

Large-scale Simulation of the Two-dimensional Kinetic Ising Model

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Abstract

We present Monte Carlo simulation results for the dynamical critical exponent z of the two-dimensional kinetic Ising model using a lattice of size $10^6 \times 10^6$ spins. We used Glauber as well as Metropolis dynamics. The z -value of 2.16 ± 0.005 was calculated from the magnetization and energy relaxation from an ordered state towards the equilibrium state at T_c .

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The precise numerical value of the dynamical critical exponent z , which characterizes the critical slowing down at a second-order phase-transition [1], has not been conclusively calculated. This note presents an effort to calculate the value of z using a system of unprecedented size.

In simulations specific attention has been given to calculate z for the Ising model because of its simplicity and its model character as a representant for a universality class. The Ising model is defined by the Hamiltonian

$$\mathcal{H}_{\text{Ising}}(s) = -J \sum_{\langle ij \rangle} s_i s_j \quad , \quad s_i = \pm 1 \quad (1)$$

where $\langle ij \rangle$ are nearest-neighbour pairs of lattice sites. The exchange coupling J is restricted to be positive (ferro-magnetic).

The dynamics of the system is specified by the transition probability of the Markov chain which will be realized by a Monte Carlo algorithm [3, 4, 5]. We used two transition probabilities

- **Metropolis** $P(s_i \rightarrow s'_i) = \min\{1, \exp\{-\Delta E\}\}$
- **Glauber** $P(s_i \rightarrow s'_i) = \frac{1}{2}\{1 - s_i \tanh(E_i/k_b T)\}$, $E_i = J \sum_{\langle i,j \rangle} s_j$

Time t in this context is measured in Monte Carlo steps per spin. One Monte Carlo step (MCS) per lattice site, i.e. one sweep through the entire lattice comprises one time unit. Neither magnetization nor energy are preserved in the model.

Our system size, on which the analysis will be based on, was $10^6 \times 10^6$. A new algorithm [9] was employed to simulate this very large lattice. Basically, instead of storing one lattice configuration and iterating in time we store only part of the lattice configuration at all time steps and iterate through the lattice. Thus we were able to reduce the memory requirements from approximately 100 GB to 20 MB.

It is generally believed that one can calculate z from the relaxation into equilibrium. In the theory of dynamical critical phenomena [10], critical slowing down is expressed as the divergence of the linear relaxation time $\tau_M^{(l)}$ of the order parameter M (the magnetization) as one approaches criticality ($\theta \rightarrow 0^+$ with $\theta = (T - T_c)/T_c$)

$$\tau_M^{(l)} \sim \theta^{-\nu z}, \quad (2)$$

where \sim stands for asymptotic proportionality and ν is the static critical exponent of the correlation length ξ . The exponent z is called the dynamical critical exponent. In analogy with finite-size scaling in the theory of static critical phenomena one may infer the following finite-size scaling relation for the linear relaxation time

$$\tau_M^{(l)} \sim L^z \tilde{f}(\theta L^{\frac{1}{\nu}}), \quad (3)$$

where $\tilde{f}(z')$ is a scaling function regular at $z' = 0$. Relation (3) is valid for $L \gg 1$ and $\theta \ll 1$.

A value for z can be obtained for very large system sizes from the relaxation of the magnetization into equilibrium from another equilibrium state [2]. If the system size tends to infinity and we are at criticality, the above scaling relaxation implies

$$M(t) \sim t^{-\beta/\nu z} \quad . \quad (4)$$

For the two-dimensional Ising model, the static critical exponents $\beta = 1/8$ and $\nu = 1$ as well as the critical temperature $T_c = 1/(\frac{1}{2} \log(1 + \sqrt{2}))$ are exactly known.

Two independent calculations were carried out by groups from Heidelberg using Metropolis dynamics and checkerboard updates and Cologne using Glauber dynamics and typewriter update.

Results from the Heidelberg group During the course of our simulation we have monitored the magnetization $M = (1/L^2) \sum s_i$ as a function of the number of sweeps t (MCS) through the lattice. We averaged over two independent configurations (cf. implementation of the algorithm in [9]). Table 1 shows the raw data.

To determine the value of z from our data we calculated the slope in a log-log plot using

$$\frac{1}{z_i} = -8 \frac{\log(m_i) - \log(m_{i-1})}{\log(i) - \log(i-1)}$$

and grouped data points for a linear least-square fit. Plotted in figure 1 is the slope and the first and second order intercepts of the linear fits to these slopes for $1/t \rightarrow 0$ against the inverse time. We obtain a value of $z \approx 2.15 \pm 0.02$. This value is in agreement with results from recent series expansion calculations [11, 12], damage spreading simulations [13] as well as other large scale simulates [6, 7].

