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A New Measurement of Dynamic Critical exponent of Wolff Algorithm by Dynamic Finite Size Scaling

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Abstract

In this work we have calculated the dynamic critical exponent z for 2-, 3- and 4-dimensional Ising models using the Wolff's algorithm through dynamic finite size scaling. We have studied time evolution of the average cluster size, the magnetization and higher moments of the magnetization. It is observed that dynamic scaling is independent of the algorithm. In this sense, universality is established for a wide range of algorithms with their own dynamic critical exponents. For scaling, we have used the literature values of critical exponents to observe the dynamic finite size scaling and to obtain the value of z . From the simulation data a very good scaling is observed leading to vanishingly small z values for all three dimensions.

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1 Introduction

One approach to observe the critical behavior of the systems exhibiting second-order phase transitions is to use dynamic scaling which exists in the early stages of the quenching process in the system. Jansen, Schaub and Schmittmann [1] showed that for a dynamic relaxation process, in which a system is evolving according to the dynamics of Model A [2] and is quenched from a very high temperature to the critical temperature, a universal dynamic scaling behavior within the short-time regime exists [3, 4, 5].

For the k^{th} moment of the magnetization of a system, the dynamic finite size relation can be written as [1]

$$M^{(k)}(t, \epsilon, m_0, L) = L^{(-k\beta/\nu)} \mathcal{M}^{(k)}(t/\tau, \epsilon L^{1/\nu}, m_0 L^{x_0}) \quad (1)$$

where L is the spatial size of the system, β and ν are the well-known critical exponents, $\epsilon = (T - T_c)/T_c$ is the reduced temperature, x_0 is a new and independent exponent which is the anomalous dimension of the initial magnetization m_0 , t is the simulation time and τ is the autocorrelation time. For second-order phase transitions autocorrelation time is given as $\tau \sim L^z$, where z is the dynamic critical exponent.

The dynamic finite size scaling requires scaling of the Monte Carlo time as well as the thermodynamic quantities. In many different dynamic finite size scaling studies Eq.(1) has been used in order to calculate the dynamic critical exponent as well as the known critical exponents. In these studies it has been shown that for a given local algorithm, dynamic critical exponents (z) are the same within the error limits for both early stages of the simulation and after the thermal equilibrium is reached [4, 5, 6, 7, 8, 9]. Since using an algorithm with a well-established dynamics

and dynamic critical exponent simplifies the scaling in all studies on the dynamic finite size scaling, the simulation algorithm is chosen as one of the local algorithms. In these studies it is established that the dynamic finite size scaling is independent of the algorithm, in this sense a universality is shown. Similarly, dynamic finite size scaling is tested on first-order phase transitions where the critical behavior is governed by the dimension rather than an exponent. In the case of first-order phase transition, the expected dynamic finite size scaling is also observed [10, 11].

Introduction of cluster algorithms [12, 13] made great improvement in the simulations of magnetic spin systems. Despite the fact that Wolff's algorithm is a modification of the Swendsen-Wang algorithm, Wolff's algorithm [13] exhibits an important difference compared to other algorithms [14]. In local algorithms and the Swendsen-Wang algorithm [12], at each Monte Carlo sweep there is an attempt to update all the spins on the lattice. On the contrary, in Wolff's algorithm only spins belonging to a certain cluster around the seed spin are considered and updated at each Monte Carlo sweep. In equilibrium simulation studies of the systems exhibiting second-order phase transitions, the dynamic critical exponent of the Wolff's algorithm can not be obtained directly from the measured autocorrelation times (τ') since only a fraction of the spins is updated. The efficiency of the Wolff's algorithm is directly related to the average cluster size ($\langle C \rangle$) at a given temperature. Hence, for comparison of the efficiencies between different algorithms and of the Wolff's algorithm, the average cluster size plays an important role. For Wolff's algorithm the ratio between the observed autocorrelation time and the actual autocorrelation time is proportional to the average cluster size.

