## Critical slowing down of the two-dimensional kinetic Ising model with Glauber dynamics

Jian Wang

Centre for the Physics of Materials and Department of Physics, McGill University, Rutherford Building, 3600 Rue Université, Montréal, Québec, Canada H3A 2T8 (Received 28 May 1991)

We calculated the autorelaxation time for the two-dimensional kinetic Ising model with Glauber dynamics using a high-temperature series-expansion technique. The series is analyzed using a differential Padé approximant. The exponent z for critical slowing down is found to be  $z = 2.207 \pm 0.008$ .

The kinetic Ising model with Glauber dynamics has been the subject of extensive studies for many years. The dynamical critical exponent z characterizing the critical slowing down has been calculated using various methods, including the Monte Carlo simulation,  $^{1-4}$  the Monte Carlo renormalization-group study,  $5^{-8}$  and the high-temperature series-expansion method.<sup>9,10</sup> Different values of z have been reported ranging from 2 to 2.24 in two dimensions. For instance, the recent Monte Carlo simulation on a  $10\,000 \times 10\,000$  square lattice by Mori and Tsuda<sup>3</sup> obtained  $z = 2.076 \pm 0.005$ . Monte Carlo finite-size scaling by Ito, Taiji, and Suzuki<sup>2</sup> predicted  $z = 2.132 \pm 0.008$ . The theoretical  $\epsilon$ -expansion prediction by Bausch et al.<sup>11</sup> based on interpolating the  $\epsilon$ -expansion results near d = 1 and 4 is z = 2.126. The series analysis by Racz and Collins<sup>12</sup> based on the twelfth-order high-temperature series<sup>10</sup> of the linear relaxation time gave  $z = 2.125 \pm 0.01$ . Most recent calculation of z by Poole and Jan<sup>13</sup> using the method of damage spreading obtained  $z = 2.24 \pm 0.04$ . Different conjectures have been proposed, e.g., z = 2 (Ref. 14 and z = 17/8.<sup>12</sup> Since the exponent z characterizes the divergence of the relaxation time near the critical point  $T_c$ , this makes the sampling near  $T_c$  very inefficient for numerical simulations and hence it is very difficult to calculate this exponent. While most studies used the Monte Carlo simulation method, little progress has been made on the calculation of z using the high-temperature series-expansion method since the work of Yahata and Suzuki<sup>9,10</sup> and Racz and Collins<sup>12</sup> in 1970s. This is because the series calculation is so complicated that only until recently did people start to retackle it using faster computers and better algorithms. Recently, Rogiers and Indekeu<sup>15</sup> have extended the existing series for the autorelaxation time to the eleventh order and obtained  $z = 2.34 \pm 0.03$ , which is higher than other recent estimates probably due to the shortness of the series. In this paper we have calculated the series for the autorelaxation time up to the seventeenth order on a square lattice which enables us to extract a very accurate exponent z from the series. We analyze the series using the differential Padé approximant and obtain the dynamical critical exponent  $z = 2.207 \pm 0.008$ . Therefore, the dynamical critical exponent predicted by our seriesexpansion method is higher than most of the simulations. For the kinetic Ising model, the Hamiltonian can be written as

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{1}$$

where J is the coupling constant. The time evolution of probability  $P(\{\sigma\}, t)$  of a spin configuration is governed by the master equation

$$\partial_t P(\{\sigma\}, t) = -\sum_j W_j(\{\sigma\}) P(\{\sigma\}, t) + \sum_j W_j(\{\sigma\}, -\sigma_j) P(\{\sigma\}, -\sigma_j, t), \qquad (2)$$

where the transition probability W obeys "detailed balance"

$$W_j(\{\sigma\})P_{\text{eq}}(\{\sigma\}) = W_j(\{\sigma\}, -\sigma_j)P_{eq}(\{\sigma\}, -\sigma_j).$$
(3)

Here  $P_{eq} = e^{-\beta H}/Tre^{-\beta H}$  is the equilibrium probability distribution. As usual, W is assumed to be

$$W_j(\{\sigma\}) = \frac{1}{2} \left[ 1 - \sigma_j \tanh\left(K \sum_{j(k)} \sigma_k\right) \right], \qquad (4)$$

where the summation is over the nearest neighbors of site k and  $K = \beta J$ .

