okano, L. Schülke, K. Yamagishi and B. Zheng, Nucl. Phys. B485 [FS] (1997) 727.
[9] J.-B. Zhang L. Wang, D.-W. Gu, H.-P. Ying and D.-R. Ji, Phys. Lett. A 262 (1999) 226.
[10] Z.B. Li, L. Schülke and B. Zheng, Phys. Rev. Lett. 74 (1995) 3396.
[11] P. Grassberger, Physica A 214 (1995) 547.
[12] M.P. Nightingale, H.W.J. Blöte, Phys. Rev. B62 (2000) 1089; Phys. Rev. Lett. 76 (1996) 4548.
[13] B. Zheng, Int. J. Mod. Phys. B12 (1998) 1419, H.P. Ying, Phys. A, 294 (2001) 111.
[14] C.S. Simões and J.R. Drugowich de Felício, Mod. Phys. Lett. B15 (2001) 487, L. Wang, J. B. Zhang, H. P. Ying and D. R. Ji, Mod. Phys. Lett. B13 (1999) 1011.
[15] P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. 49 (1977) 435.
[16] K. Okano, L. Schülke and B. Zheng, Foundations of Physics 27 (1997) 1739.
[17] Z. Li, L. Schülke, B. Zheng, Phys. Rev. E53 (1996) 2940.
[18] D. Stauffer, Physica A 186 (1992) 197.
[19] C. Münkel, D.W. Heermann, J. Adler, M. Gofman and D. Stauffer, Physica A 193 (1993) 540.
[20] L. Schülke, B. Zheng, Phys. Lett. A 215 (1996) 2940.
[21] W. Press et al., Numerical Recipes (Cambridge University Press, London, 1986).
[22] G.P. Zheng and J.X. Zhang, Phys. Rev. E 58 (1998) R1187.
[23] F.-G. Wang and C.-K. Hu, Phys. Rev. E 56 (1997) 2310.
[24] F. Wang, N. Hatano and M. Suzuki, J. Phys. A: Math. Gen. 28 (1995) 4543.
[25] N. Ito, Physica A 196 (1993) 591.
[26] K. MacIsaac and N. Jan, J. Phys. A: Math. Gen. 25 (1992) 2139.
[27] O.F. de Alcantara Bonfim, Europhys. Lett. 4 (1987) 373.
[28] L. de Arcangelis and N. Jan, J. Phys. A: Math. Gen. 19 (1986) L1179.

Figure Captions:

Figure 1. Time evolution of $F_2(t)$ for 2D three-state Potts model.

Figure 2. Time evolution of $F_2(t)$ for 2D four-state Potts model.
TABLE 1. Dynamic exponent $z$ for 2D Ising model, three and four-state Potts model.

| Reference (year) | Ising      | $q = 3$      | $q = 4$      |
|------------------|------------|--------------|--------------|
| This work        | 2.1565(7)  | 2.198(2)     | 2.290(3)     |
| [12] (2000)      | 2.1667(5)  |              |              |
| [9] (1999)       | 2.153(2)   | 2.191(6)     |              |
| [1] (1998)       | 2.153(4)   | 2.203(11)    |              |
| [13] (1998)      | 2.16(2)    | 2.14(3)      |              |
| [8] (1998)       | 2.137(8)   |              |              |
| [22] (1998)      | 2.166(7)   |              |              |
| [23] (1997)      | 2.155(3)   | 2.196(8)     |              |
| [9] (1997)       | 2.172(6)   |              |              |
| [10] (1995)      | 2.16(4)    |              |              |
| [13] (1993)      | 2.165(10)  |              |              |
| [13] (1992)      | 2.16(2)    |              |              |
| [7] (1987)       | 2.16(5)    | 2.16(4)      | 2.18(3)      |
| [11] (1986)      | 2.43(15)   | 2.36(20)     |              |

1. 2D TP lattice.
2. from scaling collapse (Table 3).
3. applying Eq. (4).
4. from HB algorithm, while $z = 2.137(11)$ and $z = 2.198(13)$, respectively for Ising and $q = 3$ model from Metropolis algorithm.
(Fig.1) 1. Time evolution of $F_2(t)$ for 2D three-state Potts model.

(Fig.2) 2. Time evolution of $F_2(t)$ for 2D four-state Potts model.