In the literature the dynamic critical exponents of cluster algorithms are well-studied by using the autocorrelation times of spin systems in thermal equilibrium [12, 13,

14, 15, 16, 17, 18]. The autocorrelation time (τ_W) for the Wolff's algorithm can be obtained by the relation

$$\tau_W = \tau_W' \frac{\langle C \rangle}{L^d} . \quad (2)$$

Considering the finite size scaling behavior of the average cluster size, $\frac{\langle C \rangle}{L^d} \sim L^{2(Y_H-d)}$, the dynamic critical exponent (z) can be calculated. In these studies, the dynamic critical exponent is observed to be much less than that of local algorithms. For measurements done in thermal equilibrium, since the correlation length is as large as the lattice size, and the fluctuations are at their maxima, finite size effects create difficulties in extracting the dynamic critical exponent. Hence for the measurement of the dynamic critical exponent, very good statistics and very large lattices are essential in order to obtain accurate results. For the 2-dimensional Ising model, Wolff showed that $z \sim 0.25$ [15]. More recently, it is suggested that data is consistent with a logarithmic divergence [16], but it is very difficult to distinguish between a logarithm and a small power [17]. For the 3-dimensional case, Tamayo et al. [18] obtained the dynamic critical exponent as $z \sim 0.44(10)$. Wolff (by using energy autocorrelations) have calculated a smaller value of $z = 0.28(2)$ [15]. In 4-dimensions, Tamayo et al. [18] obtained z with a vanishing value. This result is also consistent with the mean-field solution for the Ising model in four and higher dimensions. Recently various cluster algorithms have been tested [19] and compared to the original versions of Swendsen-Wang and Wolff's algorithms. In this study critical exponents of 2- and 3- dimensional Ising models have been observed to be small and the z values are consistent with the above mentioned values.

In the quenching process of the spin systems, very small clusters start to grow until the cluster size reaches the cluster size of the quenching temperature. Hence for the Wolff's algorithm one expects a very low efficiency at the beginning of the simulation and, as the iterations and the cluster sizes are increased, the efficiency

of the algorithm grows. Since the efficiency of the Wolff's algorithm is directly related to the size of the updated clusters, one expects that continuously increasing efficiency can be seen in dynamic processes. Considering the number of updated spins at each iteration, one can estimate the dynamic critical exponent which is characteristic of the time scale of the system. The expectation that the dynamic critical exponent is the same for both the early stages of the simulation and in thermal equilibrium (in analogy with the earlier work [4, 6, 5, 7, 8, 9]) is the main motivation of this work. In this work we aimed to discuss dynamic scaling and to obtain the dynamic critical exponent of the Wolff's algorithm by using dynamic finite size scaling relation (Eq.(1)). We plan to use the known critical exponents. Using these critical exponents and observing a good scaling behavior requires no or very little size corrections.

2 The Model and the Simulations

In this work we have employed 2- 3- and 4-dimensional Ising models described by the Hamiltonian

$$-\beta H = K \sum_{\langle ij \rangle} S_i S_j . \quad (3)$$

Here, $\beta = 1/kT$ and $K = J/kT$, where k is the Boltzmann constant, T is the temperature and J is the magnetic interaction between the spins. In the Ising model the spin variables take the values $S_i = \pm 1$.

In order to discuss time evolution of the Wolff's algorithm, we have selected a range of thermodynamic quantities. Equation (1) implies that the magnetization ($\langle S \rangle$) and its higher moments are good candidates for observing dynamic finite size scaling behavior. For this reason we have considered $\langle S \rangle$, $\langle S^2 \rangle$ and $\langle S^4 \rangle$ where,

the n^{th} moment of the magnetization is given by

$$\langle S^n \rangle = \frac{1}{L^d} \langle (\sum_i S_i)^n \rangle . \quad (4)$$

