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Monte Carlo Investigation of Dynamic Critical Phenomena in the Two-Dimensional Kinetic Ising Model

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Extending the Monte Carlo method to dynamic critical phenomena we investigated the time-dependent correlation functions in the two-dimensional one-spin-flip Ising model and the critical behavior of the associated relaxation times. These relaxation times are the following: $\tau_{\delta\mu}^{\Delta T}$, characterizing the approach of the order parameter to equilibrium after a change of temperature ΔT of the system; $\tau_{\delta\mu\delta\mu}$ and $\tau_{\delta\mu\delta\mu}^{A}$, characterizing the slowing down of the order-parameter correlation and autocorrelation functions, respectively; $\tau_{\delta\mathcal{H}\delta\mathcal{H}}$ and $\tau_{\delta\mathcal{H}\delta\mathcal{H}}^{A}$, characterizing the slowing down of the energy correlation and autocorrelation functions; and finally, $\tau_{\delta\mu\delta\mathcal{H}}$, characterizing the cross-correlation function. We give estimates for the associated exponents $\Delta_{\delta\mu}^{\Delta T} \approx \Delta_{\delta\mu\delta\mu} \approx \Delta_{\delta\mathcal{H}\delta\mathcal{H}} \approx \Delta_{\delta\mu\delta\mathcal{H}} \approx 1.90 \pm 0.10$, and $\Delta_{\delta\mu\delta\mu}^{A} \approx 1.60 \pm 0.10$, $\Delta_{\delta\mu\delta\mathcal{H}}^{A} \approx 0.95 \pm 0.10$, $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}^{A} \approx 0$, which are consistent with the dynamic scaling hypothesis and with exact inequalities. A detailed comparison with recent high-temperature-expansion estimates is performed, and the reliability of the Monte Carlo results is carefully analyzed.

I. INTRODUCTION

Much of our understanding of the static aspects or critical phenomena arises from the study of model systems.[1–3] Prominent examples are the Ising and the Heisenberg models. The former provides a useful description of systems in which a localized variable can take either of two discrete values. A highlight in any discussion of this model is Onsager's[4] solution for the zero-field partition function of a two-dimensional square lattice with periodic boundary conditions and nearest-neighbor interactions.

Although considerable progress has been made in recent years, the present "state of the art" as regards dynamic model systems is by no means as advanced as it is for static systems.[1,5] Here we shall consider the adaptation of the Ising model to the treatment of dynamic phenomena, introduced by Glauber.[6] In this model an assembly of Ising spins is in contact with a heat bath which induces random flips of the spins from one state to another. In the original Glauber model, which we consider here, only one spin is permitted to flip at once, so that neither its total magnetization nor total energy is conserved. The heat bath is not treated explicitly; it is, however, assumed that there is a transition probability $W_j(\mu_1, \ldots, \mu_N)$ that the jth spin flips from μ_j to $-\mu_j$, which is supposed not to depend on the previous history of the system. In this sense the Glauber model is Markovian.

The interest in this model lies in the fact that it is simple enough to obtain some fundamental knowledge of dynamic properties in cooperative systems, and that the equilibrium properties of the system are quite well understood.

In the work described here we used the Monte Carlo method, first introduced by Metropolis *et al.*,[7] to investigate the critical slowing down in kinetic Ising models consisting of square lattices with nearest-neighbor interactions and periodic boundary conditions (pbc). Our restriction to the critical slowing down was dictated by the desire to compare some of our results, which are expected to simulate an infinite system except in a small region around T_c, with estimates obtained by other methods. Previously, some estimates were obtained based on a high-temperature-expansion method,[8–12] and an extension of Wilson's expansion techniques.[13] Moreover, the latter results seemed to confirm the dynamic scaling hypothesis[14,15] (DSH), which in turn implies explicit relations between the critical exponents characterizing the divergencies of the relaxation times associated with, for example, the order-parameter correlation and autocorrelation functions, respectively. Both the recent series expansion[8–12] and Wilson's expansion[13] estimates predict a "kinetic slowing down," i.e., an exponent $\Delta_{\delta\mu\delta\mu}$ of the order-parameter correlation function which is larger than the exponent γ of the static susceptibility, whereas these exponents are equal in the earlier "conventional" theories.[12,16] In spite of this variety of methods, knowledge of the critical slowing down in the kinetic Ising model still seems rather incomplete; however, the high-temperature-series technique is restricted to temperatures $T > T_c$, and the only accurate exponent estimates so far available[11] are those of $\Delta_{\delta\mu\delta\mu}$ and $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$. Moreover, the Wilson expansion results[13] have so far been restricted to the order-parameter exponents $\Delta_{\delta\mu\delta\mu}$ and $\Delta_{\delta\mu\delta\mu}^{A}$, respectively. Furthermore, the accuracy of the Wilson[17] approach in two dimensions seems rather questionable since it fails to reproduce the exact result $\beta = \frac{1}{8}$.[18] We note, however, that this approach is expected to be accurate in three dimensions.[19] Even the DSH, which was first formulated by Ferrell *et al.*,[14] and reformulated and extended by Halperin and Hohenberg,[13] depends on as yet unverified assumptions concerning certain functions. In view of this, an alternative estimate of the exponents associated with the critical slowing down in the kinetic Ising model is desirable, to compare them with the previous estimates[11,13] and with rigorous inequalities.[12,20–22] Some preliminary results of this work concerning the "effective" exponents to be discussed below were presented earlier in a short communication.[23] By "effective" exponents of a diverging quantity, we denote their average slope in a given temperature interval on a log-log plot [cf. Eq. (133)].

In Sec. II we describe Glauber's kinetic Ising model, describe the extension of the Monte Carlo technique to time-dependent critical phenomena, and outline the means by which the quantities of interest may be estimated. The reliability of these estimates is then discussed. A sensitive test of the accuracy of time-dependent quantities constitutes the application to the one-dimensional kinetic Ising model, for which exact solutions exist.[6] Such calculations are presented in Appendix A. In Sec. III we summarize the formal description of the relaxation times characterizing the critical slowing down. The definitions of the various equilibrium and nonequilibrium relaxation functions are given, and the relations between their exponents are discussed. We summarize the predictions of the DSH and of the inequalities mentioned above.[12,20–22] The Monte Carlo results are presented in Sec. IV and are compared in detail to the various expansion results.[10,11,13] Our exponent estimates are derived essentially from the region $0.02 \leq |\epsilon| \leq 0.20$, where ϵ is the reduced temperature $-\epsilon = 1 - T/T_c$. Several results are of particular interest:

(i) While the "effective" exponents derived for the order-parameter and energy correlation functions are symmetric for $T < T_c$ and $T > T_c$ and presumably very close to the values of the "true" exponents, this is not the case for the "effective" exponents of the order-parameter autocorrelation function, which have significant asymmetry. It is suggested that this is due to the presence of important correction terms which are absent in the other cases. We discuss how to eliminate the influence of these corrections and thus derive tentative estimates also for the "true" exponents of the autocorrelation functions. It is shown that all these "true" exponents are consistent with the exact inequalities[12,20–22] and the DSH,[14,15] while the "effective" autocorrelation exponent turns out to be inconsistent with the DSH, as remarked earlier.[23]

(ii) Our numerical estimates of the critical exponents mentioned disagree slightly with the results obtained from the high-temperature-expansion and ratio method.[8–12] To elucidate this slight discrepancy we also present results obtained from numerical Padé approximants to these series. The formal part of the expansion approach is summarized in Appendix B, while the detailed numerical comparisons of Sec. IV show that both methods are in reasonable numerical agreement for the temperature range investigated; the above-mentioned slight discrepancy is thus reduced to a problem of extrapolating numerical results to $T \to T_c$, and we therefore feel it should be taken as a measure of the uncertainty still inherent in the determination of exponents from either method.

II. KINETIC ISING MODEL AND MONTE CARLO TECHNIQUE

A complete statistical description of the kinetic or stochastic Ising model[5,6,24] would consist of the knowledge of the probability $P(\mu_1, \ldots, \mu_N; t)$ that at time t the spin system is in the state $\{\mu_1, \ldots, \mu_N\}$. The time dependence of P is assumed to be governed by the master equation

$$\frac{d}{dt} P(\mu_1, \ldots, \mu_N; t) = \sum_{j=1}^{N} W_j(\mu_1, \ldots, -\mu_j, \ldots, \mu_N) P(\mu_1, \ldots, -\mu_j, \ldots, \mu_N; t) - \sum_{j=1}^{N} W_j(\mu_1, \ldots, \mu_j, \ldots, \mu_N) P(\mu_1, \ldots, \mu_j, \ldots, \mu_N; t), \quad (1)$$

where μ_1 takes on the values ± 1. The first summation corresponds to the total number of ways that the system can flip into the state $\{\mu_1, \ldots, \mu_N\}$, whereas the second summation corresponds to the total number of ways that the system can flip out of the state $\{\mu_1, \ldots, \mu_N\}$.

The predictions of Eq. (1) depend upon the choice for the transition probability W. A reasonable constraint is the requirement that W has such a form that it is capable of bringing the kinetic Ising model to the same equilibrium as that of the conventional static Ising model.

In equilibrium the left-hand side of Eq. (1) is by definition equal to zero. This condition corresponds to the principle of detailed balance, which asserts that

$$W_j(-\mu_j) P_0(\mu_1, \ldots, -\mu_j, \ldots, \mu_N)$$

$$= W_j(\mu_j) P_0(\mu_1, \ldots, \mu_j, \ldots, \mu_N), \quad (2)$$

where $P_0(\mu_1, \ldots, \mu_N)$ denotes the probability of finding the Ising spins in the configuration $\{\mu_1, \ldots, \mu_N\}$ when the system is in equilibrium. Observing that

$$P_0(\mu_1, \ldots, \mu_N) \sim e^{-\beta \mathcal{H}}, \quad \beta = 1/k_B T, \quad (3)$$

$$\mathcal{H} = -\sum_{i,j}{}' J_{ij}\, \mu_i \mu_j - \mu_B \sum_j \mu_j H_j, \quad (4)$$

where H_j is the external magnetic field acting on the jth spin, Eq. (2) leads to

$$\frac{W_j(\mu_j)}{W_j(-\mu_j)} = \frac{e^{-\beta E_j \mu_j}}{e^{+\beta E_j \mu_j}} = \frac{1 - \mu_j \tanh(\beta E_j)}{1 + \mu_j \tanh(\beta E_j)}. \quad (5)$$

The local field is defined by

$$E_j = \mu_B H_j + \sum_k J_{jk}\, \mu_k. \quad (6)$$

Following Suzuki and Kubo[24] one might choose for W_j a form consistent with Eq. (6):

$$W_j(\mu_j) = (1/2\tau_s)[1 - \tanh(\beta E_j)] = (1/2\tau_s)\,\varphi_j. \quad (7)$$

In a one-dimensional system Eq. (7) reduces to the choice of Glauber.[6] The parameter τ_s is the relaxation time of a single free Ising spin interacting with the heat bath, and determines the time scale of the dynamic processes. As a consequence, the time scale is determined only up to the factor τ_s.

Using Eqs. (1) and (7) and the definition of the expectation value

$$\langle \mu_j \rangle = \sum_{\{\mu\}} \mu_j P(\mu_1, \ldots, \mu_N; t),$$

where the sum is taken over all possible configurations, one can then derive the equations of motion:

$$\tau_s \frac{d}{dt} \langle \mu_j \rangle = -[\langle \mu_j \rangle - \langle \tanh(\beta E_j) \rangle], \quad (8)$$

$$\tau_s \frac{d}{dt} \langle \mu_j \mu_k \rangle = -2 \langle \mu_j \mu_k \rangle + \langle \mu_j \tanh(\beta E_k) \rangle + \langle \mu_k \tanh(\beta E_j) \rangle. \quad (9)$$

Thus the calculation problem is reduced to the problem of solving a hierarchy of differential equations, subject to certain initial conditions. This has been done exactly only in the case of one-dimensional systems by Glauber[6]; for systems with higher dimensionality one must make approximations to get explicit predictions.[5,6,24]

However, estimates of the exact results may be obtained by means of the Monte Carlo technique, which was first introduced by Metropolis *et al.*[7] in the computations of the equation of state of a hard-sphere gas. In addition, this scheme allows one to deal directly with the system at the microscopic level, and it is therefore possible to get an insight into the detailed behavior of the system which is sometimes obscure in analytical methods.[25] For a detailed discussion of this scheme we refer to Refs. 7, 26, and 27. Here we merely summarize the main points.

Following the usual procedure, we used, instead of Eq. (7), the transition probability

$$\tau_s' W_j'(\mu_j) = \begin{cases} e^{2\beta\mu_j E_j}, & \text{if } 2\beta\mu_j E_j < 0 \\ 1, & \text{otherwise.} \end{cases} \quad (10a)$$

This choice differs only slightly from that given in Eq. (7) and is of course also consistent with Eqs. (2) and (5). It has been argued[27] that the choice defined by Eq. (10a) leads near thermal equilibrium to a renormalization of the time rate with respect to that in Eq. (7). This temperature-dependent renormalization factor has been calculated to compare our Monte Carlo results with those obtained from series expansions. For this purpose Monte Carlo runs were performed with both W_j and W_j'. Equations (7) and (10a) and the renormalization factor was taken to be

$$\langle W_j \rangle / \langle W_j' \rangle = g(T). \quad (10b)$$

The exponent estimates we will derive are unaffected by $g(T)$.

In the Monte Carlo method one starts with an initial Ising spin configuration $\{\mu_1, \ldots, \mu_N\}$ and calculates W_j, where the jth spin is chosen by a random-number generator. For $\tau_s W_j < 1$ one flips the jth spin if $\tau_s W_j$ exceeds a random number between 0 and 1. If $\tau_s W_j = 1$ the jth spin is also flipped. In this manner a sequence of new spin configurations is generated. Since the system tends to equilibrium by construction, there is a correspondence between the time lapse and the number of configurations. So that the time unit does not depend on the number of spins, this unit is defined as a sequence in which, on the average, any spin has the possibility to flip once. This is the so-called Monte Carlo step per spin, containing a sequence of N spin configurations. Thus, for describing the evolution of the system we may use a parameter t, called the time, which takes on the sequential values $t_K = (k/N)\tau_s$. The kth configuration in the sequences is denoted by k, and t_N is the Monte Carlo step per spin. On this basis one may now define time-dependent averages. For example, the time-dependent magnetization at time t is defined as

$$\mu(t) = \frac{1}{N} \sum_{j=1}^{N} \mu_j(t) = \frac{1}{N} \sum_{j=1}^{N} \mu_j \left(\frac{k}{N} \tau_s \right), \quad (11)$$

where k again denotes the kth configuration in the chain of sequences. A characteristic behavior of $\mu(t)$ is shown in Fig. 1 for $T < T_c$. Three time intervals may be distinguished: a first stage, in

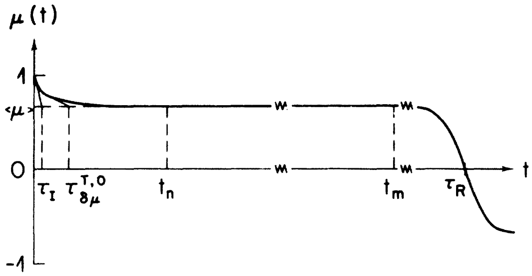

FIG. 1. Schematic sketch of the time evolution of the average order parameter $\mu(t)$. The initial state is completely ordered. Three time intervals may be distinguished: (1) The initial decay is noncritical (τ_I); (2) the decay to "equilibrium" which becomes critical $\tau_{\delta\mu}^{\Delta T,0}$; (3) this "equilibrium" state is a metastable state with lifetime τ_R. Monte Carlo averages are taken in the interval $t_n \gg \tau_{\delta\mu}^{\Delta T,0}$ and $t_m \ll \tau_R$. In practice τ_R is accessible only very close to T_c for large systems.