Results from the Cologne group Shocked by the huge lattices from the Heidelberg group, we slightly modified and adapted the step method presented in [9] to typewriter update, which was used in our previous calculations with full lattice storage [8]. The use of typewriter update instead of checkerboard update used by the Heidelberg group, simplified this method considerable. Thereby and with optimization techniques similar to multi-spin coding our program reached 3.8 MUpdate/s on an IBM RS6000/990 (Power/2). With this program we calculated 50 iterations of a $10^6 \times 10^6$ lattice on an 8 processor IBM SP1 (Glauber dynamic, user time 31 days). Beside the magnetization the energy was obtained as well. Table 2 shows the data.

Similar to the magnetization one can also calculate the exponent z from the relaxation of the energy [7]:

$$E(t) - E_{\text{critical}} \sim t^{-(1-\alpha)/\nu z} = t^{-1/z} \quad (\text{in two dimensions}) \quad (5)$$

For the determination of the value of z we calculated an arithmetic mean value of some data points. The number of gathered data points is calculated by $\lceil \text{iteration}/5 \rceil$ Figure 2 shows this and the first order intercepts. The magnetization data z_{Mag} as well as the energy data z_{Energy} lead to a z -value of 2.16 ± 0.005 for $1/t \rightarrow 0$.

| T | m_1 (Metropolis) | m_2 (Metropolis) |
|----|--------------------|--------------------|
| 0 | 1.00000000 | 1.00000000 |
| 1 | 0.92097430 | 0.92097417 |
| 2 | 0.86321233 | 0.86321220 |
| 3 | 0.83255023 | 0.83255007 |
| 4 | 0.81309636 | 0.81309770 |
| 5 | 0.79918281 | 0.79918239 |
| 6 | 0.78845203 | 0.78845225 |
| 7 | 0.77976347 | 0.77976351 |
| 8 | 0.77248408 | 0.77248426 |
| 9 | 0.76623362 | 0.76623401 |
| 10 | 0.76076646 | 0.76076750 |