The efficiency of the Wolff's algorithm is related to the average cluster size ($\langle C \rangle$), with

$$\langle C \rangle = \frac{1}{N_c} \sum_i^{N_c} \frac{1}{L^d} (C_i), \quad (5)$$

and it has been considered in our calculations. For finite size lattices, during the quenching process, very small clusters grow to the lattice size as the number of iterations increases. The rate of the cluster growth depends on the algorithm as well as the quenching temperature. More efficient the algorithm, faster the system reaches the equilibrium values. In a single-cluster Wolff's algorithm, one must consider the average number of updated spins, or the percentage of them, considering total volume. Since the number of updated spins increases at each iteration (as the system approaches the quenching temperature), repetitive calculations yield an average cluster size per iteration. Consequently in calculating the autocorrelation time, one considers the number of updated spins per iteration. In our calculations, consistent with Eq.(1) both moments of spin (Eq.(4)) and the average cluster size (Eq.(5)) are calculated as functions of iteration number. In the time-dependent forms of the above quantities, Eq.(4) and Eq.(5) take the form

$$\langle S^n \rangle (t) = \frac{1}{L^d} \langle (\sum_i S_i(t))^n \rangle \quad (6)$$

and

$$\langle C \rangle (t) = \frac{1}{N_c} \sum_i^{N_c} \frac{1}{L^d} (C_i(t)). \quad (7)$$

As it is mentioned above, in this algorithm efficiency varies and effective time changes (during the quenching process) are related to the quantities $\langle C \rangle (t)$ and $\langle S^2 \rangle (t)$.

All of the above quantities have their own anomalous dimensions and using such quantities (in order to obtain dynamic critical exponent) one may expect some ambiguities due to correction to scaling. Since our calculations are done in the early stages of the simulations, the correlation length is expected to be less than the lattice size; hence use of infinite lattice critical exponents in Eq.(1) can be sufficient to explain the critical behavior of the system. For this reason, critical exponents are taken as the Onsager solution for the 2-dimensional Ising model. For the 3-dimensional case, the critical exponent values are taken from the literature [20, 21]. The 4-dimensional case is the critical dimension for the Ising model, and above 4-dimension the critical exponents are the mean-field critical exponents. In the 4-dimensional case, the model possesses the mean-field critical exponents with logarithmic corrections. In our calculations no corrections are assumed to be necessary, since during the early stages of the quenching process the correlation length remains smaller than the lattice size.

In this work we have studied 2-, 3- and 4-dimensional Ising models evolving in time by using Wolff's algorithm. We have prepared lattices with vanishing magnetization and total random initial configurations are quenched at the corresponding infinite lattice critical temperature. We have used the lattices $L = 256, 384, 512, 640$, $L = 32, 48, 64, 80$ and $L = 16, 20, 24$, for 2-, 3- and 4-dimensional Ising models, respectively. For each dimension and size, iterations are continued until the observed quantity reaches a plateau which finalizes the evolution during the quenching process. In order to observe the plateau, the number of iterations has been chosen depending on the volume of the system. For each lattice size, initial configurations are created depending on the lattice size, but on average sixteen bins of eight to thirty thousand runs, sixteen bins of four to thirty five thousand runs and sixteen bins of five to twenty five thousand runs have been performed for 2-, 3-, and 4- di-

mensional Ising models for varying lattice sizes, respectively. Errors are calculated from the average values for each iteration obtained in different bins. Both the average cluster size and susceptibility have the same anomalous dimension, hence in obtaining the autocorrelation time (τ) from the observed behavior of the dynamic variable, one can replace $\langle S^2 \rangle$ by $\langle C \rangle$. In our simulation data both quantities have been used in order to scale time variable for the scaling of average cluster size ($\langle C \rangle$) and moments of the magnetization ($\langle S^n \rangle$).

In Figure 1 we have presented the magnetization data ($\langle S \rangle(t)$) before and after the dynamic finite size scaling for 2-dimensional Ising model for the lattice sizes considered. Figure 1(a) shows the time evolution of $\langle S \rangle(t)$ during the relaxation of the system until a plateau is reached. It is seen from this figure that the time to reach the plateau is proportional to the linear size (L) of the system. As it is seen from Eq.(1), in the dynamic finite size scaling, $\langle S \rangle(t)$ scales with factor $L^{(Y_H-d)}$ and, for the algorithms in which all spins are checked for updating the Monte Carlo time, t scales as t/L^z . For Wolff's algorithm, one obtains crossing magnetization curves but they do not scale as expected. Since one cluster is updated at each iteration, there is a need to use the average number of updated spins at each iteration, which is a factor related to $\langle C \rangle(t)$ or $\langle S^2 \rangle(t)$. If the time is not scaled by the average cluster size, using only L^z as a factor shifts the curves towards each other and curves crosses at some point, but scaling can not be observed. Figure 1(b) and (c) show the scaling of Monte Carlo time axis by using $\langle C \rangle(t)$ and $\langle S^2 \rangle(t)$ as the factor of scaling, respectively. The fluctuations in Figure 1(c) are smaller, compared to the fluctuations in Figure 1(b). In the following figures we have presented the scaling using $\langle S^2 \rangle(t)$ as the factor for time scaling. Magnetization, second and fourth moments of the magnetization, as well as the average cluster size show the same scaling behavior in all dimensions; but in order to avoid repetitive