The autorelaxation time  $\tau_A$  can be defined as

$$\tau_A = \int \langle \sigma_1(0)\sigma_1(t) \rangle_{\rm av} dt, \qquad (5)$$

where  $\langle A \rangle_{\rm av} = \sum_{\{\sigma\}} AP_{\rm eq}(\{\sigma\})$  is the thermal average. From the scaling theory,<sup>9,16–18</sup>

$$\tau_A \sim |T - T_c|^{-\Delta_A} \tag{6}$$

with

869

$$\Delta_A = \nu z - 2\beta,\tag{7}$$

where  $\nu$  and  $\beta$  are static critical exponents for the correlation length and the order parameter, respectively. De-

<u>47</u>

$$\tau_A = \left\langle \sigma_1 \frac{1}{L} \sigma_1 \right\rangle_{\rm av}.$$
(8)

In order to calculate  $\tau_A$ , we decompose the operator L as<sup>9,10</sup>

$$L = L_0 - L_a - L_c, (9)$$

where

$$L_0 = \frac{1}{2} \sum_k (1 - P_k), \tag{10}$$

$$L_a = \frac{a}{2} \sum_k \sum_{l(k)} \sigma_l \sigma_k (1 - P_k), \qquad (11)$$

$$L_{c} = \frac{c}{2} \sum_{k} \sum_{l(k)} \sigma_{l_{1}} \sigma_{l_{2}} \sigma_{l_{3}} \sigma_{k} (1 - P_{k}), \qquad (12)$$

and

$$a = \frac{1}{8}(2\tanh 2K + \tanh 4K),\tag{13}$$

$$c = -\frac{1}{8}(2\tanh 2K - \tanh 4K). \tag{14}$$

Here again the summation over l(k) refers to the nearest neighbor of site k. Expanding 1/L in terms of  $L_a$  and  $L_c$  the autorelaxation time can be expressed as a power series of  $v = \tanh K$ . Note that  $L_c$  acting on  $\sigma_1$  will generate a three-spin configuration. Hence in the seriesexpansion calculation we basically generate all spin configurations and calculate the multispin correlations. A more detailed description of how to generate the series can be found in the paper by Yahata and Suzuki.<sup>9,10</sup>

The difficulty in this calculation is that  $L_c$  generates a huge amount of multispin configurations and most of them do not contribute to the series; in other words, they are higher-order terms. For example, up to the eleventh order in our series for the autorelaxation time there are about 10000 topological inequivalent configurations. Only one-tenth contribute to the series. Therefore, we run into a memory problem as we go to higher order. To deal with this problem, we used the method of self-avoiding graphs outlined in Ref. 9 to calculate the lowest-order coefficient of the multispin correlation function. In this way, we can eliminate almost all diagrams which do not contribute to the series during the diagram generation. Specifically, we apply  $L_a$  and  $L_c$  to each configuration in a previous list to generate next-order configuration and collect all topologically inequivalent configurations as a next-order list. If the lowest-order coefficient of the multispin correlation for a configuration is higher than a predetermined order N, it will be excluded from the list. We use this method recursively until we reach the order N. The backtracking technique has been tried to save memory. We found that it is too time consum-

TABLE I. The series for the autorelaxation time.

n	c(n)	
0	1.0	
2	8.0	
4	64.0	
6	493.3333	
8	3400.2963	
10	23870.7819	
12	156974.6524	
14	1049275.3347	
16	6721093.4149	

ing that we cannot even calculate the autorelaxation time up to the eleventh order. Once all spin configurations are generated, we have to calculate the multispin correlation. We did not use the method of self-avoiding graphs of Ref. 9 because it is very time consuming and hard to program. Instead, we used the method of Ref. 10 which is based on the equation of detailed balance. The advantage of this method is that it expresses the multispin correlation of a spin configuration in terms of its next-order configuration and therefore makes it very easy to check the series. To check our series, we have calculated the quantity  $<\sigma_1 \sum_j \sigma_j >_{av}$  which can be easily obtained in our series calculated up to the fifteenth order. This series has been calculated up to the fifteenth order by Domb and Sykes.<sup>19</sup> Our result agrees with them.