Table 1: *Raw data for the calculation from the Heidelberg group.*

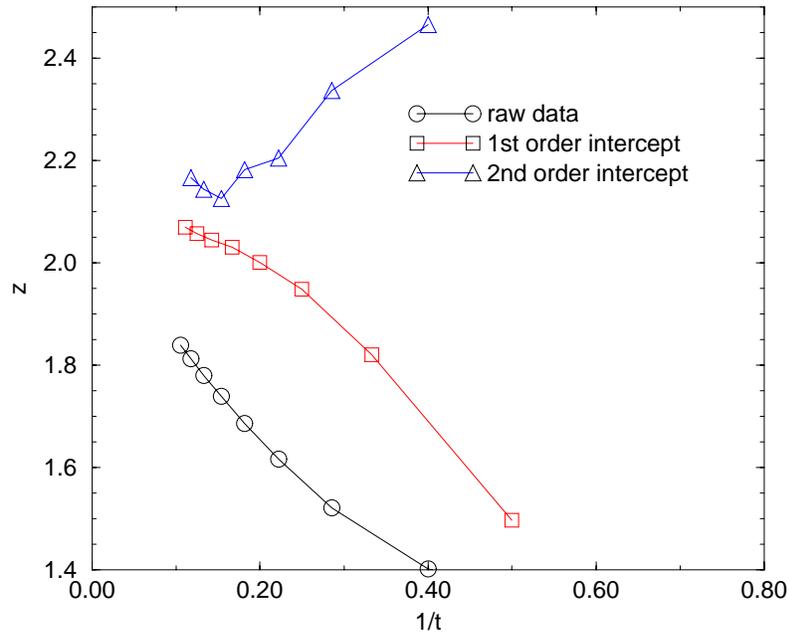


Figure 1: *Plot of the critical exponent z vs. $1/t$ (Heidelberg group).*

| T | m (Glauber) | e (Glauber) | T | m (Glauber) | e (Glauber) | T | m (Glauber) | e (Glauber) |
|----|-------------|-------------|----|-------------|-------------|----|-------------|-------------|
| 0 | 1.00000000 | 0.00000000 | 17 | 0.78287989 | 0.49666620 | 34 | 0.75161947 | 0.52225099 |
| 1 | 0.92387181 | 0.07612802 | 18 | 0.78024367 | 0.49915815 | 35 | 0.75034603 | 0.52312965 |
| 2 | 0.88930745 | 0.27878672 | 19 | 0.77775922 | 0.50144418 | 36 | 0.74910920 | 0.52396988 |
| 3 | 0.86826671 | 0.35298481 | 20 | 0.77541236 | 0.50355210 | 37 | 0.74790926 | 0.52477812 |
| 4 | 0.85343942 | 0.39143993 | 21 | 0.77318752 | 0.50550180 | 38 | 0.74674372 | 0.52555236 |
| 5 | 0.84208738 | 0.41546570 | 22 | 0.77107242 | 0.50731384 | 39 | 0.74561180 | 0.52629785 |
| 6 | 0.83292949 | 0.43221206 | 23 | 0.76905750 | 0.50900323 | 40 | 0.74450920 | 0.52701310 |
| 7 | 0.82527573 | 0.44472865 | 24 | 0.76713498 | 0.51058358 | 41 | 0.74343671 | 0.52770277 |
| 8 | 0.81871664 | 0.45453473 | 25 | 0.76529694 | 0.51206432 | 42 | 0.74238953 | 0.52836585 |
| 9 | 0.81298342 | 0.46248268 | 26 | 0.76353643 | 0.51345741 | 43 | 0.74136891 | 0.52900757 |
| 10 | 0.80789697 | 0.46910024 | 27 | 0.76184711 | 0.51476957 | 44 | 0.74037224 | 0.52962886 |
| 11 | 0.80333031 | 0.47472005 | 28 | 0.76022277 | 0.51601052 | 45 | 0.73940143 | 0.53022785 |
| 12 | 0.79918884 | 0.47957117 | 29 | 0.75865931 | 0.51718485 | 46 | 0.73845357 | 0.53080592 |
| 13 | 0.79540222 | 0.48381554 | 30 | 0.75715202 | 0.51830041 | 47 | 0.73752722 | 0.53136430 |
| 14 | 0.79191812 | 0.48756875 | 31 | 0.75569749 | 0.51936114 | 48 | 0.73662030 | 0.53190743 |
| 15 | 0.78869300 | 0.49091859 | 32 | 0.75429320 | 0.52036977 | 49 | 0.73573540 | 0.53243573 |
| 16 | 0.78568804 | 0.49393126 | 33 | 0.75293487 | 0.52133128 | 50 | 0.73486859 | 0.53294310 |

Table 2: Raw data for the calculation by the Cologne group.

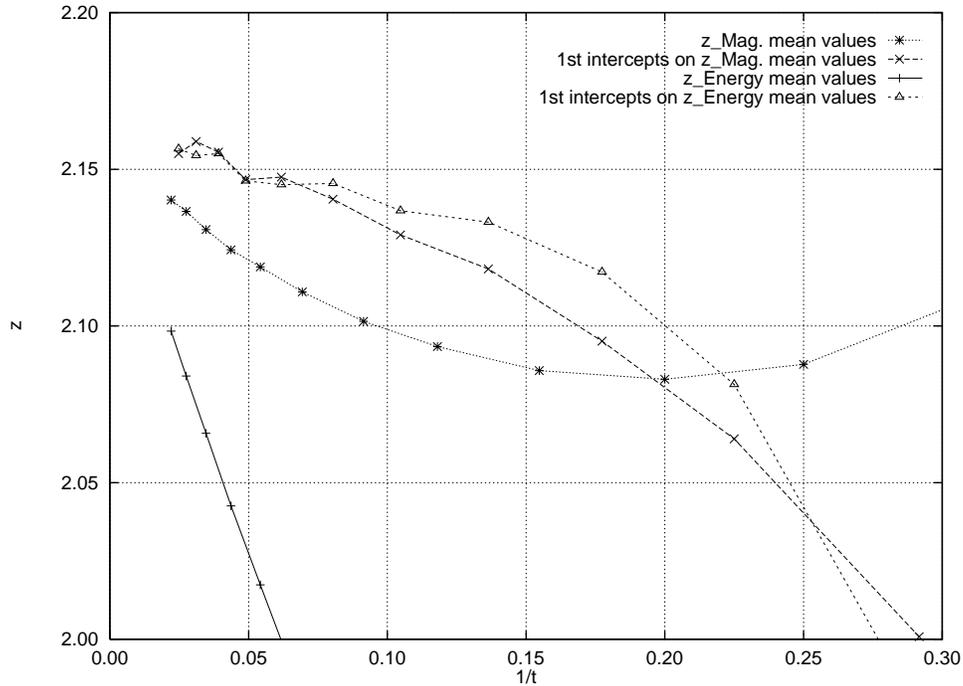


Figure 2: Plot of the critical exponent z vs. $1/t$ (Cologne group).

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