figures, we have chosen $\langle S \rangle (t)$ as an example. Only for the 2-dimensional case we have presented $\langle S^2 \rangle (t)$ in Figure 2 for comparison.

Figure 2 shows the dynamic quantity $\langle S^2 \rangle (t)$ for the 2-dimensional Ising model for the same lattice sizes given in Figure 1. Figure 2(a) shows the simulation data and Figure 2(b) shows the scaling by use of $\langle S^2 \rangle (t)$ as the factor in time scaling. As observed for $\langle S \rangle (t)$, scaling using $\langle C \rangle (t)$ and $\langle S^2 \rangle (t)$ as the factor in time scaling results in the same value of the dynamic critical exponent z . As it is mentioned above the average cluster size and the moments of the magnetization are calculated as averages at each iteration and these quantities are time-dependent during the relaxation process. In Figure 2 same factor $\langle S^2 \rangle$ appears on both the vertical and horizontal axes. Since t increases linearly, the curve in Figure 2 is linear. This also shows that the scaling is very good. Figures 3 and 4 show the simulation data and the dynamic scaling for $\langle S \rangle (t)$ for 3- and 4- dimensional Ising models, respectively. In both figures a) shows the time evolution of $\langle S \rangle (t)$ and b) shows $\langle S \rangle (t)$ after dynamic scaling.

The values of the dynamic critical exponent z for 2-, 3- and 4- dimensional Ising models are given in Table 1. In this table z' is the measured dynamic critical exponent as an average of the exponents calculated for $\langle S \rangle (t)$, $\langle S^2 \rangle (t)$, $\langle S^4 \rangle (t)$ and $\langle C \rangle (t)$. The dynamic critical exponent z is calculated using Eq.(1) by considering the number of spins updated at each iteration of the Monte Carlo simulation and by using the scaling relation for time ($\tau \sim L^z$). It is a simple relation in the form

$$z = z' - (2Y_H - d). \quad (8)$$

In this calculation, Y_H is taken as $Y_H = \frac{15}{8}$ (Onsager solution), $Y_H = 2.4808$ [20, 21],

$Y_H = 3$ (mean-field solution) for the 2-, 3- and 4- dimensional models respectively.

The errors in the values of z' are obtained from the largest fluctuations in the simulation data for $\langle S \rangle(t)$, $\langle S^2 \rangle(t)$, $\langle S^4 \rangle(t)$ and $\langle C \rangle(t)$. By considering the values of the dynamic critical exponents as the averages obtained using scaling of these four quantities and the small errors in z values, one can see from Table 1 that the scaling behavior is quite similar for these four quantities.

3 Conclusion

In this work we have observed the dynamic finite size scaling for 2-, 3- and 4- dimensional Ising models. In previous works [4, 5, 6], the dynamic finite size scaling of the Ising model has been tested by using Metropolis and the heat bath algorithms. Both algorithms are local algorithms, hence the observed similar behavior is expected. In our work we have shown for the first time that dynamic finite size scaling, exhibiting a universal behavior, is valid for use with cluster algorithms, and that both local and global algorithms show dynamic finite size scaling with their own dynamic critical exponents. In this work we have calculated the dynamic critical exponent of Wolff's cluster algorithm for 2-, 3- and 4- dimensional Ising models using dynamic scaling. In the literature, for all three dimensions, small dynamic critical exponents are obtained [12, 13, 14, 15, 16, 17, 18], but further studies of the data suggest that for all three dimensions the dynamic critical exponent of the Ising model can be considered as zero. The measurement of the dynamic critical exponent in thermal equilibrium is extremely difficult since the correlation length around the phase transition point is as large as the size of the lattice. In dynamic finite size scaling, since the correlation length remains smaller than the lattice size, it is expected that statistically independent configurations lead to better statistics since there is no finite size effects. In our calculations, we have observed that our