Using this method, we have calculated the series for the autorelaxation time up to the seventeenth order. For the autorelaxation series the odd terms are zero, we hence obtained nine nonzero coefficients which are listed in Table I. Note that the tenth-order coefficient of our series differs from that of Rogiers and Indekeu by 4%. We believe that our series is more reliable. We have analyzed the series using a differential Padé approximant<sup>20</sup> (where we did not explicitly consider the correction to scaling). The pole-residue plot for the autorelaxation time series is shown is Fig. 1. Since we know the critical point of the two-dimensional Ising model  $v_c = \sqrt{2} - 1$ , the exponent z can be obtained by reading off from the plot. We have



FIG. 1. The differential Padé pole-residue plot. In the figure we plot the differential Padé approximants based on 12, 14, and 16 terms of the series expansions. Here the critical point and the critical exponent correspond to  $v_c^2$  and  $\Delta_A$ , respectively.

 $z = 2.207 \pm 0.008$ , where the error bar comes from fitting the data. This result is different from most of the simulation results which are around z = 2.13. However, it does agree with a recent simulation by Poole and Jan.<sup>13</sup> Although our series for the autorelaxation time has only nine nonzero terms, we believe that this series behaves better than that of the linear relaxation time with twelfth order.<sup>9,10</sup> This is because the twelfth-order series for the linear relaxation time can only include six-spin correlations, whereas our seventeenth-order series for the autorelaxation time can probe eight-spin correlations.

In summary, we have calculated the series for the au-

- <sup>1</sup>S. Tang and D. P. Landau, Phys. Rev. B **36**, 567 (1987).
   <sup>2</sup>N. Ito, M. Taiji, and M. Suzuki, J. Phys. Soc. Jpn. **56**, 4218 (1987).
- <sup>3</sup>M. Mori and Y. Tsuda, Phys. Rev. B 37, 5444 (1988).
- <sup>4</sup>O. F. de Alcantara Bonfim, Europhys. Lett. 4, 373 (1987).
- <sup>5</sup>S. L. Katz, J. D. Gunton, and C. P. Liu, Phys. Rev. B **25**, 6008 (1982).
- <sup>6</sup>J. K. Williams, J. Phys. A 18, 49 (1985).
- <sup>7</sup>L. de Arcangelis and N. Jan, J. Phys. A **19**, L1179 (1986).
- <sup>8</sup>M. D. Lacasse, J. Vinals, and M. Grant (unpublished).
- <sup>9</sup>H. Yahata and M. Suzuki, J. Phys. Soc. Jpn. **27**, 1421 (1969).
- <sup>10</sup>H. Yahata, J. Phys. Soc. Jpn. **30**, 657 (1971).
- <sup>11</sup>R. Bausch, V. Dohm, H. K. Janssen, and R. K. P. Zia, Phys. Rev. Lett. **47**, 1837 (1981).

to relaxation time up to seventeenth order. The dynamical critical exponent is found to be  $z = 2.207 \pm 0.008$  which is different from most of the simulation results.

I would like to thank H. Guo, M. Grant, and M. Lacasse for useful discussions. I would also like to thank A. J. Guttmann for discussion about series analysis. This work was supported by the Natural Sciences and Engineering Research Council of Canada, le Fonds pour la Formation de Chercheurs et l'Aide à la Recherche de la Province du Québec.

- <sup>12</sup>Z. Racz and M. F. Collins, Phys. Rev. B 13, 3074 (1976).
- <sup>13</sup>P. H. Poole and N. Jan, J. Phys. A **23**, L453 (1990).
- <sup>14</sup>E. Domany, Phys. Rev. Lett. **52**, 871 (1984).
- <sup>15</sup>J. Rogiers and J. O. Indekeu, Phys. Rev. B **41**, 6998 (1990).
- <sup>16</sup>B. I. Halperin and P. C. Hohenberg, Phys. Rev. **177**, 952 (1969).
- <sup>17</sup>P. C. Hohenberg and B. I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).
- <sup>18</sup>E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973).
- <sup>19</sup>C. Domb and M. F. Sykes, J. Math. Phys. 2, 63 (1961).
- <sup>20</sup>J. -H. Chen and M. E. Fisher, J. Phys. A 14, 2553 (1981). Also see A. J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1989), Vol. 13, Chap. 1.