Critical dynamics of the two-dimensional kinetic Ising model: High-temperature series analysis of the autorelaxation time

J. Rogiers
Instituut voor Theoretische Fysika en Monitoraat Wetenschappen, Katholieke Universiteit Leuven, B-3030 Leuven, Belgium and Faculté Polytechnique, Université de Lubumbashi, Zäire

J. O. Indekeu
Laboratorium voor Molekuulfysika, Katholieke Universiteit Leuven, B-3030 Leuven, Belgium
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For the two-dimensional nearest-neighbor kinetic Ising model without conservation laws, we derive on the square lattice the high-temperature series expansion of the autorelaxation time, to the eleventh order. With use of ratio methods and Padé approximants, we obtain for the dynamical critical exponent Δ_A the value 2.09 ± 0.03, which implies the value 2.34 ± 0.03 for the linear relaxation exponent z. This value is about 10% larger than several other recent estimates. This discrepancy is possibly due to the relatively small number of nonzero coefficients in the series expansion.

I. PREVIOUS DETERMINATIONS OF THE DYNAMICAL EXPONENT z

The computation of the dynamical critical exponent z in the kinetic Ising model (or Glauber model)[1,2] has been the subject of many investigations over the past 25 years. In recent years researchers have undertaken the computation of z with the use of ever faster computers and ever more ingenious algorithms for Monte Carlo simulation,[3–5] Monte Carlo renormalization group,[6–11] Monte Carlo finite-size scaling,[12–18] or microcanonical simulation.[19–21] These massive numerical approaches have begun to overshadow other methods like, for example, real-space renormalization group,[22–28] traditional series-expansion analysis,[29,30] or field-theoretical renormalization.[31,32] The accuracy claimed by the different authors is usually rather modest (about 10–1% on the determination of z), but seems to have become a prime target in very recent works. For example, the authors of one of the latest Monte Carlo simulations[3] claim an accuracy of 0.25%. Obviously, the accuracy which is reported refers to the intrinsic statistics of the analysis and does not take into account possible systematic errors.

Our attention will be restricted to the two-dimensional kinetic Ising model (on a square lattice) without conserved densities (model A in the terminology of Hohenberg and Halperin[33]). To date the value of z for this model is still not reliably known, in our opinion, because different research groups continue to obtain different numbers which can only be made consistent with one another when sufficiently large uncertainties (typically 10%) are admitted. We will not review the different previous approaches and estimates of z, but only indicate some noteworthy facts about the value of z.

For the *linear* relaxation[34] exponent z there exists an exact lower bound[35]

$$z \geq 1.75 , \tag{1}$$

and many of the recent determinations locate z in the interval

$$2 \lesssim z \lesssim 2.2 , \tag{2}$$

with a majority of estimates close to the commonly accepted value

$$z \simeq 2.15 . \tag{3}$$

Curiously, the most recent estimate to our knowledge (and for which the smallest error bars are reported) is

$$z = 2.076\pm0.005 , \tag{4a}$$

from Mori's and Tsuda's Monte Carlo simulation in 1988.[3] This estimate was preceded in 1987 by

$$z = 2.132\pm0.008 , \tag{4b}$$

from Monte Carlo finite-size scaling work by Ito *et al.*[12] Both estimates feature very small error margins but exclude each other. Finally, there has been the intriguing conjecture of Domany[36] in 1984,

$$z = 2 , \tag{5}$$

with possibly a *logarithmic correction factor* to the algebraic divergence of the relaxation time.

II. SCALING HYPOTHESIS FOR THE AUTORELAXATION TIME

Consider a d-dimensional nearest-neighbor kinetic Ising model without conserved densities. The time evolution of the probability $P(\{s\},t)$ of a spin configuration $\{s\}$ at time t is given by the master equation

$$\partial_t P(\{s\},t) = -\sum_j W_j(\{s\})P(\{s\},t) + \sum_j W_j(\{s\},-s_j)P(\{s\},-s_j,t) . \tag{6}$$

The transition rates W obey, as usual, "detailed balance":

$$W_j(\{s\})P(\{s\}) = W_j(\{s\},-s_j)P(\{s\},-s_j) , \tag{7}$$

where $P(\{s\})$ is the equilibrium probability distribution

$\exp H(\{s\})/Z$, with $H(\{s\})$ the Hamiltonian and Z the partition function. Because of the detailed-balance condition, $P(\{s\})$ is stationary. Detailed balance still leaves a lot of freedom in the choice of W. In one dimension *and* for a special choice of W, the Glauber model is exactly solvable (Glauber's solution[1]). No exact solutions have been obtained in higher dimensions. Much attention has been devoted to the study of the critical slowing down of the relaxation of the order parameter, characterized by the dynamical exponent z (or $\Delta = z\nu$, where ν is the static correlation length exponent). Exact calculations of z have, as a rule, been possible only in the one-dimensional model or at the level of the mean-field theory.[33,34]

Scaling hypotheses or "scaling laws" for dynamical critical phenomena have been formulated by Halperin and Hohenberg.[37] Afterwards, renormalization-group theory for critical dynamics has been developed, combining space rescaling ($r \to r' = r/l$) and time rescaling ($t \to t' = t/l^z$).[33]

Consider the dynamic correlation function

$$G(K,\mathbf{r},t) \equiv \langle s_i(t) s_j(0) \rangle \ , \tag{8}$$

for Ising spins $s_i(t) = \pm 1$, with nearest-neighbor coupling $K = J/k_B T$, and where $\mathbf{r}$ is the lattice vector connecting sites i and j, and the average is defined as

$$\langle s_i(t) s_j(0) \rangle \equiv \sum_{\{s\}} s_j P(\{s\}) \sum_{\{s'\}} s_i' P(\{s'\},t|\{s\},0) \ . \tag{9}$$

In this expression $P(\{s'\},t|\{s\},0)$ is the probability of the configuration $\{s'\}$ at time t, given $\{s\}$ at $t=0$.

For the dynamic correlation function, the following scaling law applies:[37,38]

$$G(K_c + l^{y_T}(K - K_c), r/l, t/l^z) = l^{d-2+\eta} G(K,r,t) \ , \tag{10}$$

where $r = |\mathbf{r}|$, $y_T = 1/\nu$, and η is the static critical exponent of the correlation function. Relationship (10) is valid for K near the critical value K_c, and for $r \to \infty$, as well as $t \to \infty$. A time-independent scaling law can be obtained by taking the integral over t of (10), taking into account that the dominant contribution comes from the long-time domain (critical slowing down). One obtains the relaxation time Λ,

$$\Lambda(K,\mathbf{r}) \equiv \int_0^\infty G(K,\mathbf{r},t)\, dt \ , \tag{11}$$

and the scaling law

$$\Lambda(K_c + l^{y_T}(K - K_c), r/l) = l^{d-2+\eta-z} \Lambda(K,r) \ , \tag{12}$$

for $K \simeq K_c$, and $r \to \infty$. Finally, a scaling law for a normalized relaxation time τ, with

$$\tau(K,\mathbf{r}) \equiv \Lambda(K,\mathbf{r})/G(K,\mathbf{r},t=0) \ , \tag{13}$$

takes the form

$$\tau(K_c + l^{y_T}(K - K_c), r/l) = l^{-z} \tau(K,r) \ , \tag{14}$$

for $K \simeq K_c$ and $r \to \infty$. Note that $G(K,\mathbf{r},0)$ is the *static* correlation function.

The scaling law (10) applies in the same form in two other situations. The first is when $t=0$, in which case (10) reduces to the scaling law for the static correlation function. The second is for $r=0$, in which case (10) becomes the scaling law for the autocorrelation function

$$G(K,\mathbf{0},t) = \langle s_i(t) s_i(0) \rangle \ . \tag{15}$$

Because $G(K,\mathbf{0},0) = 1$, the scaling law for the autorelaxation time $\tau(K,\mathbf{0}) = \Lambda(K,\mathbf{0})$ takes the form

$$\tau(K_c + l^{y_T}(K - K_c),\mathbf{0}) = l^{-z+d-2+\eta} \tau(K,\mathbf{0}) \ , \tag{16}$$

which implies, with $\epsilon \equiv |T - T_c|/T_c$,

$$\tau(K,\mathbf{0}) \propto \epsilon^{-\Delta_A} \ , \tag{17}$$

where the autorelaxation exponent Δ_A is given by[5,30]

$$\Delta_A = (z - d + 2 - \eta)\nu = \Delta - 2\beta \ , \tag{18}$$

since $\Delta = z\nu$ and $2\beta = (d - 2 + \eta)\nu$. The exponent β is the static critical exponent of the order parameter.

III. HIGH-TEMPERATURE SERIES EXPANSION

For the kinetic Ising model on the two-dimensional square lattice we have computed the autorelaxation time $\tau(K,\mathbf{0})$, in a high-temperature series expansion to the eleventh order in $v \equiv \tanh K$. Previously this series was known to the ninth order,[22] but analyzed to the seventh order only.[30,5] This means that we have six terms at our disposal whereas previous analysis was based on four terms only.

Using the standard formalism for the Glauber model,[30] one derives

$$G(K,\mathbf{0},t) = \sum_{\{s\}} s_i \{ e^{-\mathcal{L}t} s_i \} P(\{s\}) \tag{19}$$

and

$$\tau(K,\mathbf{0}) = \sum_{\{s\}} s_i \{ \mathcal{L}^{-1} s_i \} P(\{s\}) \ , \tag{20}$$

where

$$\mathcal{L} \equiv \sum_j W_j(\{s\})(1 - p_j) \ , \tag{21}$$

with spin-flip "operators" p_j which act as follows on a function A of the spins:

$$p_j A(s_1, \ldots, s_{j-1}, s_j, s_{j+1}, \ldots) = A(s_1, \ldots, s_{j-1}, -s_j, s_{j+1}, \ldots) \ . \tag{22}$$

Consequently, τ can be expressed as a sum of static (multi)spin correlations.

We have derived the high-temperature series in the form

$$\tau(K,\mathbf{0}) = \sum_{n=0}^{N} a_n (\tanh K)^n \ , \tag{23}$$

and calculated a_n, for $n = 0, \ldots, 11$. The technique we have used follows closely the method outlined by Yahata and Suzuki,[30] and Oitmaa.[39] For the transition rate W, we have chosen a standard form

$$W_j(\{s\})=\frac{1}{2}\left[1-s_j\tanh\left[K\sum_k s_k\right]\right], \tag{24}$$

where k labels the (four) nearest neighbors of s_j. The calculation relies on the high-temperature expansion for the operator $\mathcal{L}^{-1}$,

$$\mathcal{L}^{-1}=\sum_{k=0}^{\infty}\mathcal{L}_0^{-1}(V\mathcal{L}_0^{-1})^k, \tag{25}$$

where $\mathcal{L}_0\equiv\mathcal{L}(K=0)$ and $V\equiv\mathcal{L}_0-\mathcal{L}$. Note that $V\propto 1/T$ for $T\to\infty$. When $\mathcal{L}^{-1}$ acts on a spin s_j, numerous "clusters" of spins are generated through the action of V and its powers. Finally, the thermal average of $s_i\mathcal{L}^{-1}s_i$ is obtained in the form

$$\tau(K,0)=\sum_{j=1}^{m}R_j f_j(K)\sum_{\{s\}}\left[\prod_{i=1}^{n_j}s_{j_i}\right]P(\{s\}), \tag{26}$$

where m is the number of terms relevant to the eleventh order in $v=\tanh K$, R_j is a rational number, f_j a function of K which results from the action of powers of V, and $n_j=0$, 2, 4, or 6, the number of spins in the static multispin correlation ($n_j=0$ corresponds to a factor 1). The calculation of the multispin correlations must be done to the ninth order for $n_j=2$, to the seventh order for $n_j=4$, and to the fourth order only for $n_j=6$, using standard techniques.[39] To carry out the final sum for obtaining τ, we have employed the REDUCE program for symbol manipulation.[40]

Our results for the coefficients in (23) are

$$\begin{aligned}
&a_n=0, \quad \text{for odd } n,\\
&a_0=1,\\
&a_2=8,\\
&a_4=64,\\
&a_6=1480/3,\\
&a_8=91\,808/27,\\
&a_{10}=18\,074\,824/729.
\end{aligned} \tag{27}$$

IV. ANALYSIS OF THE SERIES

We have applied the ratio method and the technique of Padé approximants to the eleventh-order series in $v=\tanh K$. Using the exact value for the critical coupling in the nearest-neighbor model ($\tanh K_c=\sqrt{2}-1$), we obtain the biased ratio-method estimates for Δ_A shown in Table I.

Clearly, the estimates based on alternating terms (third column) behave much more regularly for $n\geq 6$ than the estimates based on successive terms (second column). In a previous ratio-method analysis of the series only the terms for $n\leq 7$ were available and no conclusion could be reached.[30] Before drawing our conclusion we turn to the complementary method of Padé approximants.

Padé approximants were calculated to the logarithmic derivative of the series expansion. When this method was applied previously for $n\leq 7$, two estimates could be obtained,[5] $\Delta_A=1.25$ and $\Delta_A=1.33$. Our results are shown in Tables II and III.

TABLE I. Biased estimates of the critical exponent Δ_A for the autorelaxation time using ratios of successive (second column) and alternating (third column) terms, and $v_c=0.414\,21$ (NA means not available).

n	Δ_A	
2	1.373	NA
4	1.745	1.745
6	1.968	2.042
8	1.730	2.002
10	2.255	2.082

In Table II we show the results of an unbiased analysis, giving estimates for both the critical point $v_c=\tanh K_c$ (with exact value $\sqrt{2}-1\simeq 0.414$) and the exponent Δ_A. The estimates for the critical point are in parentheses.

The results in Table II are not well behaved. The only reasonable estimates are found for $N=D=4$. Note how strong the correlation is between the errors in the estimates of v_c and those of Δ_A. Moreover, Δ_A appears extremely sensitive to errors in the estimates of v_c. (The previously obtained estimates[5] are those for $N=0, D=4$ and $N=2, D=2$.)

Much better behavior is found in the results from the *biased* Padé analysis (where the exact v_c is assumed), in Table III. In view of the sensitivity of Δ_A to errors on v_c, this improvement is no surprise. If the analysis were restricted to the ninth-order series, the conclusions would already be quite meaningful, namely, $2.05\lesssim\Delta_A\lesssim 2.31$. Analysis of the eleventh-order series narrows this interval to

$$2.06\lesssim\Delta_A\lesssim 2.11. \tag{28}$$

We proceed to *combine* our estimates from the biased alternating ratio method with those from the biased Padé analysis to obtain, in the ninth order, $2.00\lesssim\Delta_A\lesssim 2.31$, and, in the eleventh order,

$$2.06\lesssim\Delta_A\lesssim 2.11. \tag{29}$$

Note that, in the eleventh order, the estimate from the ratio method is, for the first time, within the interval of estimates from the Padé analysis. Consequently, our final

TABLE II. Estimates of the critical point v_c (in parentheses) and exponent Δ_A using Padé approximants to the logarithmic derivative of the series.

N \ D	2	4	6
		(0.378)	Negative
0	NA	1.333	pole
	(0.375)	(0.343)	(0.453)
2	1.261	0.976	6.030
	(0.489)	(0.409)	
4	6.200	1.901	
	(0.304)		
6	0.138		

TABLE III. Biased estimates of the critical exponent Δ_A from the residues of the Padé approximants to the logarithmic derivative at the pole $v_c = 0.41421$.

N \ D	2	4	6
2	4.205	2.313	2.063
4	2.049	2.112	
6	2.101		

conclusion (29) is not different from the conclusion (28) reached on the basis of the Padé analysis alone.

We can summarize our result in the form

$$\Delta_A = 2.09 \pm 0.03 \ . \tag{30}$$

For the exponent z this implies, in view of (18),

$$z = 2.34 \pm 0.03 \ . \tag{31}$$

This result is about 10% larger than several recent results from other works.[3,4,6–8,12–14] Clearly, the number of estimates on which our result is based is rather small and therefore both the numerical value and the error margin cannot be considered authoritative. Qualitatively, our result agrees with those of other recent works in indicating that $z > 2$, and thus suggesting that Domany's conjecture[36] ($z = 2$) is not valid in the $d = 2$ Ising model. However, if it is true, as Domany suggested, that a logarithmic correction factor is present, then it would be more difficult to rule out his conjecture because such corrections may lead to a serious overestimation of the exponent.[41] We have not searched for the possible presence of such corrections because the series expansions are too short for this.

In conclusion, our main result has been the derivation of a longer series for the *autorelaxation time,* which allowed us, for the first time, to carry out a meaningful computation of its dynamical critical exponent Δ_A by means of high-temperature series analysis. In the highest order of our analysis the estimates from ratio method and Padé approximants are mutually consistent and lead to an estimate for the linear relaxation exponent z which lies about 10% away from the majority of recent authoritative estimates. As far as comparison of our work with previous series analyses is concerned, we would like to remark the following. Clearly, our analysis of the autorelaxation time is much better than previous analyses for that particular function,[5,30] simply because our series is substantially longer. However, for other functions, namely the linear relaxation time (and the nonlinear one), the "old" series analysis by Rácz and Collins[29] predicted a value of z which agrees with the commonly accepted value today. They obtained $z = 2.125 \pm 0.01$. For explaining why our result differs by about 10% from theirs, one must take into account that (i) different thermodynamic functions have been used, (ii) in both cases the analyses were based on series of reasonable but still short length (twelfth order at most), (iii) a twelfth-order series for the linear relaxation time contains 13 nonzero terms, whereas our eleventh-order series for the autorelaxation time has only six nonzero terms [see Eqs. (27)], and (iv) the quoted error bars always refer to the intrinsic statistics of the analysis and ignore possible systematic errors due to possible errors in the series coefficients or to the shortness of the series, for example.

In the light of the foregoing, it is plausible that our statistics and hence our result suffer from the relatively small number of terms in our series. This would then mean that the autorelaxation time is intrinsically more difficult to analyze, having only "even" coefficients in the series expansion. It would certainly be worthwhile to derive a still longer series in order to improve the accuracy, but this appears too costly within the present computational scheme.

It is important to pursue the direction we have taken and to obtain eventually much more accurate values of Δ_A. Indeed, one can then use that information and combine it with the most reliable estimate of Δ in order to test the scaling relation (18), which we have taken for granted in our discussion so far.

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