data is consistent with vanishing dynamic critical exponent. Despite the fact that obtaining good statistics is extremely time consuming for large lattices, data is free of errors due to finite size effects. One can see from the results of dynamic scaling that scaling is very good and the errors are very small, hence this method is a good candidate to calculate the dynamic critical exponent for any spin model and for any algorithm.

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Table Captions

Table 1. The values of measured (z') and calculated (z) dynamic exponents for 2-, 3- and 4-dimensional Ising models.

Figure Captions

Figure 1 a) Magnetization data $\langle S \rangle(t)$ for 2-dimensional Ising Model for linear lattice sizes $L = 256, 384, 512, 640$ as a function of simulation time t , b) scaling of $\langle S \rangle(t)$ data given in a) using $\langle C \rangle(t)$ as the factor in time scaling, c) scaling of $\langle S \rangle(t)$ data given in a) using $\langle S^2 \rangle(t)$ as the factor in time scaling.

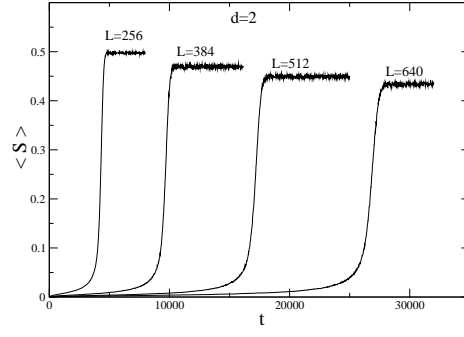
Figure 2 a) Simulation data for $\langle S^2 \rangle(t)$ as a function of simulation time t for 2-dimensional Ising model for linear lattice sizes $L = 256, 384, 512, 640$, b) scaling of $\langle S^2 \rangle(t)$ data given in a) using $\langle S^2 \rangle(t)$ as a factor in time scaling.

Figure 3. Simulation data for $\langle S \rangle(t)$ as a function of simulation time t for 3-dimensional Ising model for linear lattice sizes $L = 32, 48, 64, 80$, b) scaling of $\langle S \rangle(t)$ data given in a) using $\langle S^2 \rangle(t)$ as the factor in time scaling.

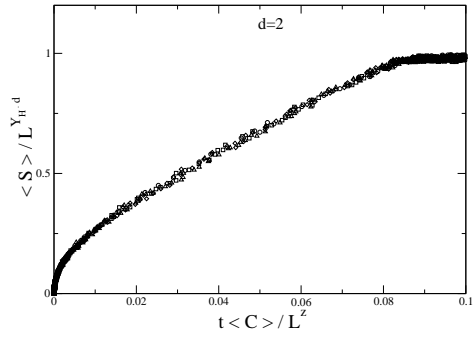
Figure 4. Simulation data for $\langle S \rangle(t)$ as a function of simulation time t for 4-dimensional Ising model for linear lattice sizes $L = 16, 20, 24$, b) scaling of $\langle S \rangle(t)$ data given in a) using $\langle S^2 \rangle(t)$ as the factor in time scaling.

d	z'	$z = z' - (2Y_H - d)$
2	1.73 ± 0.05	0.02 ± 0.05
3	1.94 ± 0.09	0.02 ± 0.09
4	2.13 ± 0.19	-0.13 ± 0.19

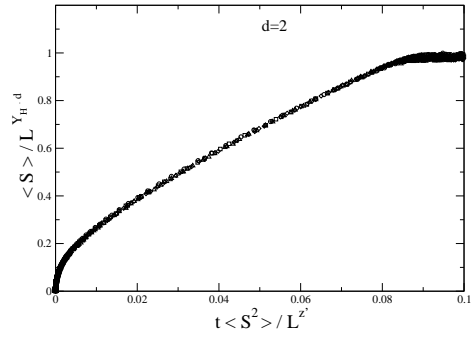
Table 1.