which the system relaxes rapidly from the nonequilibrium initial configuration towards "equilibrium" (τ_I); a second interval $\tau_{\delta\mu}^{\Delta T}$, where the relaxation becomes slower and the system develops towards a metastable state; this metastable state may be so long lived (τ_R, the third interval) that time averages, such as

$$\langle \mu \rangle = \frac{1}{t_m - t_n} \int_{t_n}^{t_m} \mu(t)\, dt, \tag{12}$$

become meaningful quantities. However, at τ_R the system may undergo a "first-order transition." This behavior expresses the fact that in any finite system at zero field, the canonical ensemble average of μ vanishes ($\langle\mu\rangle = 0$). Nevertheless, as long as

$$\tau_R \gg t_m - t_n \quad (T < T_c) \tag{13}$$

and the interval $t_m - t_n$ permits reasonable time averages, $\langle\mu\rangle$ [Eq. (12)] should provide a reliable estimate for the canonical ensemble average of the infinite system. However, by approaching the transition temperature of the infinite system, τ_R becomes shorter and $\tau_{\delta\mu}^{\Delta T}$ increases. As a consequence, very close to T_c, condition (13) can no longer be fulfilled. The actual region depends, of course, on the number of spins N and decreases with increasing N. For $T > T_c$ condition (13) must be reversed:

$$\tau_R \ll t_m - t_n \quad (T > T_c). \tag{14}$$

In this case $\langle\mu\rangle$ represents an estimate for $\langle\mu\rangle = 0$. However, by approaching T_c from above, τ_R increases. Consequently, close to T_c condition (14) can no longer be fulfilled. It now becomes evident that the Monte Carlo technique provides a very direct technique for estimating $\langle\mu\rangle$ and $\mu(t)$ of an infinite system, except in a very narrow region around T_c. The actual extension of this region depends on the number of spins N. In a 110×110 square lattice with pbc and nearest-neighbor interactions, it extends from $T/T_c \approx 0.99$–1.02.[28] Moreover, this technique may be used to estimate many other properties, such as the isothermal susceptibility

$$\chi_{\delta\mu\delta\mu} = \frac{N}{k_B T} \frac{1}{t_m - t_n} \int_{t_n}^{t_m} [\mu(t) - \langle\mu\rangle]^2 dt = \left(\frac{\partial\langle\mu\rangle}{\partial \mu_B H}\right)_T, \tag{15}$$

and the correlation functions

$$\hat{\phi}_{\delta\mu\delta\mu}(t) = \frac{N}{k_B T \chi_{\delta\mu\delta\mu}} \left(\frac{1}{t_m - t - t_n}\right) \times \int_{t_n}^{t_m - t} [\mu(t') - \langle\mu\rangle][\mu(t+t') - \langle\mu\rangle]\, dt', \tag{16}$$

$$\hat{\phi}^A_{\delta\mu\delta\mu}(t) = \frac{t_m - t}{t_m - t - t_n} \frac{\sum_{j=1}^N \int_{t_n}^{t_m - t} [\mu_j(t') - \langle\mu\rangle][\mu_j(t+t') - \langle\mu\rangle]\, dt'}{\sum_{j=1}^N \int_{t_n}^{t_m} [\mu_j(t') - \langle\mu\rangle]^2 dt'} . \tag{17}$$

$\hat{\phi}^A_{\delta\mu\delta\mu}(t)$ is the order-parameter autocorrelation function. Since the relaxation behavior of both $\phi_{\delta\mu\delta\mu}(t)$ and $\hat{\phi}^A_{\delta\mu\delta\mu}(t)$ is polydispersive, an unambiguous measure of the relaxation rate is the area under the relaxation curve.[29] Thus the slowing down manifested in the magnetization correlation and autocorrelation functions may be characterized

$$\tau_{\delta\mu\delta\mu} = \int_0^{t_m - t_n} dt\, \hat{\phi}_{\delta\mu\delta\mu}(t) \tag{18}$$

and

$$\tau^A_{\delta\mu\delta\mu} = \int_0^{t_m - t_n} dt\, \hat{\phi}^A_{\delta\mu\delta\mu}(t). \tag{19}$$

In Fig. 2 we show as an example the calculated temperature dependence of the isothermal susceptibility [Eq. (15)] for the square 55×55 lattice. It should be emphasized that the susceptibility is a second derivative of the energy and is therefore harder to calculate accurately than first derivatives, like magnetization or energy. In view of this, agreement between simulated and "exact" results[2] is satisfactory and reveals again the possibility to estimate critical exponents with the Monte Carlo method.[28,30]

In full analogy to Eqs. (11) and (12) we define the time-dependent energy at time t [$\mathcal{H}_j \equiv -\mu_j E_j$, see Eq. (6)]

$$\mathcal{H}(t)=\frac{1}{N}\sum_{j=1}^{N}\mathcal{H}_j(t)=\frac{1}{N}\sum_{j=1}^{N}\mathcal{H}_j\left(\frac{k}{N}\,\tau_s\right) \qquad (20)$$

and its time average

$$\langle\mathcal{H}\rangle=\frac{1}{t_m-t_n}\int_{t_n}^{t_m}\mathcal{H}(t)\,dt. \qquad (21)$$

From the fluctuation of this quantity we may estimate the specific heat

$$\chi_{\delta\mathcal{H}\delta\mathcal{H}}(=C_H T)=\frac{N}{k_B T}\left(\frac{1}{t_m-t_n}\right)\int_{t_n}^{t_m}[\mathcal{H}(t)-\langle\mathcal{H}\rangle]^2\,dt. \qquad (22)$$

The slowing down of the energy is characterized by the correlation functions

$$\hat{\phi}_{\delta\mathcal{H}\delta\mathcal{H}}(t)=\frac{N}{k_B T\chi_{\delta\mathcal{H}\delta\mathcal{H}}}\left(\frac{1}{t_m-t-t_n}\right)\times\int_{t_n}^{t_m-t}[\mathcal{H}(t')-\langle\mathcal{H}\rangle][\mathcal{H}(t'+t)-\langle\mathcal{H}\rangle]\,dt', \qquad (23)$$

$$\hat{\phi}^{A}_{\delta\mathcal{H}\delta\mathcal{H}}(t)=\frac{t_m-t_n}{t_m-t-t_n}\;\frac{\sum_{j=1}^{N}\int_{t_n}^{t_m-t}[\mathcal{H}_i(t')-\langle\mathcal{H}\rangle][\mathcal{H}_i(t'+t)-\langle\mathcal{H}\rangle]\,dt'}{\sum_{j=1}^{N}\int_{t_n}^{t_m}[\mathcal{H}_i(t')-\langle\mathcal{H}\rangle]^2\,dt'}\;, \qquad (24)$$

which are analogous to Eqs. (16) and (17). Again we measure the associated energy relaxation times by the area under the relaxation curves,

$$\tau_{\delta\mathcal{H}\delta\mathcal{H}}=\int_0^{t_m-t_n}dt\,\hat{\phi}_{\delta\mathcal{H}\delta\mathcal{H}}(t) \qquad (25)$$

and

$$\tau^{A}_{\delta\mathcal{H}\delta\mathcal{H}}=\int_0^{t_m-t_n}dt\,\hat{\phi}^{A}_{\delta\mathcal{H}\delta\mathcal{H}}(t). \qquad (26)$$

In addition to the order parameter and energy fluctuations which are characterized by Eqs. (15)–(19) and Eqs. (22)–(26), respectively, it is interesting to consider the coupling between order parameter and energy fluctuations. This is done by defining the quantity

$$\chi_{\delta\mu\delta\mathcal{H}}=\frac{N}{k_B T}\left(\frac{1}{t_m-t_n}\right)\int_{t_n}^{t_m}[\mu(t)-\langle\mu\rangle][\mathcal{H}(t)-\langle\mathcal{H}\rangle]\,dt \qquad (27)$$

and the associated time-dependent correlation functions

$$\hat{\phi}_{\delta\mu\delta\mathcal{H}}(t)=\frac{N}{k_B T\chi_{\delta\mu\delta\mathcal{H}}}\left(\frac{1}{t_m-t-t_n}\right)\times\int_{t_n}^{t_m-t}[\mu(t')-\langle\mu\rangle][\mathcal{H}(t'+t)-\langle\mathcal{H}\rangle]\,dt', \qquad (28)$$

$$\hat{\phi}^{A}_{\delta\mu\delta\mathcal{H}}(t)=\frac{t_m-t}{t_m-t-t_n}\;\frac{\sum_{j=1}^{N}\int_{t_n}^{t_m-t}[\mu_i(t')-\langle\mu\rangle][\mathcal{H}_i(t'+t)-\langle\mathcal{H}\rangle]\,dt'}{\sum_{j=1}^{N}\int_{t_n}^{t_m}[\mu_i(t')-\langle\mu\rangle][\mathcal{H}_i(t')-\langle\mathcal{H}\rangle]\,dt'}\;. \qquad (29)$$

In analogy to Eqs. (18), (19) and (25), (26) we define the relaxation times

$$\tau_{\delta\mu\delta\mathcal{H}}=\int_0^{t_m-t_n}dt\,\hat{\phi}_{\delta\mu\delta\mathcal{H}}(t) \qquad (30)$$

and

$$\tau^{A}_{\delta\mu\delta\mathcal{H}}=\int_0^{t_m-t_n}dt\,\hat{\phi}^{A}_{\delta\mu\delta\mathcal{H}}(t). \qquad (31)$$

In Fig. 3 we show as an example the calculated temperature dependence of the specific heat [Eq. (22)] for the square 55×55 lattice. In this case an exact solution for this finite lattice (with pbc) is available from the work of Ferdinand and Fisher[31] and is included in the figure. The close agreement of the numerical estimates with the exact solution again gives confidence in the accuracy of the Monte Carlo calculations.

In addition to these relaxation times Eqs. (18), (19), (25), (26), and (30), (31), which characterize the decay of fluctuations in the thermal equilibrium state, we may also introduce relaxation times which characterize the approach to thermal equilibrium. Suppose at time $t=0$ a sudden change of the magnetic field ΔH or the temperature ΔT is performed. Then we describe the relaxation of magnetization by the function

$$\hat{\phi}^{\Delta T,\Delta H}_{\delta\mu}(t)=\frac{\mu(t)-\mu(t_n)}{\mu(0)-\mu(t_n)}\;, \qquad (32)$$

and the associated relaxation time is

$$\tau^{\Delta T,\Delta H}_{\delta\mu}=\int_0^{t_n}dt\,\hat{\phi}^{\Delta T,\Delta H}_{\delta\mu}(t). \qquad (33)$$

In the short communication[23] the time $\tau^{T,0}_{\delta\mu}$ was denoted by τ_{nl}, following Suzuki.[29] A similar "nonlinear" autocorrelation function can be defined in an analogous fashion but will not be considered explicitly in this paper. Finally, we describe the relaxation of the energy,

$$\hat{\phi}^{\Delta T,\Delta H}_{\delta\mathcal{H}}(t)=\frac{\mathcal{H}(t)-\mathcal{H}(t_n)}{\mathcal{H}(0)-\mathcal{H}(t_n)}\;, \qquad (34)$$

and introduce the relaxation time

$$\tau_{\delta\mathfrak{X}}^{\Delta T,\Delta H} = \int_0^{t_n} dt\, \hat{\phi}_{\delta\mathfrak{X}}^{\Delta T,\Delta H}(t). \tag{35}$$

So far we have explained how we estimate the quantities of interest using the Monte Carlo method and have given the appropriate definitions. Comparing static susceptibility and specific heat to exact results[2,31] we have asserted the accuracy of our Monte Carlo methods as applied to static quantities of the two-dimensional Ising model. However, no analogous exact results exist for dynamic properties. But a very sensitive test of the accuracy of the Monte Carlo method with respect to time-dependent quantities is the application to the *one*-dimensional kinetic Ising model, for which exact solutions exist.[6] Such calculations have been performed for various temperatures and are summarized in Appendix A. From the very good agreement with the exact results we conclude that our Monte Carlo programs provide reliable estimates for dynamic quantities, too.

III. SUMMARY OF ANALYTIC RESULTS CONCERNING CRITICAL SLOWING DOWN

A. Formal Introduction

In this subsection we summarize the formal description of the relaxation times characterizing the critical slowing down of the fluctuations. The relaxation function associated with the dynamic variables B and C may be defined by[10]

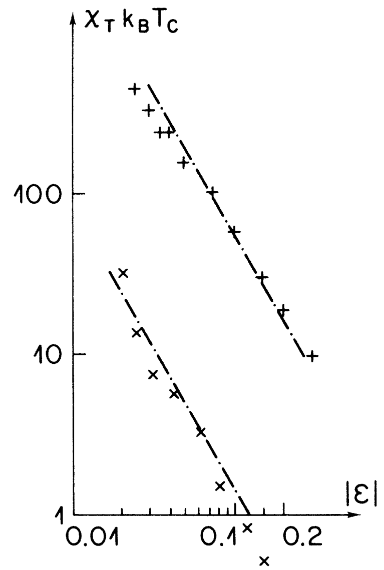

FIG. 2. Calculated temperature dependence of the isothermal susceptibility for a square 55×55 lattice with nearest-neighbor interactions subjected to periodic boundary conditions, +: $T>T_c$, X: $T<T_c$. The broken lines correspond to the asymptotic behavior obtained from series expansions and exact solutions, respectively (see Ref. 2).

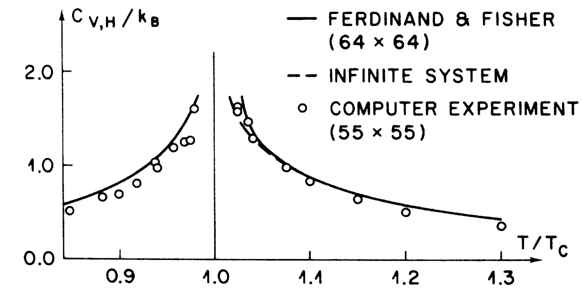

FIG. 3. Calculated temperature dependence of the specific heat for a square 55×55 lattice with nearest-neighbor interactions subjected to periodic boundary conditions. The full curve is the exact solution obtained by Ferdinand and Fisher (Ref. 31) and the dashed curve is the result for the infinite system.

$$\phi_{\delta B,\delta C}(\vec{k},t) = \frac{\langle \delta B(-\vec{k},0)\,\delta C(\vec{k},t)\rangle}{\langle \delta B(-\vec{k},0)\,\delta C(\vec{k},0)\rangle}, \tag{36}$$

where for any operator D,

$$\delta D = D - \langle D\rangle, \tag{37}$$

and

$$\delta D(t) = e^{-Lt}\,\delta D(0). \tag{38}$$

The operator L, playing the role of a Liouville operator, is defined by[10]

$$L = \sum_{j=1}^{N} W_j(\mu_j)(1-P_j), \tag{39}$$

P_j being the spin-flip operator of the jth spin:

$$P_j\,\mu_k = -\mu_k\delta_{jk} + \mu_k(1-\delta_{jk}). \tag{40}$$

The transition probability $W_j(\mu_j)$ has been discussed in Sec. II [see Eqs. (5)–(7) and (10)]. From Eq. (36) the relaxation time associated with the variables B and C is deduced to be [cf., Eq. (38)]

$$\tau_{\delta B\delta C} = \int_0^\infty \hat{\phi}_{\delta B\delta C}(0,t)\,dt \equiv \int_0^\infty \hat{\phi}_{\delta B\delta C}(t)\,dt$$

$$= \frac{\langle \delta B(1/L)\,\delta C\rangle}{\langle \delta B\delta C\rangle}. \tag{41}$$

This relaxation time is expected to diverge as

$$\tau_{\delta B\delta C} \propto \begin{cases} (-\epsilon)^{-\Delta'}{}_{\delta B\delta C} & \text{for } T_c - T \to 0^+ \\ (\epsilon)^{-\Delta}{}_{\delta B\delta C} & \text{for } T - T_c \to 0^+, \end{cases} \tag{42}$$

where

$$\epsilon = \frac{T-T_c}{T_c}. \tag{43}$$

$\Delta_{\delta B\delta C}$ is the critical exponent of the relaxation time $\tau_{\delta B\delta C}$. It is also necessary to define the corresponding autocorrelation function

$$\phi^A_{\delta B\delta C}(t) = \frac{\langle \delta B_i(0)\,\delta C_i(t)\rangle}{\langle \delta B_i(0)\,\delta C_i(0)\rangle}$$

$$=\frac{\sum_k\langle\delta B(-\vec{k},0)\,\delta C(\vec{k},t)\rangle}{\sum_k\langle\delta B(-\vec{k},0)\,\delta C(\vec{k},0)\rangle}\,. \tag{44}$$

The second part of Eq. (44) follows immediately using the definition of Fourier transform

$$\delta D(\vec{k})=\frac{1}{N}\sum_i e^{i\vec{k}\cdot\vec{R}_i}\,\delta D_i\,. \tag{45}$$

The relaxation time characterizing the decay of the autocorrelation function is then

$$\tau^A_{\delta B\delta C}=\int_0^\infty dt\,\phi^A_{\delta B\delta C}(t), \tag{46}$$

and its exponents $\Delta^A_{\delta B\delta C}$ and $(\Delta^A_{\delta B\delta C})'$ follow from the relations

$$\tau^A_{\delta B\delta C}\propto\begin{cases}(-\epsilon)^{-(\Delta^A_{\delta B\delta C})'}, & \text{for } T_c-T\to 0^+\\ (\epsilon)^{-\Delta^A_{\delta B\delta C}}, & \text{for } T-T_c\to 0^+\,.\end{cases} \tag{47}$$

The variables in which we are actually interested, δB and δC, are the order parameter and energy, respectively:

$$\delta B(\vec{k},t)\text{ or }\;\delta C(\vec{k},t)=\begin{cases}\delta\mu(\vec{k},t)=\dfrac{1}{N}\sum_i e^{i\vec{k}\cdot\vec{R}_i}\delta\mu_i(t)\\ \delta\mathcal{H}(\vec{k},t)=\dfrac{1}{N}\sum_i e^{i\vec{k}\cdot\vec{R}_i}\delta\mathcal{H}_i(t)\,,\end{cases} \tag{48}$$

where, according to Eq. (37)

$$\delta\mu_i(t)=\mu_i(t)-\langle\mu\rangle \tag{49}$$

and

$$\delta\mathcal{H}_i(t)=-\sum_j J_{ij}\,\mu_i\,\mu_j(t)-\langle\mathcal{H}\rangle\,. \tag{50}$$

Using Eqs. (48)–(50) in Eqs. (36)–(47), we have the formal definitions of all relaxation functions and relaxation times introduced on a phenomenological basis in Sec. II [Eqs. (16)–(37)]. While these quantities are derived experimentally from time averages over a metastable state of a finite system, we give these quantities in this section their conventional meaning as ensemble averages taken in a canonic ensemble, namely,

$$\langle D\rangle=\operatorname{Tr}\rho D=\frac{\operatorname{Tr}e^{-\mathcal{H}/k_BT}D}{\operatorname{Tr}e^{-\mathcal{H}/k_BT}}\,. \tag{51}$$

Since the kinetic Ising system is ergodic by construction, the definitions given in Secs. II and III become equivalent in the thermodynamic limit $N\to\infty$. We are now in a position to discuss several important concepts concerning the theory of critical slowing down.

B. Conventional Theory

This concept has been first derived by van Hove[32] for the critical slowing down of the order parameter. It states that the slowing down of the order-parameter relaxation is determined by the static fluctuation of the order parameter, i.e., the susceptibility

$$\tau_{\delta\mu\delta\mu}\propto\langle\delta\mu(0,0)\,\delta\mu(0,0)\rangle=k_BT\chi_T, \tag{52}$$

and thus implies

$$\Delta_{\delta\mu\delta\mu}=\gamma. \tag{53}$$

These results, Eqs. (52) and (53), turn out to be correct in the mean-field theory,[24] which should be a reasonable description for an Ising system with long-range interactions. In this case the stronger result is found that $\delta\mu(0,0)$ is an eigenvector of the Liouville operator L; i.e., we have

$$L\delta\mu(0,0)=\lambda\delta\mu(0,0), \tag{54}$$

and thus it follows

$$\delta\mu(0,t)=e^{-\lambda t}\delta\mu(0,0) \tag{55}$$

and

$$\phi_{\delta\mu\delta\mu}(0,t)=e^{-\lambda t} \tag{56}$$

turn out to be a simple exponential. From Eq. (54) it is easy to determine the eigenvalue λ deriving the first moment which is a finite and nonvanishing constant at T_c:

$$\lambda=\frac{\langle\delta\mu(0,0)\,L\delta\mu(0,0)\rangle}{\langle\delta\mu(0,0)\,\delta\mu(0,0)\rangle}\propto\frac{1}{\chi_T}\,. \tag{57}$$

Equation (56) further implies that all moments can be simply expressed in terms of the first one; specifically, it is found that

$$\langle\delta\mu(0,0)\,L^2\delta\mu(0,0)\rangle=\lambda^2\langle\delta\mu 0,0)\,\delta\mu(0,0)\rangle$$

$$=\frac{\langle\delta\mu(0,0)\,L\delta\mu(0,0)\rangle^2}{\langle\delta\mu(0,0)\,\delta\mu(0,0)\rangle}\,, \tag{58}$$

i.e., the ratio of the second and first moments should tend to zero as T approaches T_c. Of course it is not expected that this result of a random-phase approximation is actually correct for an Ising magnet with short-range (nearest-neighbor!) interactions. Abe and Hatano[20] succeeded in calculating $\langle\delta\mu(0,0)\,L\delta\mu(0,0)\rangle$ and $\langle\delta\mu(0,0)\,L^2\delta\mu(0,0)\rangle$ exactly at T_c. The temperature dependence of these quantities can also be estimated with the aid of the Monte Carlo technique as shown in Fig. 4.

For comparison we also included high-temperature-expansion results (see Appendix B) and Monte Carlo results obtained from the average transition probability $\langle W_j\rangle$ [Eq. (7)]. We note that

$$2\langle W_j\rangle=\langle\delta\mu(0,0)\,L\delta\mu(0,0)\rangle. \tag{59}$$

The good agreement between the results obtained by three different methods (Fig. 4) proves the consistency of our Monte Carlo calculation. The finite second moment [Fig. 4(b)] shows that Eq. (58) and thus Eqs. (54)–(57) are not correct. As

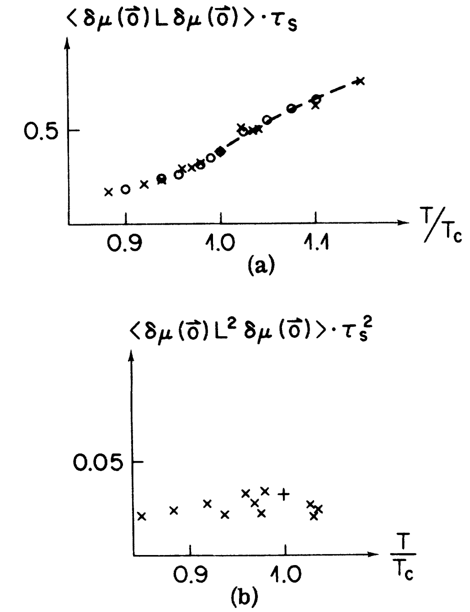

FIG. 4. Calculated temperature dependence of (a) $\langle \delta\mu(0) L \delta\mu(0) \rangle$ and (b) $\langle \delta\mu(0) L^2 \delta\mu(0) \rangle$ for a 55×55 square Ising lattice with nearest-neighbor interactions and periodic boundary conditions. For comparison we included the exact results (+) of Abe and Hatano:,[20] O denotes $2\langle W_j \rangle$ and the broken line the series-expansion results [Eq. (B28)]. These results have been renormalized by the factor $1/g(T)$ [Eq. (10b)].

a consequence, $\mu(0,0)$ is not an eigenvector of L, so that a cumulant representation[33] of the relaxation function would require the knowledge of all moments. However, the failure of Eqs. (54)–(58) does not necessarily imply that also Eqs. (52) and (53) are invalid. It only states that the decay time $\tau_{\delta\mu\delta\mu}$ is different from the decay-time constant $\tau^I_{\delta\mu\delta\mu}$ of the initial decay, defined by

$$\phi_{\delta\mu\delta\mu}(0,t) \sim e^{-t/\tau^I_{\delta\mu\delta\mu}}, \tag{60}$$

in the small t limit, with

$$\tau^I_{\delta\mu\delta\mu} = \frac{k_B T \chi_T}{\langle \delta\mu(0,0)\,\delta\mu(0,0)\rangle}, \tag{61}$$

and defining its exponent $\Delta^I_{\delta\mu\delta\mu}$ by

$$\tau^I_{\delta\mu\delta\mu} \propto |\epsilon|^{-\Delta^I_{\delta\mu\delta\mu}} \tag{62}$$

we immediately get from Eq. (61) the exact result[10]:

$$\Delta^I_{\delta\mu\delta\mu} = \gamma. \tag{63}$$

While it is always true that $\Delta^I_{\delta\mu\delta\mu} = \gamma$, $\Delta_{\delta\mu\delta\mu}$ can be different from $\Delta^I_{\delta\mu\delta\mu}$, depending on the precise asymptotic temperature dependence of the moments. If $\Delta_{\delta\mu\delta\mu} > \Delta^I_{\delta\mu\delta\mu} = \gamma$ we speak of a "kinetic slowing down" of the order-parameter fluctuations.

Finally, we briefly mention some extensions[12,16,34] of the conventional theory to include energy fluctuations. It is suggested[12,16] that in this case equations analogous to Eqs. (52) and (53) hold, i.e. [cf. also Eqs. (22) and (27)],

$$\tau_{\delta\mu\delta\mu} \propto \langle \delta\mu(0,0)\,\delta\mu(0,0)\rangle = k_B T \chi_{\delta\mu\delta\mu}, \tag{64}$$

$$\tau_{\delta\mathcal{H}\delta\mathcal{H}} \propto \langle \delta\mathcal{H}(0,0)\,\delta\mathcal{H}(0,0)\rangle = C_H k_B T^2, \tag{65}$$

since

$$k_B T\,|\chi_{\delta\mu\delta\mathcal{H}}| \equiv \frac{\partial\langle\mu\rangle}{\partial(1/k_B T)} \propto |\epsilon|^{\beta-1} \quad \text{for } T \to T_c^-. \tag{66}$$

Equations (64) and (65) imply

$$\Delta_{\delta\mu\delta\mathcal{H}} = 1-\beta, \quad \Delta_{\delta\mathcal{H}\delta\mathcal{H}} = \alpha. \tag{67}$$

However, recently it has been shown[22] that this extension of the conventional theory does not even hold in the mean-field theory.

C. Rigorous Inequalities

While an exact calculation of the relaxation functions defined in Eqs. (44) and (46) is possible in one dimension only[6] [here Eqs. (54)–(57) hold, but there is no phase transition; for explicit results see Appendix A], rigorous lower bounds for various relaxation functions and times, respectively, can be obtained[12,20–22] also for higher-dimensional systems. This approach makes use of rather general properties of the problem, for example, the semipositive-definiteness of L, together with such well-known mathematical relations as the Schwarz inequality.[20,21] For the derivation of inequalities involving the energy fluctuations[22] it turned out to be convenient to use a generalized Mori[35] two-variable theory.[22] These rigorous lower bounds for the critical exponents of slowing down are summarized in Eqs. (68)–(74). Abe and Hatano[20] derived

$$\Delta_{\delta\mu\delta\mu} \geq \gamma, \quad (\Delta_{\delta\mu\delta\mu})' \geq \gamma, \tag{68}$$

Suzuki[12] derived

$$2(\Delta_{\delta\mu\delta\mathcal{H}})' \leq (\Delta_{\delta\mu\delta\mu})' + (\Delta_{\delta\mathcal{H}\delta\mathcal{H}})', \tag{69}$$

and Schneider[22] derived

$$\Delta_{\delta\mathcal{H}\delta\mathcal{H}} \geq \gamma, \quad (\Delta_{\delta\mathcal{H}\delta\mathcal{H}})' \geq \gamma, \quad (\Delta_{\delta\mu\delta\mathcal{H}})' \geq \gamma. \tag{70}$$

Note that $\phi_{\delta\mu\delta\mathcal{H}}(\vec{0},t)$ is defined only below T_c. It has been pointed out[22] that the aforementioned extension[16] of the conventional theory [Eqs. (64)–(67)] is inconsistent with the exact result Eq. (70).

Corresponding inequalities may be derived for the autocorrelation functions [Eq. (44)] by invoking the static scaling hypothesis,[2] which is exact in the 2d case. These inequalities are due to Halperin,[21]

$$\Delta^A_{\delta\mu\delta\mu} \geq \gamma - 2\beta, \quad (\Delta^A_{\delta\mu\delta\mu})' \geq \gamma - 2\beta, \tag{71}$$

and Schneider,[22]

$$(\Delta^A_{\delta\mu\delta\mathcal{H}})' \geq 1 - 2\beta, \tag{72a}$$

$$\Delta^A_{\delta\mathcal{K}\delta\mathcal{K}} \geq 0, \quad (\Delta^A_{\delta\mathcal{K}\delta\mathcal{K}})' \geq 0, \tag{72b}$$

$$2(\Delta^A_{\delta\mu\delta\mathcal{K}})' - (\Delta^A_{\delta\mu\delta\mu})' + (\Delta^A_{\delta\mathcal{K}\delta\mathcal{K}})' \leq 2\beta. \tag{73}$$

The zero in (72b) includes the possibility that there might be no divergence at all. Emphasizing the small value of β $[=\frac{1}{8}]$ in the two-dimensional Ising model and noting the trivial inequalities

$$\Delta^A_{\delta\mu\delta\mu} \leq \Delta_{\delta\mu\delta\mu}, \quad (\Delta^A_{\delta\mu\delta\mu})' \leq (\Delta_{\delta\mu\delta\mu})',$$
$$\Delta^A_{\delta\mathcal{K}\delta\mathcal{K}} \leq \Delta_{\delta\mathcal{K}\delta\mathcal{K}}, \quad (\Delta^A_{\delta\mathcal{K}\delta\mathcal{K}})' \leq (\Delta_{\delta\mathcal{K}\delta\mathcal{K}})', \tag{74}$$
$$(\Delta^A_{\delta\mu\delta\mathcal{K}})' \leq (\Delta_{\delta\mu\delta\mathcal{K}})',$$

which follow from the definitions (36), (41), (42), (44), (46), and (47), it becomes clear that the lower bounds (71) and (72a) are rather restrictive.

These rigorous inequalities [Eqs. (68)–(74)] are very helpful in discussing the validity of the numerical data [Sec. IV]; it will be pointed out that the "effective critical exponents" as deduced from a log-log plot of the relaxation function for $|\epsilon| \geq 0.01$ can be different from the "true" critical exponents considered in the present section. This difference is due to the existence of correction terms[2] to the leading critical behavior near T_c. Therefore "effective exponents" might violate the exact inequalities [Eqs. (68)–(74)], indicating the existence of important corrections.

D. Dynamic Scaling Hypothesis

The dynamic scaling hypothesis (DSH) was first formulated by Ferrell *et al.* in their study of the λ point of He^4.[14] Here we follow the reformulation of their approach due to Halperin and Hohenberg.[15] For this purpose we introduce the Fourier transform of the order-parameter relaxation function,

$$S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega) = (1/2\pi)\int_{-\infty}^{+\infty} dt\, e^{i\omega t}\, \phi_{\delta\mu\delta\mu}(\vec{k}, t). \tag{75}$$

The superscripts denote the sign of $T - T_c$. It is convenient to express its dependence on temperature as a dependence on the inverse correlation length κ. Then a "characteristic frequency" $\omega^c_{\delta\mu\delta\mu}$ is defined by

$$\frac{\int_{-\omega^c_{\delta\mu\delta\mu}}^{+\omega^c_{\delta\mu\delta\mu}} S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega)d\omega}{\int_{-\infty}^{+\infty} S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega)d\omega} = \frac{1}{S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k})} \times \int_{-\omega^c_{\delta\mu\delta\mu}}^{+\omega^c_{\delta\mu\delta\mu}} S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega)\, d\omega = \tfrac{1}{2}. \tag{76}$$

The shape function $F^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega/\omega^c_{\delta\mu\delta\mu})$ is defined by[15]

$$S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega) = \frac{1}{\omega^c_{\delta\mu\delta\mu}(\kappa, \vec{k})} S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}) \times F^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega/\omega^c_{\delta\mu\delta\mu}). \tag{77}$$

Equations (76) and (77) imply

$$\int_{-1}^{+1} F^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, x)\, dx = \tfrac{1}{2}, \quad \int_{-\infty}^{+\infty} F^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, x)\, dx = 1. \tag{78}$$

The DSH involves the following assumptions:

$$F^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, x) = f^{\pm}_{\delta\mu\delta\mu}(\vec{k}/\kappa, x), \tag{79}$$

$$\omega^{c\pm}_{\delta\mu\delta\mu}(\lambda\kappa, \lambda\vec{k}) = \lambda^{Z_{\delta\mu\delta\mu}}\, \omega^{c\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}); \tag{80}$$

$Z_{\delta\mu\delta\mu}$ denotes the critical exponent associated with $\omega^c_{\delta\mu\delta\mu}$. In addition, scaling of the static correlation function $S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k})$, implies[1–3]

$$S^{\pm}_{\delta\mu\delta\mu}(\lambda\kappa, \lambda\vec{k}) = \lambda^{V_{\delta\mu\delta\mu}}\, S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}), \quad V_{\delta\mu\delta\mu} = -2 + \eta. \tag{81}$$

Using these expressions, the relaxation times of critical slowing down of the order-parameter correlation function $\tau^{\pm}_{\delta\mu\delta\mu}$, Eqs. (18) and (41) and of the associated autocorrelation function $\tau^{A\pm}_{\delta\mu\delta\mu}$, Eqs. (19) and (46) assume the following forms:

$$2\tau^{\pm}_{\delta\mu\delta\mu} \equiv \frac{S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}=0, \omega=0)}{S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}=0)} = 2\,\frac{\int_0^\infty dt\, \langle \delta\mu(0,0)\delta\mu(0,t)\rangle}{\langle \delta\mu(0,0)\delta\mu(0,0)\rangle}$$
$$= 2\int_0^\infty \phi_{\delta\mu\delta\mu}(0,t)\, dt = \kappa^{-Z_{\delta\mu\delta\mu}}\, \frac{f^{\pm}_{\delta\mu\delta\mu}(0,0)}{\omega^{c\pm}_{\delta\mu\delta\mu}(1,0)} \tag{82}$$

and

$$2\tau^{A\pm}_{\delta\mu\delta\mu} \equiv \frac{\sum_k S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k}, \omega=0)}{\sum_k S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k})} = 2\,\frac{\int_0^\infty dt\, \langle \delta\mu_i(0)\delta\mu_i(t)\rangle}{\langle \delta\mu_i(0)\delta\mu_i(0)\rangle}$$
$$= 2\int_0^\infty \phi^A_{\delta\mu\delta\mu}(t)\, dt \sim \kappa^{-(Z_{\delta\mu\delta\mu} - V_{\delta\mu\delta\mu} - d)} \times \sum_{k/\kappa} \frac{S^{\pm}_{\delta\mu\delta\mu}(1, \vec{k}/\kappa)\, f^{\pm}_{\delta\mu\delta\mu}(\vec{k}/\kappa, 0)}{\omega^{c\pm}_{\delta\mu\delta\mu}(1, \vec{k}/\kappa)}. \tag{83}$$

d denotes the dimensionality of the k summation. In Eq. (83) we used the fact that $\sum_k S^{\pm}_{\delta\mu\delta\mu}(\kappa, \vec{k})$ is nonzero and finite at T_c. Also the sum in Eq. (83) is only a slowly varying function of temperature near T_c[15] so that according to Eqs. (81)–(83),

$$\frac{\tau^{\pm}_{\delta\mu\delta\mu}}{\tau^{A\pm}_{\delta\mu\delta\mu}} \sim \kappa^{-(V_{\delta\mu\delta\mu}+d)} \sim |\epsilon|^{-\nu(V_{\delta\mu\delta\mu}+d)} \sim |\epsilon|^{-\nu(d-2+\eta)}, \tag{84}$$

where we used $\kappa = \kappa_0^{\pm}|\epsilon|^{\nu}$. This DSH prediction, Eq. (84), implies for the critical exponents $\Delta_{\delta\mu\delta\mu}$ and $\Delta^A_{\delta\mu\delta\mu}$ [Eqs. (42) and (47)]

$$\nu Z_{\delta\mu\delta\mu} - \Delta^A_{\delta\mu\delta\mu} = \Delta_{\delta\mu\delta\mu} - \Delta^A_{\delta\mu\delta\mu} = \nu(d-2+\eta) = 2\beta. \tag{85}$$

In the last step we used the scaling relations[1–3] $\gamma = (2-\eta)\nu$ and $\gamma + 2\beta = d\nu$ to derive the equality between exponents

$$\Delta_{\delta\mu\delta\mu} - \Delta^A_{\delta\mu\delta\mu} = 2\beta \ (=\tfrac{1}{4} \ \text{for}\ d=2). \tag{86}$$

Furthermore, it implies symmetry above and below T_c; i.e.,

$$\Delta_{\delta\mu\delta\mu} = (\Delta_{\delta\mu\delta\mu})', \quad \Delta^A_{\delta\mu\delta\mu} = (\Delta^A_{\delta\mu\delta\mu})'. \tag{87}$$

Similar predictions can be derived for the energy relaxation times using an "extended dynamic" scaling hypothesis." The derivation is completely analogous to Eqs. (75)–(87) but Eq. (81) has to be replaced by

$$S^{-}_{\delta\mu\delta\mathcal{H}}(\lambda\kappa,\lambda\vec{k})=\lambda^{V_{\delta\mu\delta\mathcal{H}}}S^{-}_{\delta\mu\delta\mathcal{H}}(\kappa,\vec{k}),\quad V_{\delta\mu\delta\mathcal{H}}=\frac{-1+\beta}{\nu} \tag{88}$$

or

$$S^{\pm}_{\delta\mathcal{H}\delta\mathcal{H}}(\lambda\kappa,\lambda\vec{k})=\lambda^{V_{\delta\mathcal{H}\delta\mathcal{H}}}S^{\pm}_{\delta\mathcal{H}\delta\mathcal{H}}(\kappa,\vec{k}),\quad V_{\delta\mathcal{H}\delta\mathcal{H}}=-\alpha/\nu. \tag{89}$$

The case $\alpha=0$ corresponds to the logarithmic anomaly of the specific heat in the $2d$ Ising model.[1–3] The results corresponding to Eqs. (86) and (87) are

$$(\Delta_{\delta\mu\delta\mathcal{H}})'-(\Delta^{A}_{\delta\mu\delta\mathcal{H}})'=1-\alpha, \tag{90}$$

where the result

$$\langle\delta\mu_i(0)\delta\mathcal{H}_i(0)\rangle\propto(-\epsilon)^{\beta},\quad T\to T_c^- \tag{91}$$

has to be used in the analog of Eq. (83), and

$$\Delta_{\delta\mathcal{H}\delta\mathcal{H}}-\Delta^{A}_{\delta\mathcal{H}\delta\mathcal{H}}=2(1-\alpha), \tag{92}$$

$$\Delta_{\delta\mathcal{H}\delta\mathcal{H}}=(\Delta_{\delta\mathcal{H}\delta\mathcal{H}})',\quad \Delta^{A}_{\delta\mathcal{H}\delta\mathcal{H}}=(\Delta^{A}_{\delta\mathcal{H}\delta\mathcal{H}})'. \tag{93}$$

Of course, a critical slowing down of the energy autocorrelation function is inferred only if $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}\geq 2(1-\alpha)$ and $\Delta^{A}_{\delta\mathcal{H}\delta\mathcal{H}}\geq 0$; otherwise the autocorrelation time of the energy has a finite cusp at T_c. Since the numerical calculation is performed rather in time than in frequency space it is helpful to translate the DSH from the $(\vec{k},\omega)$ into a $(\vec{k},t)$ representation. The equation analogous to Eq. (77) is

$$\langle\delta\mu(\vec{k},0)\delta\mu(\vec{k},t)\rangle=S^{\pm}_{\delta\mu\delta\mu}(\kappa,\vec{k})\,G^{\pm}_{\delta\mu\delta\mu}(\kappa,\vec{k},t/\tau^{c\pm}_{\delta\mu\delta\mu}). \tag{94}$$

Again it is required [cf. Eq. (78)] that

$$\int_0^{\infty}G^{\pm}_{\delta\mu\delta\mu}(\kappa,\vec{k},x)\,dx=1,\quad \int_0^{1}G^{\pm}_{\delta\mu\delta\mu}(\kappa,\vec{k},x)\,dx=\tfrac{1}{2}. \tag{95}$$

The DSH involves assumptions equivalent to Eqs. (79) and (80):

$$G^{\pm}_{\delta\mu\delta\mu}(\kappa,\vec{k},x)=g^{\pm}_{\delta\mu\delta\mu}(\vec{k}/\kappa,x), \tag{96}$$

$$\tau^{c\pm}_{\delta\mu\delta\mu}(\lambda\kappa,\lambda\vec{k})=\lambda^{-Z_{\delta\mu\delta\mu}}\,\tau^{c\pm}_{\delta\mu\delta\mu}(\kappa,\vec{k}). \tag{97}$$

From Eqs. (94)–(97) we immediately derive the scaling behavior of the function $\phi_{\delta\mu\delta\mu}(0,t)=\hat{\phi}_{\delta\mu\delta\mu}(t)$ [cf. Eq. (36)],

$$\hat{\phi}_{\delta\mu\delta\mu}(t)=g^{\pm}_{\delta\mu\delta\mu}\left(0,\ \frac{t}{\kappa^{-Z}\tau^{c\pm}_{\delta\mu\delta\mu}(1,0)}\right)$$
$$\cong g^{\pm}_{\delta\mu\delta\mu}(0,t|\epsilon|^{\Delta_{\delta\mu\delta\mu}}), \tag{98}$$

i.e., we may test the scaling behavior of the function $\hat{\phi}_{\delta\mu\delta\mu}(t)$ itself, suitably renormalizing the time scale. The order-parameter relaxation functions at all temperatures of the critical region should fit a single curve, thus determining the shape function $g^{\pm}(0,x)$, which does not depend on temperature. In order to save space we do not write down all the definitions and derivations for the other functions, but merely quote the results

$$\hat{\phi}^{A}_{\delta\mu\delta\mu}(t)\cong|\epsilon|^{2\beta}h^{\pm}_{\delta\mu\delta\mu}(t|\epsilon|^{\Delta_{\delta\mu\delta\mu}}), \tag{99}$$

where the function $h^{\pm}_{\delta\mu\delta\mu}(x)$, which is obtained from Eqs. (44) and (94)–(97) carrying out the integration over $\vec{k}$, should be, again, independent of temperature, and

$$\hat{\phi}_{\delta\mu\delta\mathcal{H}}(t)\cong g^{\pm}_{\delta\mu\delta\mathcal{H}}(0,t|\epsilon|^{\Delta_{\delta\mu\delta\mathcal{H}}}), \tag{100}$$

$$\hat{\phi}_{\delta\mathcal{H}\delta\mathcal{H}}(t)\cong g^{\pm}_{\delta\mathcal{H}\delta\mathcal{H}}(0,t|\epsilon|^{\Delta_{\delta\mathcal{H}\delta\mathcal{H}}}). \tag{101}$$

E. Determination of Exponents by Expansion Techniques

The technique of high-temperature series expansions[36] has been generalized by Suzuki, Yahata, and others (Refs. 8–11) to derive exponent estimates for the critical slowing down in the kinetic Ising model. In order to perform a comparison of these results with our numerical data which is as detailed as possible, we outline their method and our reanalysis of their results in Appendix B. The main results of those investigations[8–11] are

$$\Delta_{\delta\mu\delta\mu}=2.00\pm0.05,\quad \Delta_{\delta\mathcal{H}\delta\mathcal{H}}=2.00\pm0.05. \tag{102}$$

Also a series expansion for $\tau^{A}_{\delta\mu\delta\mu}$ is given[10] but does not allow for making precise statements about the exponent. The remarkable feature of Eq. (102) is that it disagrees with the conventional theory [Eq. (53)] and its extension [Eq. (67)]. Both relaxation times exhibit the phenomenon of a "kinetic slowing down," contrary to conjectures based on mode-mode coupling approach for anisotropic magnets[37] that the conventional theory for the order-parameter relaxation should be valid. Suzuki[12] conjectured ("similarity hypothesis") that the kinetic slowing down [i.e., deviation from Eqs. (53) and (67)] should have the same amount both for order parameter and energy fluctuations, which is also borne out to be incorrect. However, Eq. (102) is consistent with the rigorous inequalities Eqs. (68) and (70), respectively.

Another expansion technique which has been applied recently is the generalization of Wilson expansions[17] to dynamic critical phenomena.[13] This method does not apply to the kinetic Ising model directly but to a continuous analog[13]: from the universality[38] argument it is concluded[13] that the critical exponents should be the same as in the kinetic Ising model. These expansions are either expansions in $\epsilon = 4 - d$ (where d is the dimensionality of the system)[17] or in $1/n$ (where n is the "dimensionality of the spin").[39] From these expansions it is found[13] that the DSH is correct to order ϵ^2 or n^{-1}; for the exponent $Z_{\delta\mu\delta\mu}$ [Eq. (80)] it is found[13] that

$$Z_{\delta\mu\delta\mu} = 2 + (6\ln\tfrac{4}{3} - 1)\eta + O(\epsilon^3) \tag{103}$$

and

$$Z_{\delta\mu\delta\mu} = 2 + O(1/n^2) \quad (d=2), \tag{104}$$

while the conventional theory implied [Eqs. (53), (80), and (82)]

$$Z_{\delta\mu\delta\mu} = 2 - \eta. \tag{105}$$

These results [Eqs. (103) and (104)] support the existence of a kinetic slowing down and agree with the high-temperature series-expansion result [Eq. (102)], at least in the order of magnitude. The accuracy of Eqs. (103) and (104) for the $2d$ Ising model ($\epsilon = 2$, $n = 1$) seems questionable, however, since, for example, the prediction for the order-parameter exponent β is

$$\beta = \frac{1}{2}\left(1 - \frac{3}{4(n+8)}\epsilon + \frac{(2n+1)(n+2)}{4(n+8)^3}\epsilon^2\right) \approx 0.19, \tag{106}$$

which disagrees with the exact value[18] $\beta = \frac{1}{8} = 0.125$. This approach [Eqs. (103) and (104)] is expected to be more reliable for $d = 3$.

F. Nonequilibrium Relaxation

A critical behavior does not only show up in equilibrium relaxation functions, but also in the nonequilibrium relaxation. This relaxation occurs if a sudden change ΔT, ΔH in the intensive variables T, H is performed. This is a very common procedure in Monte Carlo calculations, since equilibrium configurations of the state to be investigated are not available at the very beginning of the procedure [cf. Sec. II and Fig. 1]. In the formal description of a nonequilibrium process, one assumes that the system is in thermal equilibrium at times $t < 0$, described by some initial Hamiltonian $\mathcal{H}_0$ and initial density matrix ρ_0:

$$\rho(t) = \rho(0) = \rho_0 = \frac{e^{-\mathcal{H}_0/k_B T}}{\mathrm{Tr}\, e^{-\mathcal{H}_0/k_B T}} \quad \text{for} \quad t < 0. \tag{107}$$

Generalizing a treatment of Suzuki[29] we allow for sudden changes ΔH_j and ΔT_j (which may depend on the lattice site j). We then consider the evolution in time for some variable $B(\vec{k})$,

$$\langle B(\vec{k}, t)\rangle = \mathrm{Tr}\, \rho(t) \sum_i e^{i\vec{k}\cdot\vec{R}_i} B_i . \tag{108}$$

We may identify the density matrix $\rho(t)$ with the time-dependent probability $P(\sigma_1, \ldots, \sigma_N, t)$ obeying the master equation [Eq. (1)]. Since the system is constructed to be ergodic via the detailed balance condition [Eq. (2)], $P(t)$ will evolve towards the final probability distribution P_∞ or density matrix ρ_∞,

$$\rho_\infty = \frac{\exp(-\sum_j \mathcal{H}_j / k_B T_j)}{\mathrm{Tr}\exp(-\sum_j \mathcal{H}_j / k_B T_j)}, \quad t \to \infty \tag{109}$$

where

$$T_j = T + \Delta T_j, \quad H_j = H + \Delta H_j \tag{110}$$

and [cf. Eq. (6)]

$$\mathcal{H}_j = -\sum_{1(\neq j)} J_{1j}\, \mu_1 \mu_j - H_j \mu_j \mu_B . \tag{111}$$

It is now convenient to introduce a reduced function $\varphi(t)$ by[29]

$$\rho(t) = \varphi(t)\, \rho_\infty . \tag{112}$$

If we rewrite the master equation [Eq. (1)] in terms of the operator L introduced in Eq. (39),

$$\frac{d}{dt}\rho(t) = -L\rho(t), \tag{113}$$

we get an equation for $\varphi(t)$ in terms of a new operator L':

$$\frac{d}{dt}\varphi(t) = -L'\varphi(t), \tag{114}$$

with

$$L'\varphi = \rho_\infty^{-1} L \varphi \rho_\infty . \tag{115}$$

The formal solution of Eq. (114) is

$$\varphi(t) = e^{-L't}\varphi(0) = e^{-L't}\rho_0\rho_\infty^{-1} \tag{116}$$

and from Eqs. (108), (112), and (116) it follows that

$$\langle B(\vec{k}, t)\rangle = \mathrm{Tr}\,\rho(t)\, B(\vec{k}) \equiv \sum_{\{\mu_j\}} P(\mu_1, \ldots, \mu_N, t) B(\{\mu_j\}, \vec{k})$$
$$= \sum_{\{\mu_j\}} B(\{\mu_j\}, \vec{k}) P(\mu_1, \ldots, \mu_N, t) \tag{117a}$$
$$= \mathrm{Tr}\, B(\vec{k})\rho(t) = \mathrm{Tr}\, B(\vec{k})\varphi(t)\rho_\infty$$

or

$$\langle B(\vec{k}, t)\rangle = \mathrm{Tr}\, B(\vec{k})\, e^{-L't}\rho_0 = \mathrm{Tr}\,\rho_0\, e^{-L't} B(\vec{k}), \tag{117b}$$

where in the last step the symmetry relation[40] enters,

$$\langle f L' g\rangle = \langle g L' f\rangle, \tag{118}$$

which can be derived from arbitrary spin functions f, g from the detailed balance principle [Eq. (2)]. The meaning of the expectation brackets in Eqs. (108) and (117) is thus shown to be an average in the *initial* ensemble

$$\langle B(\vec{k},t)\rangle = \langle e^{-L't}B(k)\rangle_{T,H} \equiv \langle B(\vec{k},t)\rangle_{T,H}. \quad (119)$$

Now the nonequilibrium relaxation function is defined by

$$\phi_{\delta B}^{\Delta H_j,\Delta T_j}(\vec{k},t) \equiv \frac{\langle B(\vec{k},t)\rangle_{T,H} - \langle B(\vec{k},\infty)\rangle_{T,H}}{\langle B(\vec{k},0)\rangle_{T,H} - \langle B(\vec{k},\infty)\rangle_{T,H}}. \quad (120)$$

In close analogy to Eq. (41) we define its relaxation time

$$\tau_{\delta B}^{\Delta H_j,\Delta T_j} = \int_0^\infty \phi_{\delta B}^{\Delta H_j,\Delta T_j}(0,t)\,dt \equiv \int_0^\infty \hat{\phi}_{\delta B}^{\Delta H_j,\Delta T_j}(t)\,dt \quad (121)$$

and its critical exponent $\Delta_{\delta B,\Delta H,\Delta T}$ [cf. Eq. (12)],

$$\tau_{\delta B}^{\Delta H,\Delta T} \propto \begin{cases} (-\epsilon)^{(-\Delta_{\delta B,\Delta H,\Delta T})'} & \text{for } T_c - T \to 0^+, \\ (\epsilon^{-\Delta_{\delta B,\Delta H,\Delta T}} & \text{for } T - T_c \to 0^+. \end{cases} \quad (122)$$

In Ref. 29 it was conjectured that $\Delta_{\delta\mu,\Delta H,0}$ should be equal to $\Delta_{\delta\mu\delta\mu}$, and a series expansion for $\tau_\mu^{\Delta H,0}$ was given. In the Monte Carlo calculation usually $\tau_B^{0,\Delta T}$ is important and we thus proceed to relate the nonequilibrium relaxation function $\phi_B^{\Delta H_j,\Delta T_j}(\vec{k},t)$ to the appropriate equilibrium relaxation function $\phi_{\delta B\delta C}(\vec{k},t)$ considering the limiting case of $\Delta H_j \to 0$, $\Delta T_j \to 0$. First, one notes from the ergodicity property[41] that

$$\langle B(\vec{k},\infty)\rangle_{T,H} = \langle B(\vec{k})\rangle_{T+\Delta T_j,H+\Delta H_j}, \quad (123)$$

and then one uses the expansion

$$\langle B(\vec{k},t)\rangle_{T,H} = \langle B(\vec{k})\rangle_{T,H} - \frac{1}{k_BT}\sum_j [\langle B(\vec{k},t)\mu_j(0)\rangle_{T_j,H_j} - \langle B(\vec{k})\rangle_{T_j,H_j}\langle \mu_j\rangle_{T_j,H_j}]\Delta H_j$$
$$- \frac{1}{k_BT}\sum_j [\langle B(\vec{k},t)\mathcal{H}_j(0)\rangle_{T_j,H_j} - \langle B(\vec{k})\rangle_{T_j,H_j}\langle \mathcal{H}_j\rangle_{T_j,H_j}]\Delta T_j/T, \quad (124)$$

which is valid in the limit $\Delta H_j \to 0$, $\Delta T_j \to 0$, where the density matrix may be linearized

$$e^{-\mathcal{H}/k_BT} = \exp\Big(\sum_j \mathcal{H}_j/k_BT_j\Big) \times \Big(1 - \sum_j \frac{\mathcal{H}_j}{k_BT}\frac{\Delta T_j}{T} - \sum_j \frac{\mu_j}{k_BT}H_j\Big). \quad (125)$$

Introducing the Fourier transforms of ΔT_j and ΔH_j one derives from Eq. (124) [cf. Eq. (37)]

$$\langle \delta B(\vec{k},t)\rangle_{T,H} = -\frac{1}{k_BT}\Delta H(\vec{k})\langle \delta B(\vec{k},t)\delta\mu(\vec{k},0)\rangle - \frac{1}{k_BT}\frac{\Delta T(\vec{k})}{T}\langle \delta B(\vec{k},t)\delta\mathcal{H}(-\vec{k},0)\rangle. \quad (126)$$

Thus we get the relations

$$\lim_{\Delta H_j\to 0}\phi_{\delta B}^{\Delta H_j,0}(\vec{k},t) = \phi_{\delta B\delta\mu}(\vec{k},t), \quad (127a)$$

$$\lim_{\Delta T_j\to 0}\Phi_{\delta B}^{0,\Delta T_j}(k,t) = \phi_{\delta B\delta\mathcal{H}}(\vec{k},t). \quad (127b)$$

It is plausible to assume that the exponents $\Delta_{\delta B,\Delta H,\Delta T}$ introduced in Eq. (122) should be independent of the magnitude of ΔH or ΔT. Equations (127) thus imply abbreviating $\Delta_{\delta\mu,\Delta H,0} \equiv \Delta_{\delta\mu}^{\Delta H}$, $\Delta_{\delta\mu,0,\Delta T} \equiv \Delta_{\delta\mu}^{\Delta T}$, etc.,

$$\Delta_{\delta\mu}^{\Delta H} = \Delta_{\delta\mu\delta\mu}, \quad \Delta_{\delta\mu}^{\Delta T} = (\Delta_{\delta\mu\delta\mathcal{H}})' = \Delta_{\delta\mu}^{\Delta T'}, \quad \Delta_{\delta\mathcal{H}}^{\Delta T} = \Delta_{\delta\mathcal{H}\delta\mathcal{H}}. \quad (128)$$

A further equality of exponents is derived if one assumes the validity of Eq. (128) not only for finite changes ΔH, $\Delta T/T$ but also for infinite changes ($\Delta H = \infty$, $\Delta T = T$); the initial state of a fully aligned ferromagnet is achieved either by $T = 0$ or $H = \infty$, all correlations being identical in both cases. Thus heating the system at $H = 0$ from $T = 0$ to T abruptly or switching off an infinite field $H = \infty$ for a system at temperature T leads precisely to the same behavior. Thus we have

$$\Delta_{\delta\mu}^{\Delta H=\infty} = \Delta_{\delta\mu}^{\Delta T=T}, \quad \Delta_{\delta\mathcal{H}}^{\Delta H=\infty} = \Delta_{\delta\mathcal{H}}^{\Delta T=T}. \quad (129)$$

The assumption that Eq. (128) also holds in this case now implies that all exponents $\Delta_{\delta\mu\delta\mu}$, $(\Delta_{\delta\mu\delta\mathcal{H}})'$, and $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$ are equal,

$$\Delta_{\delta\mu\delta\mu} = (\Delta_{\delta\mu\delta\mathcal{H}})' = \Delta_{\delta\mathcal{H}\delta\mathcal{H}}. \quad (130)$$

IV. MONTE CARLO RESULTS

To estimate the critical exponents associated with the relaxation times $\tau^{\pm}_{\delta\mu\delta\mu}$, $\tau^{A\pm}_{\delta\mu\delta\mu}$, $\tau_{\delta\mu\delta\mathcal{H}}$, $\tau^{A}_{\delta\mu\delta\mathcal{H}}$, and $\tau^{\pm}_{\delta\mathcal{H}\delta\mathcal{H}}$, $\tau^{A\pm}_{\delta\mathcal{H}\delta\mathcal{H}}$, respectively, we used the Monte Carlo technique outlined in Sec. II. As pointed out in the last part of Sec. III these exponents may also be estimated considering nonequilibrium relaxation, and since this approach was used in the previous investigation of Ogita *et al.*[25] (without the justification given in Sec. III, however) we first present some results derived in this way.

In Fig. 5 we plotted the time dependence of $\hat{\phi}_{\delta\mu}^{0,T}(t)$ [Eqs. (32) and (120)], where we used the scaling representation [Eq. (98)], for a variety of temperatures $T > T_c$ and a 220×220 square lattice with nearest-neighbor interactions and pbc. For some temperatures two independent runs are shown to illustrate the magnitude of "statistical" errors. Within these errors all functions fit to one curve for all temperatures in the critical region; this fact demonstrates the statement [stronger than Eqs. (79)–(101)] that even nonequilibrium relaxation functions seem to obey the DSH in the critical region. It is important to note that for large times, $\hat{\phi}_{\mu}^{0,T}(t)$ may be approximated very well by a simple exponential. For each temperature the time integrations were performed in accordance with Eqs. (33) and (121) to derive the associated relaxation time $\tau_{\delta\mu}^{0,\Delta T}$. The calculated temperature dependence of $\tau_{\delta\mu}^{0,\Delta T\pm}$ is shown in Fig. 6 for $T > T_c$ and for $T < T_c$. Since one expects [Eq. (122)] a power-law divergence

$$\tau_{\delta\mu}^{0,\Delta T} = |\epsilon|^{-\Delta_{\delta\mu}^{\Delta T}} \{C_0 + C_1|\epsilon|^{x_1} + C_2|\epsilon|^{x_2} + \cdots\}, \quad (131)$$

it is appealing to plot $\Delta_{\delta\mu}^{\Delta T}$ in a log-log plot well known from experimental investigations, in order to estimate the critical exponent $\Delta_{\delta\mu}^{\Delta T}$,

$$\ln \tau_{\delta\mu}^{0,\Delta T} = -\Delta_{\delta\mu}^{\Delta T,\mathrm{eff}}(|\epsilon|) \ln|\epsilon| + \ln c_0, \quad (132)$$

where

$$\Delta_{\delta\mu}^{\Delta T,\mathrm{eff}}(|\epsilon|) = \Delta_{\delta\mu}^{\Delta T} - \ln[1 + (C_1/C_0)|\epsilon|^{x_1} + (C_2/C_0)|\epsilon|^{x_2} + \cdots]/\ln|\epsilon| \quad (133)$$

is an "effective" temperature-dependent "exponent"; in practice one takes the average of $\Delta_{\delta\mu}^{\Delta T,\mathrm{eff}}(|\epsilon|)$ over a certain temperature interval. One wants to estimate the "true" exponent $\Delta_{\delta\mu}^{\Delta T}$, of course; the effect of correction terms in Eq. (133) can be neglected if either their amplitudes are very small ($C_i/C_0 \ll 1$) or their exponents

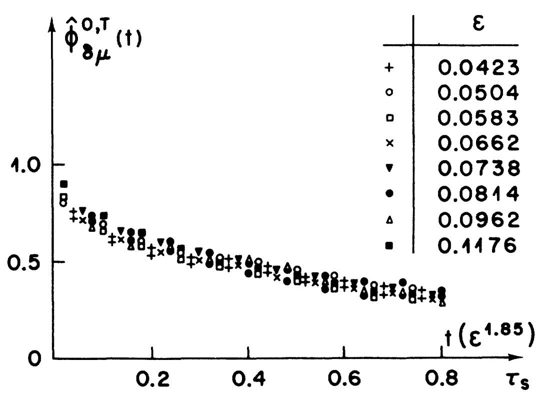

FIG. 5. Calculated time dependence of the nonequilibrium relaxation function [Eqs. (32) and (120)] for various temperatures above T_c and a 55×55 square lattice with nearest-neighbor interactions and periodic boundary conditions. At two temperatures two independent runs are plotted to display the magnitude of the statistical errors. The time scale was renormalized according to Eq. (98) in order to exhibit the dynamic scaling behavior.

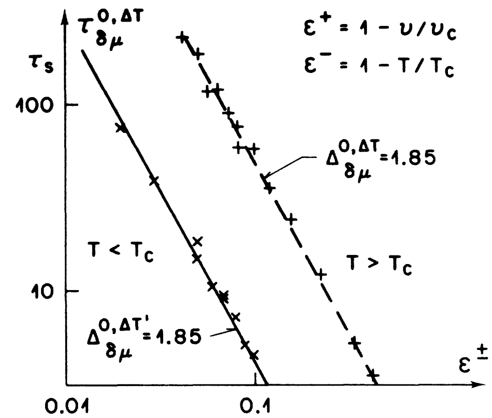

FIG. 6. Calculated temperature dependence of the relaxation time $\tau_{\delta\mu}^{0,\Delta T\pm}$ associated with $\hat{\phi}_{\mu}^{0,T}(t)$ shown in Fig. 7. The slopes indicated by the full and broken lines correspond to $\Delta_{\delta\mu}^{0,\Delta T} = 1.85$.

rather large ($x_i \approx 1$) or $|\epsilon|$ is made very small. In our computer simulation which is always done on finite systems, $|\epsilon|$ cannot be made arbitrarily small, there is an unattainable temperature interval of about $|\epsilon| \lesssim 0.02$. This restriction is simply understood since near T_c all relaxation times become large, and as a consequence accurate estimates require an increasing number of Monte Carlo steps (MCS) per spin. In practice, this requirement can only be met as long as conditions (13) and (14) are satisfied: this expresses the fact that T_c cannot be reached using a model system of finite size. Thus to make the correction terms in Eqs. (131) and (133) as small as possible we found it convenient to make plots versus $\epsilon^+ = 1 - v/v_c$ above T_c, where v is the high-temperature expansion variable $\tanh(2J/k_B T)$. From Fig. 6 no indication of important correction terms can be seen, and thus we tentatively estimate the critical exponent $\Delta_{\delta\mu}^{\Delta T}$:

$$\Delta_{\delta\mu}^{\Delta T} \approx \Delta_{\delta\mu}^{\Delta T'} \approx 1.85 \pm 0.10, \quad (134)$$

as indicated in the figure. This result is consistent with the previous estimate,[25] and combining it with Eq. (130) is consistent with the inequality Eq. (70).

Next we turn to the slowing down of the equilibrium relaxation functions. The relaxation functions defined in Sec. II were calculated at several temperatures, and integrating them the associated relaxation times were estimates. In Fig. 7 the temperature dependence of the order-parameter relaxation time $\tau_{\delta\mu\delta\mu}^{\pm}$ is plotted for $T < T_c$ and $T > T_c$. Since it might be conjectured that our data are seriously affected by the finite-size rounding phenomena,[31,42,43] we perform calculations for systems of various size, e.g., $N = 20\times20$, 55×55, and

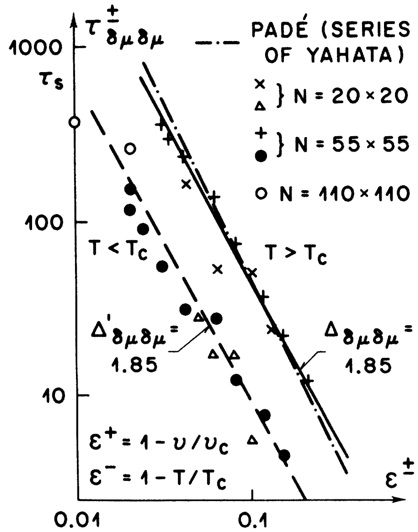

FIG. 7. Calculated temperature dependence of the relaxation time $\tau^{\pm}_{\delta\mu\delta\mu}$ [Eq. (18)] associated with the magnetization correlation function. The slopes indicated by the full and broken lines correspond to $\Delta_{\delta\mu\delta\mu}=1.85$. For comparison we included the Padé approximants to the series expansions of Yahata (Ref. 11). These estimates have been renormalized by $g(T)$ [Eq. (10b)].

110×110. Including the data of the smallest system above T_c, it turned out to be essential to take the "shift" of T_c into account. This shift was taken from the exact calculation[37] to be

$$\Delta T_c/T_c=-0.36/\sqrt{N}\,. \tag{135}$$

Then it appears that independent of N all data points fit the same curves both above and below T_c, yielding the estimate

$$\Delta_{\delta\mu\delta\mu}\approx(\Delta_{\delta\mu\delta\mu})'\approx 1.85\pm 0.10. \tag{136}$$

Even if we neglect the shift of T_c [Eq. (135)] the same result [Eq. (136)] is obtained, provided N is greater than 55×55, as in our preliminary communication,[23] where it was stressed that our result [Eq. (136)] does not rule out the validity of the conventional theory [Eq. (53)]. It is also important to note that the data of Fig. 7 should not be invalidated by the rounding phenomena, since our smallest $|\epsilon|\approx 0.03$ and, according to Ref. 31, $|\epsilon|^{\text{rounding}}\lesssim|\epsilon|^{\text{shift}}$ holds. This result can be understood qualitatively from the fact that, for example, at $T/T_c=1.07$ the correlation length has the value $\xi\sim 8$, which is still small compared to the linear dimensions of our systems. On the low-temperature side this situation is even more favorable, because $2\xi_0^-=\xi_0^+=1/1.76$.[2] These facts exclude the possibility that our results are seriously affected by the rounding phenomena. We note that the same conclusion is evident from Figs. 2 and 3.

The kinetic slowing down predicted by Eq. (136) is somewhat smaller than the high-temperature series prediction, Eq. (102). In order to elucidate this slight numerical discrepancy we reanalyzed the series expansions [Appendix B] and formed Padé approximants to them; the dashed-dotted curve included in Fig. 7 is a numerical approximation obtained in this way. It is seen that the numerical agreement between the series result and our data points is, in fact, remarkably good, in spite of the slightly different exponents. Since other curves also fit better to exponents near 1.85 than to 2.0, we are in favor of the value of Eq. (136) instead of 2.0; the possibility of effects due to corrections [Eqs. (131)–(133)] should not be forgotten, however, and as also pointed out in Appendix B, the series extrapolation approach suffers from several uncertainties. Therefore the slight discrepancy between Eqs. (102) and (136) should be taken as a measure of the uncertainty still inherent in the determination of exponents by numerical techniques.

In Fig. 8 the calculated temperature dependence of the order-parameter autocorrelation time $\tau^{A}_{\delta\mu\delta\mu}$ is shown. Again the two systems $N=20\times 20$ and $N=55\times 55$ yielded results consistent with each other. From Fig. 8 it is seen that the "effective exponents" are

$$\begin{aligned}\Delta^{A,\text{eff}}_{\delta\mu\delta\mu}&=1.35 \text{ for } T>T_c,\\ \Delta^{A,\text{eff}}_{\delta\mu\delta\mu}&=1.0 \text{ for } T<T_c,\end{aligned} \tag{137}$$

implying a pronounced asymmetry of the effective exponents above and below T_c.[44] Above T_c a series expansion of $\tau^{A}_{\delta\mu\delta\mu}$ is available.[10] However, as noted by these authors, the series for $\tau^{A}_{\delta\mu\delta\mu}$ has too few terms to yield reliable estimates from the ratio method. This fact is also evident from our Padé approximants to this series. In fact, only two Padé approximants could be formed, which in turn led to exponents $\Delta^{A}_{\delta\mu\delta\mu}=1.25$ and 1.33. Nevertheless, we included these estimates in Fig. 8. Combining Eqs. (137) and (136) we find

$$\Delta^{\text{eff}}_{\delta\mu\delta\mu}-\Delta^{A,\text{eff}}_{\delta\mu\delta\mu}\approx\begin{cases}1.85-1.35=0.5 & \text{for } T>T_c\\ 1.85-1.00=0.85 & \text{for } T<T_c,\end{cases} \tag{138}$$

which strongly implies that the effective exponents do not fulfill the dynamic scaling hypothesis [which predicted for the difference in Eq. (138) a value of $2\beta=\frac{1}{4}$, Eq. (86)]. In the absence of any rigorous knowledge about the exponents one would have to consider the possibility that Eq. (137) might indicate also a violation of the DSH for the "true" exponents.[23] From the rigorous inequality Eq. (71), $\Delta^{A}_{\delta\mu\delta\mu}\geq\frac{3}{2}$, owing to Halperin[21] it is immediately clear that the true value of $\Delta^{A}_{\delta\mu\delta\mu}$ must be con-

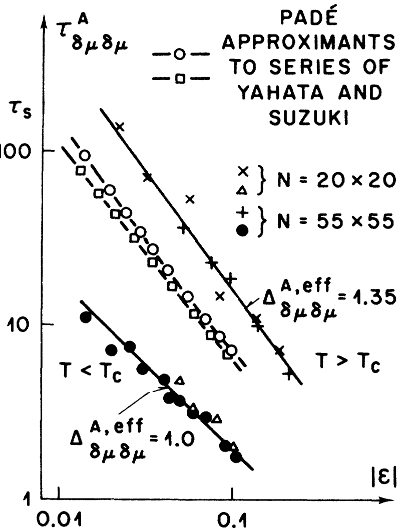

FIG. 8. Calculated temperature dependence of the order-parameter autocorrelation time $\tau^{A\pm}_{\delta\mu\delta\mu}$. The slopes indicated by the full and broken lines correspond to "effective" exponents $\Delta^{A,\mathrm{eff}}_{\delta\mu\delta\mu}=1.0$ for $T<T_c$ and $\Delta^{A,\mathrm{eff}}_{\delta\mu\chi\mu}=1.35$ for $T>T_c$, respectively. For comparison we also included Padé approximants to the series of Yahata and Suzuki (Ref. 10). O lead to $\Delta^{A}_{\delta\mu\delta\mu}=1.33$ and □ lead to $\Delta^{A}_{\mu\delta\mu}=1.25$. These estimates have been normalized by $g(T)$ [Eq. (10b)].

siderably larger than its "effective" value in the temperature range $0.02\leq|\epsilon|\leq 0.20$, Eq. (137). Such deviations between a "true" exponent Δ and an "effective" exponent Δ^{eff} are due to considerable correction terms, as explained in Eqs. (131)–(133). In order to also provide an estimate for the true exponent $\Delta^{A}_{\delta\mu\delta\mu}$, it is necessary to estimate the main correction terms. First we note that below T_c a correction will be caused from the temperature dependence of the normalizing denominator of $\tau^{A}_{\delta\mu\delta\mu}$, which is [Eqs. (17), (19), (44), (46), and (83)]

$$\sum_k S(\vec{k})=\langle\delta\mu_i(0)\delta\mu_i(0)\rangle=1-B^2\epsilon^{2\beta}, \quad T<T_c \tag{139}$$

where $B\approx 1.22$ is the critical amplitude of the spontaneous magnetization.[2] For $\tau_{\delta\mu\delta\mu}$, etc., the leading temperature dependence of the denominator does not give rise to corrections, since the denominator is critical and thus its temperature dependence changes the "true" exponent, while the cusp-shaped temperature dependence of Eq. (139) enters only into the correction terms. Thus it seems preferable to plot $\tau^{A}_{\delta\mu\delta\mu}\sum_k S(\vec{k})$ below T_c instead of $\tau^{A}_{\delta\mu\delta\mu}$ itself to remove this correction term.[45] Furthermore, it is useful to note that $\tau^{A}_{\delta\mu\delta\mu}$ is an even function of v for $T>T_c$.[10] This fact implies that the effective exponent $\Delta^{A,\mathrm{eff}}_{\delta\mu\delta\mu}$ tends to zero for $\epsilon=1-|T_c/T|\to 1$. Therefore it seems reasonable to plot $\tau^{A}_{\delta\mu\delta\mu}$ on a $\epsilon_+=|1-v^2/v_c^2|$ scale in order to remove this trivial source of changeover of the effective exponent. In Fig. 9 the result of this removal of correction terms is shown: Again, $\tau^{A}_{\delta\mu\delta\mu}\sum_k S(\vec{k})$ fits to straight lines both above and below T_c, but the slopes are now very different from those given in Fig. 8. Instead of Eq. (137) we find

$$\Delta^{A}_{\delta\mu\delta\mu}=1.60\pm 0.10,\quad (\Delta^{A}_{\delta\mu\delta\mu})'=1.60\pm 0.10, \tag{140}$$

i.e., symmetric exponents, which are consistent with both the rigorous inequality of Halperin [Eq. (71)] and the predictions of the DSH [Eq. (86)]. In fact, from Eqs. (136) and (140) it follows that

$$\Delta_{\delta\mu\delta\mu}-\Delta^{A}_{\delta\mu\delta\mu}\approx 0.25\pm 0.15. \tag{141}$$

In order to test the accuracy of the present calculation, we included in Fig. 9 the rigorous lower bound for $\tau^{A}_{\delta\mu\delta\mu}$ derived by Halperin[21]:

$$\tau^{A}_{\delta\mu\delta\mu}\geq\frac{1}{N\Gamma}\sum_k S^2(\vec{k})\sim|\epsilon|\Delta^{A,\mathrm{L.B.}}_{\delta\mu\delta\mu}, \tag{142}$$

where the abbreviation L. B. denotes lower bound and Γ denotes [cf. Eqs. (59) and (7)]

$$\Gamma=2\langle W_j\rangle. \tag{143}$$

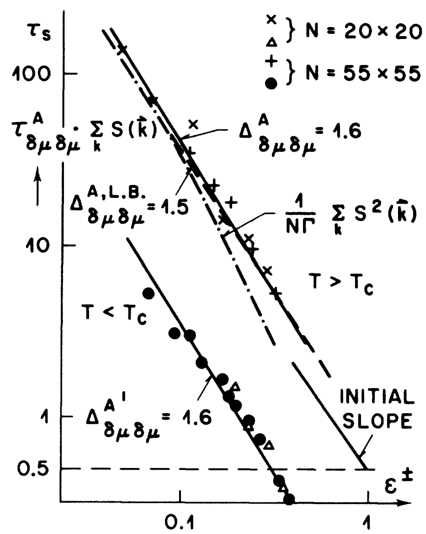

FIG. 9. Calculated temperature dependence of the "critical part" $\tau^{A}_{\delta\mu\delta\mu}\sum_k S(\vec{k})$ of the relaxation time $\tau^{A\pm}_{\delta\mu\delta\mu}$, where $\epsilon^+=1-(v/v_c)^2$ and $\epsilon^-=1-u/u_c$. The slopes indicated by the full lines correspond to $\Delta^{A}_{\delta\mu\delta\mu}=1.6$. The rigorous lower bound Eq. (142) is represented by the dashed-dotted line; its asymptotic slope is indicated by the broken line and corresponds to $\Delta^{A,\mathrm{LB}}_{\delta\mu\delta\mu}=1.5$; L. B. denotes the lower bound.

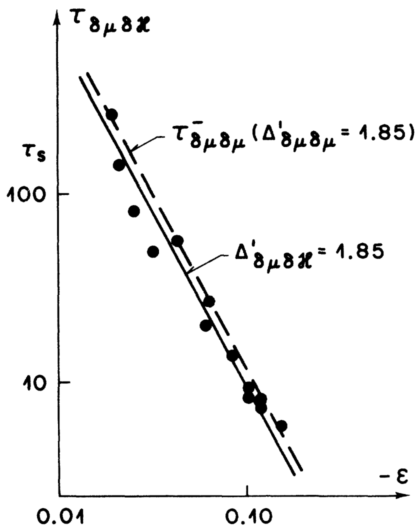

FIG. 10. Calculated temperature dependence of the relaxation time $\tau^-_{\delta\mu\delta\mathcal{H}}$ [Eq. (30)]. The slope indicated by the full line corresponds to $(\Delta_{\delta\mu\delta\mathcal{H}})' = 1.85$. For comparison we include the result obtained for $\tau^-_{\delta\mu\delta\mu}$ [broken line].

Noting that the available explicit exact solutions for pair correlations in the square lattice[46] apply to certain directions of $\vec{k}$ only, we evaluated the sum in Eq. (142) using the so-called "second Fisher-Burford approximant"[47] for $S(\vec{k})$:

$$S(\vec{k}) = \frac{1}{r_1^{2-\eta}} \frac{[\kappa^2 + \Phi^2 K^2(\vec{k})]^{\eta/2}}{[\kappa^2 + \Psi^2 (\vec{k})]}, \tag{144}$$

with[48]

$$\Psi^2 = 1 + \tfrac{1}{2}\eta\Phi^2 \tag{145}$$

and $[v \equiv \tanh(2J/k_B T)]$

$$\Phi^2 = 4\sqrt{2}\, v^4 \frac{1 - 2.360217 v}{1 - 0.360217 v - 4.220435 v^2}, \tag{146}$$

$$r_1 = 0.57959[1 - 0.350(T/T_c - 1)], \tag{147}$$

$$\log_{10}\kappa = \nu \log_{10}(T/T_c - 1) + 0.24640 - 0.299(T/T_c - 1). \tag{148}$$

The angular-dependent momentum $K^2(\vec{k})$ is in the case of the square lattice given by[47]

$$K^2(\vec{k}) = 4 - 2(\cos k_x + \cos k_y). \tag{149}$$

The accuracy of the expression Eq. (144) is by far sufficient, since for Γ we had to take the numerical values of the Monte Carlo calculation [see Fig. 4]. Figure 9 shows that all data points satisfy the rigorous inequality Eq. (142). It is further seen that the effective exponent of the lower bound is at high temperatures considerably higher ($\Delta^{\mathrm{eff}} \approx 1.7$) than its exact asymptotic value $\Delta^{A,\,\mathrm{L.B.}}_{\delta\mu\delta\mu} = 1.5$. Therefore it is clear that data of even higher statistical precision would not allow to give more accurate exponent estimates than the ones given in Eqs. (136) and (140). A higher accuracy can be obtained only from data which are closer to T_c, requiring considerably larger systems because of the conditions Eqs. (13) and (14); this is outside the scope of present computing possibilities.

In Fig. 9 we included also the initial slope of $\tau^A_{\delta\mu\delta\mu}$ at $v^2 \to 0$ [note that the limiting value of $\tau^A_{\delta\mu\delta\mu}$ $(v^2 \to 0) = 0.5$ and not 1.0 due to the renormalization of the time scale, Eq. (10b)].

Next we turn to the correlations involving energy correlations. In Fig. 10 the calculated temperature dependence of $\tau_{\delta\mu\delta\mathcal{H}}$ is plotted. Note that this relaxation time is defined below T_c only. Again we find

$$(\Delta_{\delta\mu\delta\mathcal{H}})' = 1.85 \pm 0.10, \tag{150}$$

which is consistent with inequality (70) and the estimate for $\Delta^{\Delta T}_{\delta\mu}$ [Eq. (134)] as expected [see Sec. III, Eq. (128)]. Furthermore we included our result for $\tau^-_{\delta\mu\delta\mu}$ in Fig. 10 to show that the critical amplitudes of $\tau^-_{\delta\mu\delta\mu}$ and $\tau^-_{\delta\mu\delta\mathcal{H}}$ are nearly equal. The coincidence of the values found for the exponents confirms Eq. (130).

In Fig. 11 the temperature dependence of the associated autocorrelation function $\tau^A_{\delta\mu\delta\mathcal{H}}$ is shown. From these data it is seen that the "effective"

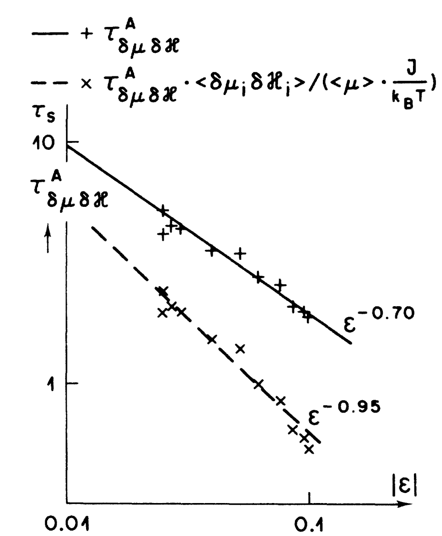

FIG. 11. Calculated temperature dependence of the relaxation time $\tau^{A-}_{\delta\mu\delta\mathcal{H}}$ [Eq. (31)] of the autocorrelation function [Eq. (29)]. The slope indicated by the full line corresponds to $(\Delta^A_{\delta\mu\delta\mathcal{H}})' = 0.95$.

exponent in the temperature regime investigated is $\Delta^{A,\mathrm{eff}}_{\delta\mu\delta\mathcal{H}} \approx 0.70 \pm 0.10$. In the case of $\tau^{A}_{\delta\mu\delta\mu}$ the effective exponent was considerably smaller [Eq. (137)] than the rigorous lower bound [Eq. (71)], while $\Delta^{A,\mathrm{eff}}_{\delta\mu\delta\mathcal{H}}$ is only slightly smaller than the associated lower bound $\tau^{A,\mathrm{L.B.}}_{\delta\mu\delta\mathcal{H}} = 0.75$ [Eq. (72a)]. Nevertheless it is easy to see that the denominator of $\tau^{A}_{\delta\mu\delta\mathcal{H}}$ (which can be calculated exactly) leads again to important correction terms. Therefore it is useful to eliminate these corrections as was done in the case of $\tau^{A}_{\delta\mu\delta\mu}$; here we have to consider the quantity $\Delta^{A}_{\delta\mu\delta\mathcal{H}} \langle \delta\mu_i\, \delta\mathcal{H}_i\rangle / (J/k_B T \langle \mu \rangle)$, which is also plotted in Fig. 11. From this plot we find

$$(\Delta^{A}_{\delta\mu\delta\mathcal{H}})' = 0.95 \pm 0.10. \qquad (151)$$

Combining the estimates (150) and (151) we obtain $(\Delta_{\delta\mu\delta\mathcal{H}})' - (\Delta^{A}_{\delta\mu\delta\mathcal{H}})' = 0.9 \pm 0.15$, which is consistent with the prediction of the extended DSH [$(\Delta_{\delta\mu\delta\mathcal{H}})' - (\Delta^{A}_{\delta\mu\delta\mathcal{H}})' = 1 - \alpha$; Eq. (90)].

In Fig. 12 the temperature dependence of the energy relaxation time $\tau_{\delta\mathcal{H}\delta\mathcal{H}}$ [Eq. (25)] is shown. Here we plotted the low-temperature data versus $\epsilon^{-} = 1 - u/u_c$, where $u = e^{-8J/k_B T}$. These data are less accurate than the order-parameter relaxation data, since they involve four spin correlations. The straight lines shown in the figure correspond to exponents

$$\Delta_{\delta\mathcal{H}\delta\mathcal{H}} \approx (\Delta_{\delta\mathcal{H}\delta\mathcal{H}})' \approx 2.00 \pm 0.10, \qquad (152)$$

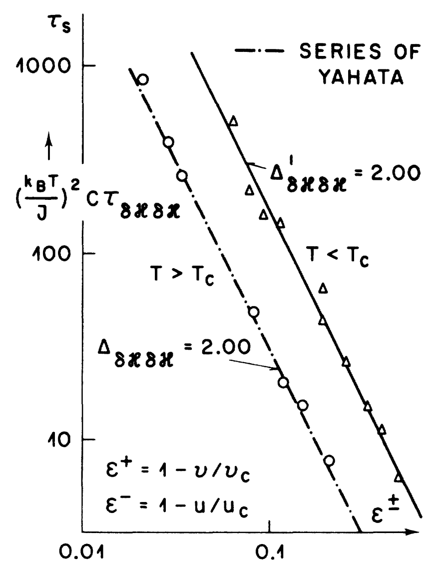

FIG. 12. Calculated temperature dependence of the energy relaxation time $\tau^{\pm}_{\delta\mathcal{H}\delta\mathcal{H}}$ [Eq. (25)]. The slopes indicated by the full and broken lines correspond to $\Delta_{\delta\mathcal{H}\delta\mathcal{H}} = 2.00$ and $(\Delta_{\delta\mathcal{H}\delta\mathcal{H}})' = 2.00$, respectively. The broken curve is the result of the series expansion (see Ref. 11).

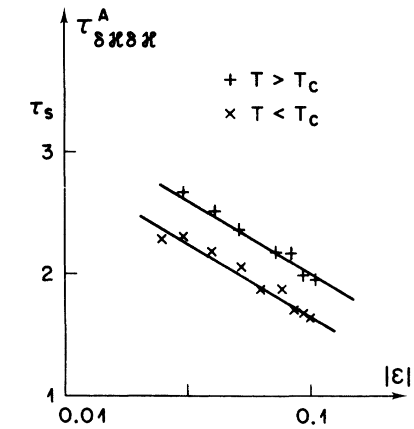

FIG. 13. Calculated temperature dependence of the relaxation time $\tau^{A\pm}_{\delta\mathcal{H}\delta\mathcal{H}}$ [Eq. (26)] of the energy autocorrelation function [Eq. (24)]. Note that the scale of $\tau^{A}_{\delta\mathcal{H}\delta\mathcal{H}}$ is here linear; thus the full lines correspond to a logarithmic divergence of $\tau^{A}_{\delta\mathcal{H}\delta\mathcal{H}}$.

which are consistent with the inequalities (72b) and in rough agreement with the conjecture expressed in Eq. (130). The estimates (136), (150), and (152) reveal that the exponents $\Delta_{\delta\mu\delta\mu}$, $(\Delta_{\delta\mu\delta\mathcal{H}})'$, and $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$ are nearly equal.

In Fig. 13 the temperature dependence of the energy autocorrelation time $\tau^{A}_{\delta\mathcal{H}\delta\mathcal{H}}$ [Eq. (26)] is shown. From the extended DSH [Eq. (92)] and the result (152) it is expected that $\Delta^{A}_{\delta\mathcal{H}\delta\mathcal{H}} \approx 0$, i.e., the energy autocorrelation time should diverge with a logarithmic singularity. This prediction is obviously consistent with our results shown in Fig. 13 and the lower bound (72b).

Finally, let us comment on the ratios of the relaxation times at corresponding temperatures above and below T_c. Conventional theory of slowing down predicts, according to Eq. (64),

$$\tau^{+}_{\delta\mu\delta\mu} / \tau^{-}_{\delta\mu\delta\mu} = \chi^{+}_{\delta\mu\delta\mu} / \chi^{-}_{\delta\mu\delta\mu}. \qquad (153)$$

In the two-dimensional Ising square lattice the ratio is 36.8.[2] From Fig. 14, it is seen that the calculated ratio is considerably smaller than that predicted by the conventional theory of slowing down. This result again indicates the failure of the conventional theory and is more reliable than the conclusions drawn from the dynamic exponents.

In judging the reliability of our estimates we recall the arguments why the following error sources do not invalidate our results.

(i) Correlation between pseudo-random-numbers: We used a random-number generator[49] by suitable mixing of several pseudo-random-number sequences, which was carefully tested. If serious correlations between the random numbers existed,

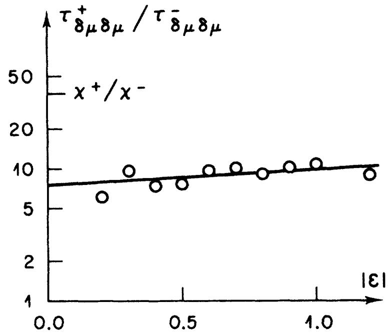

FIG. 14. Calculated ratio of the relaxation time of the order-parameter fluctuations at temperatures above and below T_c.

they should be visible in the calculations of the one-dimensional Ising model, described in Appendix A. No effect of such correlations could be detected. Such correlations would enhance the time-dependent spin correlations at short times.

(ii) Statistical inaccuracy: Since conditons (13) and (14) allow only time averages over finite-time intervals, the question arises whether or not the intervals considered are large enough to guarantee small statistical errors. It was shown in Sec. II and Refs. 28 and 30 that our choice of the time intervals leads to an accurate description of static properties like the static susceptibility (see also Fig. 2). The accuracy of our time-dependent quantities has been asserted in Appendix A. A further test of consistency is provided by Figs. 3 and 4.

(iii) Finite-size rounding phenomena: According to usual theories[31,42,43] these effects should occur only if the correlation length ξ is comparable to the linear dimension $N^{1/2}$ of the system. In fact, it has been shown[3] that rounding corrections are of the order $e^{-N^{1/2}/\xi}$. As shown above, this factor is very small in our case provided $|\epsilon| \geq 3\times10^{-2}$ This argument is well established with respect to static quantities; the results of Appendix A show that it also holds for dynamic quantities.

(iv) Time integration: In order to calculate the relaxation times, one has to perform time integrations [Eqs. (18), (19), (25), (26), (30), (31), and (35)] over time intervals t, which are short compared to the intervals available to perform time averages. It was found that the decay is exponential for large times. Using this fact we integrated to infinity in Eqs. (18), (19), (25), (26), (30), (31), and (35) by extrapolating this exponential. To justify this procedure it must be shown that the correlation functions already exhibit the asymptotic decay in the time intervals considered. Next we analyze the problem in more detail.

For this purpose it is interesting to estimate the time when the asymptotic decay shows up, using the series expansions where the critical exponents of initial and asymptotic decay are different. In doing so we consider the ratios of the critical amplitudes of the coefficients a_κ in the frequency expansion [Eq. (B22)]. From the expansion coefficients[11] f_n^κ we get for the order-parameter relaxation function

$$f_n^2/n^\Delta f_n^1 \approx 0.1, \quad f_n^3/n^{2\Delta} f_n^1 \approx 0.07. \tag{154}$$

The smallness of these coefficients indicates a rapid convergence of the series Eq. (B22). This, in turn, implies that the changeover of $f(x)$, defined in Eq. (B24), from the low- to the high-frequency behavior occurs for rather large x values, namely, $x \gg 1$. Consequently, we conclude that [Eq. (16)]

$$\hat{\phi}_{\delta\mu\delta\mu}(t) \approx \text{const} \exp[-(t/\tau_s) C_1 \epsilon^{\Delta_{\delta\mu\delta\mu}}] \tag{155}$$

for

$$(t/\tau_s)\epsilon^{\Delta_{\delta\mu\delta\mu}} \gtrsim 1. \tag{156}$$

C_1 is a constant of order unity. From Eq. (155) we may now estimate the time when the asymptotic decay as predicted by the series expansion should show up. The result is

$$t/\tau_s \approx (|\epsilon|^{7/4} - |\epsilon|^2). \tag{157}$$

Exponent $\frac{7}{4}$ is the exponent of the initial decay of $\hat{\phi}_{\delta\mu\delta\mu}(t)$ [Eq. (63)], and exponent 2 is series expansion estimate for $\Delta_{\delta\mu\delta\mu}$.[10,11] We note that the time when our exponential extrapolation was taken was always larger than t [Eq. (157)]. Consequently, our results for $\tau^\pm_{\delta\mu\delta\mu}$ cannot be seriously affected by calculating $\hat{\phi}_{\delta\mu\delta\mu}(t)$ for a very large but finite time only.

In summary, we conclude from remarks (i)–(iv) that sufficient accuracy has been achieved tc predict effective exponents with reliability of about 5%. These exponents refer to the temperature region $|\epsilon| \gtrsim 2\times10^{-2}$. It has to be stressed that possible experiments refer to a similar temperature region as our Monte Carlo calculations.

V. CONCLUDING REMARKS

It is clear that the kinetic Ising model in which each spin can flip according to prescribed transition probabilities should not be regarded as a model which faithfully simulates phenomena occurring in certain real systems. The value of the kinetic Ising model lies in the fact that it provides us with a precisely defined model in which no statistical approximations enter. This allows us the study of dynamic critical phenomena with techniques such as the high-temperature series-expansion approach, which was first developed for the study of static critical phenomena, and the Monte Carlo method. Since the alternative approaches to dynamic critical phenomena are still highly phenomenological, studies of the kinetic Ising model can be regarded as complementary and are expected to open a door towards a better understanding of the dynamics of phase transitions and critical phenomena.

In this work we extended the Monte Carlo technique to time-dependent critical phenomena. Among other tests of this method we calculated the one-dimensional kinetic Ising system and obtained striking agreement with the exact solution of Glauber.[6] The main purpose of this investigation was then to calculate various relaxation times of slowing down in the two-dimensional kinetic Ising system. The associated "effective" critical exponents have been determined with reasonable accuracy. Tentative arguments have been provided that these "effective" exponents should agree with the "true" ones within the given accuracy, except in the case of the order-parameter autocorrelation time: here, correction terms whose nature could be investigated in detail lead to pronounced changeover of critical exponents. Nevertheless, in the latter case also, a reasonable estimate for the "true" exponent $\Delta^A_{\delta\mu\delta\mu}$ could be obtained. A detailed comparison with all available results of other methods (for example, series expansions) has been performed. For the sake of clarity we collect in Table I all these exponent estimates so far available. It is seen that a large number of new exponents could be determined which have not been estimated by any other method previously. We found slight discrepancies with recent series-expansion estimates[10,11] for $\Delta_{\delta\mu\delta\mu}$ and $\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$. Therefore we gave a detailed discussion of reliability for both methods [Sec. IV, Appendix B], suggesting that the slight discrepancies indicate the magnitude of uncertainty still inevitable in the derivation of estimates for the exponents of slowing down with both methods. It is emphasized that the estimates of the (true) exponents in this paper are symmetric (with respect to the change of the sign of $T - T_c$), are consistent with the exact inequalities[12,20–22] and consistent with the dynamic scaling hypothesis.[14,15] While we have been able to derive all the relaxation times of interest, it was beyond present possibilities to determine the full $S(\kappa, \vec{k}, \omega)$ functions and the characteristic frequency [Eqs. (75) and (76)]. Nevertheless, the numerical results presented may promote a better understanding of dynamic critical phenomena in stochastic models, which so far have "remained a mystery."

ACKNOWLEDGMENTS

We express our sincere gratitude to B. I. Halperin for sending the detailed derivation of his inequality [Ref. 21] prior to publication. We

TABLE I. Relaxation times and exponents in the kinetic two-dimensional Ising model.

Relaxation time	Definition	Exponent	Previous investigations Kawasaki[a]	Suzuki[b,c]	Yahata[d]	4-d-exp.[e]	$1/n$-exp.[e]	Present investigations
$\tau^{+}_{\delta\mu\delta\mu}$	$\frac{\langle \delta\mu(1/L)\delta\mu \rangle}{\langle \delta\mu\delta\mu \rangle}$	$\Delta_{\delta\mu\delta\mu}$	1.75	2.00 ± 0.05	~ 2.0	~ 2.18	~ 2.0	1.85 ± 0.10
		$(\Delta_{\delta\mu\delta\mu})'$	1.75	⋯	⋯	~ 2.18	~ 2.0	1.85 ± 0.10
$\tau^{-}_{\delta\mu\delta\mathcal{H}}$	$\frac{\langle \delta\mu(1/L)\delta\mathcal{H} \rangle}{\langle \delta\mu\delta\mathcal{H} \rangle}$	$(\Delta_{\delta\mu\delta\mathcal{H}})'$	0.875[b]	1.125 ± 0.05	⋯	⋯	⋯	1.85 ± 0.10
$\tau^{\pm}_{\delta\mathcal{H}\delta\mathcal{H}}$	$\frac{\langle \delta\mathcal{H}(1/L)\delta\mathcal{H} \rangle}{\langle \delta\mathcal{H}\delta\mathcal{H} \rangle}$	$\Delta_{\delta\mathcal{H}\delta\mathcal{H}}$	0(log)	0.25 ± 0.05	~ 2.0	⋯	⋯	2.00 ± 0.10
		$(\Delta_{\delta\mathcal{H}\delta\mathcal{H}})'$	0(log)	⋯	⋯	⋯	⋯	2.00 ± 0.10
$\tau^{A\pm}_{\delta\mu\delta\mu}$	$\frac{\langle \delta\mu_i(1/L)\delta\mu_i \rangle}{\langle \delta\mu_i\delta\mu_i \rangle}$	$\Delta^A_{\delta\mu\delta\mu}$	⋯	⋯	⋯	~ 1.93	~ 1.75	1.60 ± 0.10
		$(\Delta^A_{\delta\mu\delta\mu})'$	⋯	⋯	⋯	~ 1.93	~ 1.75	1.60 ± 0.10
$\tau^{A-}_{\delta\mu\delta\mathcal{H}}$	$\frac{\langle \delta\mu_i(1/L)\delta\mathcal{H}_i \rangle}{\langle \delta\mu_i\delta\mathcal{H}_i \rangle}$	$(\Delta^A_{\delta\mu\delta\mathcal{H}})'$	⋯	⋯	⋯	⋯	⋯	0.95 ± 0.10
$\tau^{A\pm}_{\delta\mathcal{H}\delta\mathcal{H}}$	$\frac{\langle \delta\mathcal{H}_i(1/L)\delta\mathcal{H}_i \rangle}{\langle \delta\mathcal{H}_i\delta\mathcal{H}_i \rangle}$	$\Delta^A_{\delta\mathcal{H}\delta\mathcal{H}}$	⋯	⋯	⋯	⋯	⋯	~ 0(log)
		$(\Delta^A_{\delta\mathcal{H}\delta\mathcal{H}})$	⋯	⋯	⋯	⋯	⋯	~ 0(log)
$\tau^{0,T}_{\delta\mu}$ $[\tau^{\infty,0}_{\delta\mu}]^{c}$	see Eqs. (33) and (121)	$\Delta^{\Delta T}_{\delta\mu}$	⋯	~ 2.0[c]	⋯	⋯	⋯	1.85 ± 0.10
		$(\Delta^{\Delta T}_{\delta\mu})'$	⋯	⋯	⋯	⋯	⋯	1.85 ± 0.10

[a]Reference 16 (extended conventional theory; see Sec. III B).

[b]Reference 12 (similarity hypothesis: generalizes the treatment of Ref. 16 to take the kinetic slowing down as found from Refs. 8–11 into account).

[c]Reference 29 (high-temperature-series extrapolation; see Appendix B).

[d]Reference 11 (high-temperature-series extrapolation; see Appendix B).

[e]Reference 13 ("Wilson expansions" of Halperin, Hohenberg, and Ma; see Sec. III E).

should like to thank P. C. Hohenberg for helpful discussions and correspondence as well as for sending the preprint, Ref. 13. We acknowledge fruitful discussions with Y. Imry, R. Kubo, P. Meier, and H. Yahata. We thank P. Heller for a careful reading of the manuscript.

APPENDIX A: MONTE CARLO STUDY OF THE ONE-DIMENSIONAL KINETIC ISING MODEL

An exact solution for the kinetic Ising chain with the transition probability Eq. (7) has been given by Glauber[6]: all time-dependent pair correlation functions are thus known. A Monte Carlo calculation will not reveal new results in this case, but it will provide a sensitive test of the accuracy which can be achieved evaluating time-dependent quantities by the use of this technique. It is important to perform such a test, since several sources of inaccuracy have to be considered.

(i) No true random-number sequences are available for the Monte Carlo method, but only sequences produced by pseudo-random-number generators. If there existed any (higher-order) correlations between these numbers, time-dependent quantities would be seriously affected, while static pair correlations and similar quantities are less affected (these static quantities would be affected by low-order correlations between these numbers). Therefore the tests that have been made in connection with the calculation of static quantities[28,30] cannot rule out completely the possibility of such correlations.

(ii) Since the length of the Markov chain used for the Monte Carlo averages is finite, all quantities are affected by some statistical error. It is rather difficult to estimate this statistical inaccuracy precisely.[27] It can also be difficult to judge whether one is close enough to thermal equilibrium or whether there is still some influence of the starting configuration.

(iii) As discussed in Secs. II and IV the calculation is done for a finite lattice. As long as the correlation length ξ is much smaller than the linear dimension N of the lattice, this finite lattice is expected to simulate an infinite system very well. While this idea is well established with respect to static properties,[31,42,43] little is known about the finite-size effects upon dynamic quantities.

All these problems can be investigated very well considering the kinetic Ising chain. The time-dependent pair correlation function is given in terms of modified Bessel functions $I_l(x)$,[6]

$$\langle \mu_0(0)\mu_n(t)\rangle = e^{-t/\tau_s} \sum_{l=-\infty}^{+\infty} (\tanh \beta J)^{|n-l|} \times I_l((t/\tau_s)\tanh(2\beta J)). \quad \text{(A1)}$$

From Eq. (A1) it is shown that the correlation length ξ is given by

$$\xi = [\ln \tanh(\beta J)]^{-1}. \quad \text{(A2)}$$

Thus the finite-size rounding effects (iii) can be studied conveniently, since ξ gets very large at low temperatures.

In the computer simulation of the kinetic Ising chain the transition probability of Eq. (7) was used instead of Eq. (10a). There is no need to renormalize[27] the time scale as discussed in Sec. II. At several temperatures, systems with $N = 20$, 55, and 220 spins were calculated. As an example, the correlation functions are plotted for $N = 220$, $\beta J = 1$ in Fig. 15. The exact solution [Eq. (A1)] is represented by the dashed-dotted curves. Agreement between the exact calculation and the simulated results is very good. In this case 2.5×10^3 Monte Carlo steps per spin have been used. Note that in the two-dimensional case the total number of steps per spin was typically as large. It turned out that the autocorrelation function $\langle \mu_0(0)\mu_0(t)\rangle$ was already most accurate for very short Markov chains, while the inaccuracy increased with the distance n between the spins. But within the drawing accuracy of Fig. 15 the results of various shorter independent runs agreed with one another and also with the results for the $N = 55$ and $N = 20$ systems. It is interesting to mention that the correlation length ξ is $\xi \cong 3.7$ [Eq. (A2)] in the present example, which would correspond to $T/T_c \cong 0.92$ in the two-dimensional case.[2] These results prove convincingly that all three sources of inaccuracy mentioned above [(i)–(iii)] have quite negligible

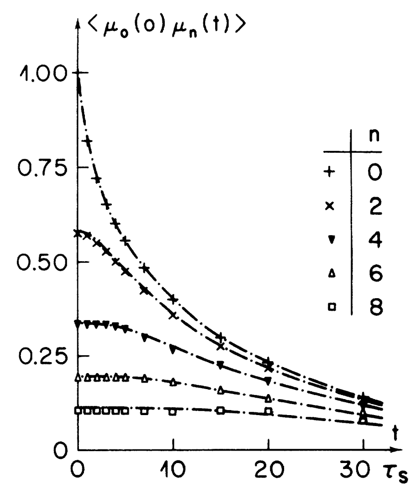

FIG. 15. Calculated time dependence of various pair correlation functions in the one-dimensional kinetic Ising model ($N = 220$) with nearest-neighbor interactions and periodic boundary conditions. The curves represent the exact solution of the infinite system [Eq. (A1)].

effects in our case.

It is also useful to study the time-dependent correlation function of the magnetization itself, which is given by[6]

$$\chi_T \hat{\phi}_{\delta\mu\delta\mu}(t) = \langle \delta\mu(0,0)\delta\mu(0,t)\rangle = \chi_T \exp[-(1/\tau_s)t(1-\tanh 2\beta J)], \quad \text{(A3)}$$

and the static susceptibility χ_T given by

$$\chi_T = \frac{N}{k_B T}\,\mu_B^2\,\frac{1+\tanh(\beta J)}{1-\tanh(\beta J)} \quad . \quad \text{(A4)}$$

This correlation function is plotted in Fig. 16 at several temperatures and compared to the results of the Monte Carlo calculation. Again good agreement is observed. It turned out that this correlation function is more sensitive to the error source (ii), i.e., the statistical error due to short Markov-chain lengths. In most cases a rather large number (~ 10^3 Monte Carlo steps per spin) of configurations had to be discarded at the beginning of the calculation until thermal equilibrium was obtained. In addition, short runs (500 Monte Carlo steps per spin) have not yet yielded accurate results. Most of this error is due to that of the static susceptibility χ. However, the error in the normalized correlation function $\hat{\phi}_{\delta\mu\delta\mu}(t) = \langle\delta\mu(0,0)\delta\mu(0,t)\rangle/\chi_T$ is considerably smaller. This observation strongly indicates that the inaccuracy of the relaxation time $\tau^{\pm}_{\delta\mu\delta\mu}$ should be smaller than the inaccuracy of the corresponding static susceptibility. Thus Fig. 2 (in which the static susceptibilities are compared to "exact" asymptotic expressions[2] in the two-dimensional case) also presents convincing evidence of accuracy with respect to dynamic quantities.

In conclusion, we have shown that in the one-dimensional case any time-dependent correlation

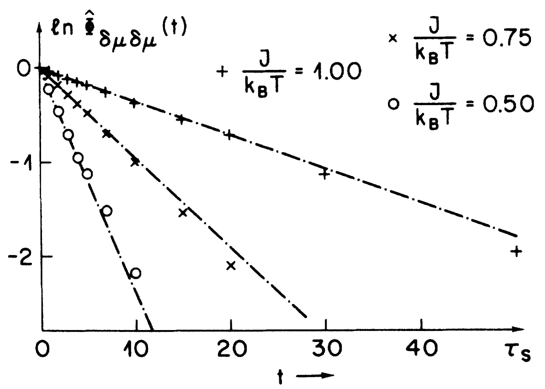

FIG. 16. Calculated time dependence of the magnetization correlation for three temperatures in the linear Ising chain with $N = 220$, nearest-neighbor interaction, and periodic boundary conditions. The straight lines represent the exact solution of Glauber (Ref. 6).

functions could be calculated with reasonable accuracy.

APPENDIX B: APPLICATIONS OF THE HIGH-TEMPERATURE-SERIES-EXPANSION TECHNIQUE

Here we briefly discuss the extension[8–12] of the well-known high-temperature-series-expansion technique[1,36] to time-dependent correlations in the kinetic Ising model. It will turn out that the comparison between the extended and conventional expansion methods clarifies the slight discrepancies between our Monte Carlo results and the estimates obtained from the extended expansion method.[8–12]

The conventional high-temperature-series-expansion method starts from

$$\langle A\rangle = \frac{\mathrm{Tr}\, e^{-\beta\mathcal{H}}A}{\mathrm{Tr}\, e^{-\beta\mathcal{H}}} = \frac{\mathrm{Tr}\exp[(2J/k_BT)\sum'_{i,j}\mu_i\mu_j]A}{\mathrm{Re}\exp[(2J/k_BT)\sum'_{i,j}\mu_i\mu_j]} \quad . \quad \text{(B1)}$$

Expansion of the exponential and the identity

$$\exp[(2J/k_BT)\mu_i\mu_j] = \cosh(2J/k_BT)\times[1+\mu_i\mu_j\tanh(2J/k_BT)] \quad \text{(B2)}$$

leads to

$$\langle A\rangle = \frac{\mathrm{Tr}\prod_{i,j}[1+\mu_i\mu_jV]A}{\mathrm{Tr}\prod_{i,j}[1+\mu_i\mu_jV]}\ , \quad \text{(B3)}$$

where

$$V = \tanh(2J/k_BT). \quad \text{(B4)}$$

Expressing the quantity A in terms of μ_k, rearranging terms of products in Eq. (B3) according to the power of V and performing the traces, one obtains the high-temperature expansion

$$\langle A\rangle = \sum_{l=0}^{\infty} f_l^A V^l. \quad \text{(B5)}$$

We note that the lth order term in this expansion can contain contributions from all powers of $\mathcal{H}$ up to $\mathcal{H}^l$. In most cases the coefficients f_l^A can be obtained only numerically, up to some order L. A finite series, however, cannot exhibit any singularity at the critical point $V_c = \tanh(2J/k_BT)$. Thus, the series must be extrapolated in order to study the nature of the singularity. Suppose that

$$\langle A\rangle \approx C_A\,\epsilon_{V,T}^{-\varphi_A}, \quad \text{(B6)}$$

where

$$\epsilon_T = \left|\frac{T-T_c}{T_c}\right| \to 0 \quad \text{or} \quad \epsilon_V = \left|\frac{V_c - V}{V_c}\right| \to 0. \quad \text{(B7)}$$

This implies that the f_l^A behave like

$$\frac{f_l^A}{f_{l-1}^A} \to \frac{1}{V_c}\left(1+\frac{\varphi_A - 1}{l}\right) \quad \text{(B8)}$$

or

$$\frac{f_l^A}{f_{l-1}^A} V_c - l + 1 \approx \varphi_A \tag{B9}$$

for large l. Equation (B9) indicates how the ratio of subsequent coefficients can be used to estimate the critical exponent φ_A.[1,36]

A second familiar technique of extrapolating a finite series starts from the observation that logarithmic derivative of $\langle A\rangle$ should diverge like

$$\frac{d}{dv}\ln\langle A\rangle \sim \frac{\varphi_A}{V_c - V}, \quad V \to V_c . \tag{B10}$$

This suggests that a useful extrapolation might be obtained by approximating the auxiliary series for $d\ln\langle A\rangle/dv$ by a polynomial, i.e., forming a Padé approximant[1,36]

$$\frac{d}{dv}\ln\langle A\rangle = \sum_{l=0}^{L-1} g_l^A V^l = \frac{\varphi_0^A + a_1^A V + \cdots + a_M^A V^M}{1 + b_1^A V + \cdots + b_N^A V^N} . \tag{B11}$$

The new coefficients a_l^A, b_l^A are determined by comparing the coefficients on both sides in Eq. (B11), which requires $N+M=L-1$. The degrees M and N of the polynomials in this (M,N) Padé approximant are otherwise arbitrary. From Eqs. (B10) and (B11) it becomes clear that φ_A may be estimated from the residue of Eq. (B11) at V_c. The advantages of this technique for our purpose are twofold: (i) the consistency can be checked to some extent, because various choices of (M,N) should lead to consistent results; (ii) by integrating (B11) over V one obtains a numerical interpolation formula which holds in the whole range $0 \leqslant V < V_c$, while Eq. (B6) only holds asymptotically near T_c.

The number of coefficients L (order of the expansion) which typically is taken into account lies between 10 and 20. The accuracy of these methods has been tested on several nontrivial models exhibiting phase transitions and for which exact solutions exist (two-dimensional Ising model, $d \geqslant 3$ spherical model).[1-3] Difficulties arise only in cases where additional parameters are introduced[50] (e.g., next-neighbor exchange interaction).

The extension of this method to dynamic properties is hampered by the fact that there are no such exactly soluble models. Furthermore, one has an additional parameter (the time or the frequency). Since we need these expansion results for comparison, we briefly sketch the procedure to obtain the series-expansion coefficients.[8-12] Furthermore, we outline our method to obtain an interpolation scheme for the temperature dependence of the relaxation times and discuss the reliability of these series techniques.

The susceptibility associated with a dynamic variable A may be defined by

$$\chi_{\delta A\delta A}(\omega) = \beta\int_0^\infty e^{-i\omega t}\langle \delta A e^{-Lt} L\delta A\rangle dt = \beta\left(\langle\delta A\delta A\rangle - i\omega\left\langle \delta A \frac{1}{i\omega + L}\delta A\right\rangle\right), \tag{B12}$$

where

$$\delta A = A - \langle A\rangle, \quad L = \sum_{j=1}^N W_j(\mu_j)(1-P_j). \tag{B13}$$

L is the Liouville operator and P_j is the spin-flip operator of the jth spin, so that [Eq. (40)]

$$P_j\,\mu_k = -\mu_k\delta_{jk} + \mu_k(1-\delta_{jk}), \qquad \tfrac{1}{2}(1-P_j)\,\mu_k = \delta_{jk}\,\mu_k . \tag{B14}$$

To derive a series expansion of χ one constructs in a first step a perturbation expansion for Eq. (B12). For this purpose one may split L into an "unperturbed" part L_0 and perturbation terms L_1 and L_3,

$$L = (1/\tau_s)(L_0 - L_1 - L_3), \tag{B15}$$

where

$$L_0 = \frac{1}{2}\sum_{j=1}^N (1-P_j), \tag{B16}$$

$$L_1 = \tfrac{1}{32}(\tanh 6\beta J + 4\tanh 4\beta J + 5\tanh 2\beta J) \times \sum_{j=1}^N \sum_{(k)_j} \mu_k\mu_j \tfrac{1}{2}(1-P_j), \tag{B17}$$

$$L_3 = \tfrac{1}{32}(\tanh 6\beta J - 3\tanh 2\beta J) \times \sum_{j=1}^N \sum_{(k_1k_2k_3)_j} \mu_{k_1}\mu_{k_2}\mu_{k_3}\mu_j \tfrac{1}{2}(1-P_j). \tag{B18}$$

$\sum_{(k)_j}$ denotes a summation over such k which are nearest neighbors of j. Equations (B16)–(B18) follow from Eq. (B13) by expanding $W_j(\mu_j)$ with the aid of Eq. (B2). In deriving an expansion in powers of V it should be emphasized that the coefficient of L_1 yields a coefficient of V^1 (+higher-order terms), whereas L_3 starts with V^3 (+higher-order terms). If L_0 acts on an n-spin product $\mu_1\times\mu_2\times\cdots\times\mu_N$ one finds from (B14) and (B16)

$$L_0(\mu_1\times\mu_2\times\cdots\times\mu_N) = n(\mu_1\times\mu_2\times\cdots\times\mu_N) \tag{B19}$$

or

$$\frac{1}{Z\tau_s + L_0}(\mu_1\times\mu_2\times\cdots\times\mu_N) = \frac{1}{Z\tau_s + n}(\mu_1\times\mu_2\times\cdots\times\mu_N). \tag{B20}$$

This property of L_0 suggests the following expansion:

$$\frac{1}{i\omega + L} = \left(\frac{\tau_s}{i\omega\tau_s + L_0}\right)\left(1 + \frac{L_1 + L_3}{i\omega\tau_s + L_0} + \cdots\right). \tag{B21}$$

Substituting Eq. (B21) into (B12) one may now perform the trace, using the conventional expansion technique [Eqs. (B1)–(B5)]. We note that each term in the expansion [Eq. (B21)] contributes a factor $(i\omega\tau_s+L_0)^{-L}$, or using Eq. (B20), $(i\omega\tau_s+n)^{-L}$. These terms are then expanded in powers of $i\omega\tau_s$ because one is interested only in the low-frequency region. Rearranging terms (for details we refer to Refs. 8–12) one obtains the final result

$$\chi_{\delta A\delta A}(\omega)=\beta\left[a_0+\sum_{k=1} a_k(i\omega\tau_s)^k\right], \tag{B22}$$

where all a_k are series in V, with non-negative coefficients f_n^k. The a_k's have been calculated up to $k=3$, both for the order parameter and the energy. a_0 determines the static susceptibility or specific heat. For including L_3 up to third order in the perturbation expansion one must already go to higher than ninth order in the common high-temperature variable V. This property [following from Eq. (B18)] has no analog in the expansions of static quantities. It also indicates that the question of how many terms are necessary for reliable expansion estimates must be studied with care.[51]

The expansion of the a_k's has been given up to twelfth[51] order in V. Applying the ratio estimates [Eqs. (8) and (9)] it was found that

$$a_k\sim\epsilon^{-\varphi_k},\quad \varphi_k=\varphi_0+k\Delta, \tag{B23}$$

leading to the conjecture

$$\chi(\omega)=\chi(\omega=0)f(i\omega\tau_s/\epsilon^{\Delta}). \tag{B24}$$

The case where $\chi(\omega)$ represents the order-parameter susceptibility deserves particular interest. Here $\varphi_0\equiv\gamma=\frac{7}{4}$. Ratio estimates seem to indicate that[11]

$$\Delta_{\delta\mu\delta\mu}\approx 2,\quad \Delta_{\delta\mathcal{H}\delta\mathcal{H}}\approx 2. \tag{B25}$$

However, from Ref. 11 it is not clear in what temperature region the asymptotic form (23) holds and how important correction terms are. In view of this, we applied the Padé analysis [Eqs. (B10) and (B11)] to derive an explicit interpolation formula for $\tau^{+}_{\delta\mu\delta\mu}=a_1/a_0$ and also valid for $V\to 0$, from the coefficients tabulated in Ref. 11. Several Padé approximants have been evaluated for both a_0 and a_1, yielding consistent results among one another and with Eq. (B25). It was found sufficient to take the (3, 4) approximants

$$\ln a_0\equiv\ln\chi_{\delta\mu\delta\mu}(V)=\int_0^V\frac{4-42V'-102V'^2-88V'^3}{1-12.5V'-7.5V'^2+68.5V'^3+24.5V'^4}\,dV' \tag{B26}$$

and

$$\ln a_1\equiv\ln[\chi_{\delta\mu\delta\mu}(V)\tau_{\delta\mu\delta\mu}]=\int_0^V\frac{8+51.3423V'+113.262V'^2+222.098V'^3}{1-34.1779V'-3.09565V'^2-0.875392V'^3-64.5533V'^4}\,dV'. \tag{B27}$$

The estimates for $\ln\tau_{\delta\mu\delta\mu}$ following from these expressions are shown in Fig. 7. Evidently, these series-expansion estimates of $\tau_{\delta\mu\delta\mu}$ are in close numerical agreement with the Monte Carlo results, although the predicted exponents differ slightly. Therefore we believe this slight discrepancy does not violate the credibility of both methods, but is rather an estimate of the error involved in the extrapolation $T\to T_c$.

Similarly, we formed Padé approximants to the series for $\tau_{\delta\mu}^{\delta H,0}$[29] and $\tau^{A}_{\delta\mu\delta\mu}$,[10] which did not yield reliable results due to the brevity of the available series. The result for $\tau_{\delta\mathcal{H}\delta\mathcal{H}}$[11] is included in Fig. 12 and is in full agreement with our data.

In addition, we performed series expansions for $\langle W_j\rangle$ Eq. (7). This quantity was needed to provide the series estimates shown in Figs. 4 and 9. The standard procedure outlined in Eqs. (B1)–(B5) leads to the result

$$2\langle W\rangle=1-4V^2+4V^4-44V^6+180V^8-+\cdots. \tag{B28}$$

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