(a)



(b)



(c)

Figure 1:

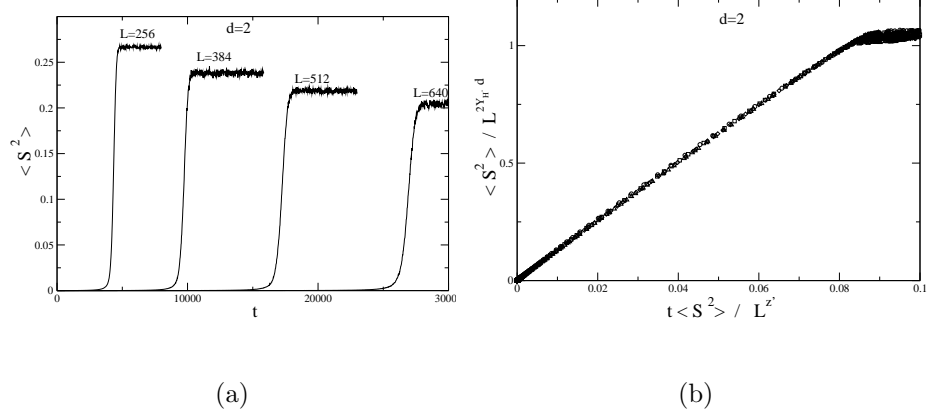


Figure 2:

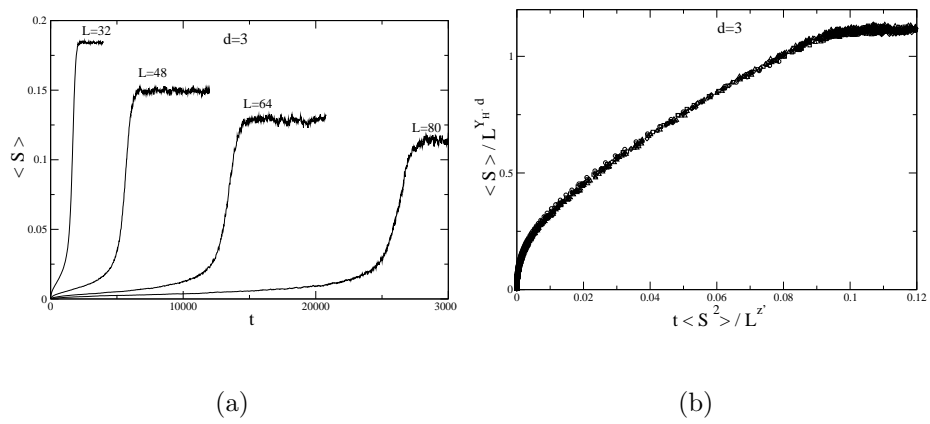


Figure 3:

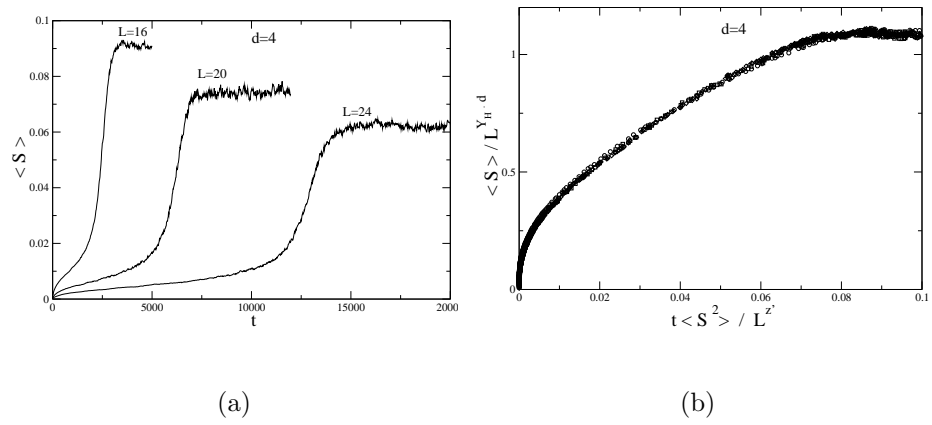


Figure 4: