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Critical Dynamics of Finite Ising Model

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The Glauber kinetics of Ising spins is considered as a queueing process and simulated "event by event" as first proposed by Bortz, Kalos, and Lebowitz. The advantage of this algorithm compared to the standard single-flip Monte Carlo method is discussed for the situation of slowing down of dynamics. This process is used to generate fluctuations of magnetization and energy in the critical regime $T = T_c$ of two-dimensional Ising models. The analysis of these fluctuations leads to numerical determination of the critical exponents for dynamics: for the size dependence of correlation time at T_c, and μ for frequency dependence of the power spectrum $S(\omega) \sim \omega^{-\mu}$. From the finite-size scaling hypothesis, scaling relations are settled which are confirmed by this numerical experiment.

KEY WORDS: Ising; critical dynamics; spectral powers; queueing process.

1. INTRODUCTION

The concept of scaling invariance in the critical regime predicts very precise behavior for finite-size systems of interacting particles. This behavior has been discussed by Fisher[1] in terms of scaling theory involving the critical exponents of the corresponding infinite systems. It is remarkable that for a very small-size system one accesses very easily to critical exponents of the infinite system by varying the size of the samples studied. The numerical simulation is therefore very well adapted for these types of study and the finite-size scaling theory has been verified[2] for magnetic and thermal properties of the Ising model. Only very few attempts[3] have been developed for the critical dynamics which is based similarly on the finite-size scaling hypothesis proposed by Suzuki.[4] The aim of this article is to test

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this hypothesis and to determine the critical dynamical exponent by using a new algorithm for generating kinetics of Ising spins. Since this work includes the determination of the characteristic correlation time of a finite sample, it gives in addition indication for proper use of the time average for static thermodynamic variables.

The kinetics of the Ising model is based on the Glauber[5] model where the time evolution is created by a single-spin-flip transition matrix. This kinetics is simulated by the Monte Carlo method which generates sequences of configuration states for the system by using a single-spin transition probability obeying the Boltzmann law. In general the study of static critical phenomena is performed by the same method which leads to time average instead of ensemble average. We are primarily interested by the critical slowing down which is the strongest at $T_{\mathrm{MAX}}(L)$, a temperature corresponding to the peak of the specific heat and L the linear size of the system [the correlation time $\tau(L)$ must diverge as L^z when L goes to infinity]. We need very long records of fluctuations, longer than the correlation time $\tau(L)$. Owing to the long and expensive computer time involved in the standard Monte Carlo method, we have chosen a different stochastic process for simulating the time evolution of the system. In this process each step corresponds to a real flip of one spin instead of frequent unsuccessful trials of spin flip in the standard method, particularly at low temperature. The acceleration rate gained by this process first proposed by Bortz, Kalos, and Lebowitz[6] is about 5 at T_c. In Section 2, the method is presented in some detail and a comparison with the standard Monte Carlo method is given. In Section 3, the fundamental hypothesis of the dynamical scaling invariance for finite-size systems is recalled. New scaling relations are obtained for the critical exponent μ_M and μ_E of the power spectrum $S(\omega) = \omega^{-\mu}$ of magnetization and energy. Finally, in Section 4, the results obtained for this model of critical kinetics are presented and the numerical values of z and μ_E and μ_M are given. The value $z = 2 \pm 0.1$ confirms Suzuki's prediction while the values $\mu_M = 15/8$ and $\mu_E = 1$ are obtained for the first time.

2. QUEUING PROCESS—METHOD OF BORTZ, KALOS, AND LEBOWITZ[6] (BKL)

In Glauber kinetics, spins behave like customers waiting to be served. Service consists in a state change (flip of spin, for example). Two possible transitions exist: "period by period" or "event by event." The Monte Carlo method is a "period-by-period" simulation at discrete times while the BKL process is an "event-by-event" simulation with continuous time. Let us consider the continuous time model for N interacting Ising spins.

A configuration $\{X_t\}$ is the state of all the spins at the time t $t \in \mathbb{R}$, where $x_t \in \{-1, 1\}^N$.

The process generates a set $\{X_t\}$ of configurations. It is a continuous, Markovian and homogeneous process, i.e., satisfying the following two conditions:

(I) For any $t_1 < t_2 < t_3 < \cdots < t_n < t$

$$\Pr(X_t = \beta \mid X_{t_n} = \alpha_n, X_{t_{n-1}} = \alpha_{n-1}, \ldots, X_{t_1} = \alpha_1) = \Pr(X_t = \beta \mid X_{t_n} = \alpha_n)$$

where $\beta \in \{-1, 1\}^N$ and $\alpha_k \in \{-1, 1\}^N$ $1 \leqslant k \leqslant n$ (Markovian continuous process).

(II) For any $t > 0$ and $s > 0$

$$\Pr(X_{s+t} = \beta \mid X_s = \alpha) = \Pr(X_t = \beta \mid X_0 = \alpha)$$

(homogeneous continuous process).

Let us recall that a queueing process is conventionally defined by[7]

the arrival process
the service process
the number of servants
the largest number of customers in the system
the interaction between number of customers in the system and the arrival process
the discipline

These different characteristics of the BKL process are identified as follows:

(a) Arrival Process. Let $\Theta_\alpha > 0$ be the "persistence" of the state α:

(III) $$\Pr(\Theta_\alpha > t + \eta \mid \Theta_\alpha > t) = \Pr(X_\tau = \alpha;\ t \leqslant \tau \leqslant t + \eta \mid X_s = \alpha;\ 0 \leqslant s \leqslant t)$$

Using (I) we get

$$\Pr(X_\tau = \alpha;\ t \leqslant \tau \leqslant t + \eta \mid X_s = \alpha;\ 0 \leqslant s \leqslant t) = \Pr(X_\tau = \alpha;\ t \leqslant \tau \leqslant t + \eta \mid X_t = \alpha)$$

and using (II)

$$\Pr(X_\tau = \alpha;\ t \leqslant \tau \leqslant t + \eta \mid X_t = \alpha) = \Pr(X_\tau = \alpha;\ 0 \leqslant \tau \leqslant \eta \mid X_0 = \alpha)$$

and so (III) becomes

(IV) $$\Pr(\Theta_\alpha > t + \eta \mid \Theta_\alpha > t) = \Pr(\Theta_\alpha > \eta)$$

(IV) is a characterization of exponential distribution.

Then $\exists \lambda \in \mathbb{R}$

$$\text{(V)} \qquad \Pr(\Theta_\alpha \leqslant t) = 1 - e^{-\lambda t}$$
$$\Pr(\Theta_\alpha > t) = \exp(-\lambda t)$$

Let us notice that generally λ depends on α. In the case of Ising interacting spins, we get

$$\begin{aligned}\Pr(\Theta_\alpha > t) &= \Pr(\text{no spins will be flipped before the instant } t) \\ &= \prod_{\text{all } i} \Pr(\text{the spin } \sigma_i \text{ will not be flipped before } t) \\ &= \prod_i (\exp\{-P_i^\alpha t\})\end{aligned}$$

with

$$P_i^\alpha = \inf\left[\exp(-(\Delta E_i / T), 1)\right] \qquad \text{(Boltzmann)}$$

where ΔE_i is the variation of energy associated to the flip of the spin σ_i; T is the temperature. So

$$\Pr(\Theta_\alpha > t) = \exp\left[-\left(\sum_i P_i^\alpha\right)\right] \equiv \exp(-S_\alpha t)$$

$$S_\alpha \equiv \sum_{i=1}^{N} P_i^\alpha$$

is *the rate of evolution of the system* in the state α (during the relaxation of the system S_α changes of value at each event). At high temperature $\Delta E_i \ll T$, then $P_i \sim 1$ and $S \sim N$.

(b) Service Process. Here the service process is obvious. We admit that the flip is instantaneous. The service process is determinist with a duration equal to zero.

(c) Number of Servants. There is only one servant. We exclude the simultaneous flip of n spins. Therefore, notice that the duration between two flips can be very short.

(d) Number of Customers in the System. This number is simply the number N of spins.

(e) Interaction. There is no interaction between the number of customers and the arrival process.

(f) Discipline. Because the duration of one flip is zero, there is no discipline. Therefore, this queueing process is

$$(M(S_\alpha), D(0), 1, N, \infty, \text{indifferent})$$

S_α is the characteristic parameter of this queueing process and $M(S_\alpha)$ is conventionally the rate of the exponential decay: $\exp(-S_\alpha t)$.

Description of a BKL Algorithm

The principle is simple: the duration of the present event and the choice of the spin which will be flipped at the next step is computed.

The persistence of the current event obeys the following exponential law: $M(S_\alpha)$. The spins are chosen with relative probability as compared with all likelihood (Fig. 1).

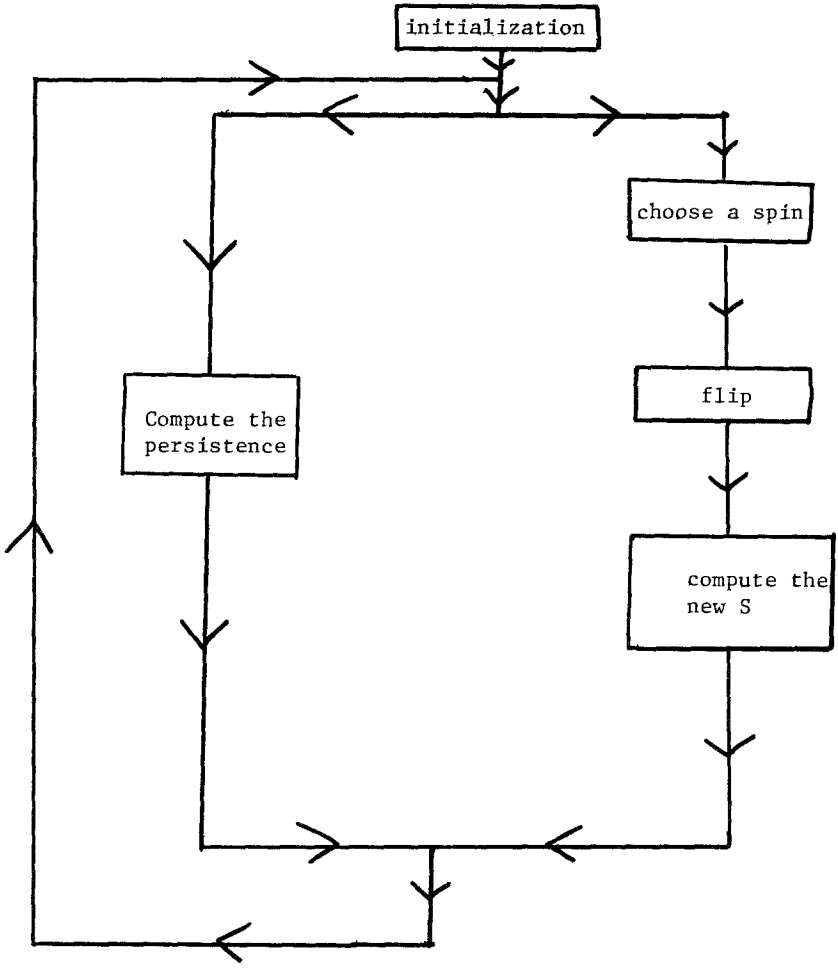

Fig. 1. Chart flow for the queueing process of BKL.

(a) Initialization. For external conditions fixed (temperature, magnetic field, etc. . . .) an initial configuration of spins is chosen at random.

(b) Calculation of the Persistence of the Current Event. We chose a random number T obeying the exponential law (parameter 1); then $t = T/S$ is the persistence of the current event. This is the basic difference between the Monte Carlo method and the BKL method. Indeed, the time units used in the two methods are different: In the Monte Carlo (MC) method, the spin i is chosen with uniform probability among the set of N spins: it is the elementary step. The "MCS/spin" corresponds to N consecutive steps; in the BKL method, *each step corresponds to a real flip*.

Let τ be the mean time till the next event (i.e., the mean time of persistence).

(i) With the BKL process, τ is given by

$$\tau = \int_0^\infty ue^{-Su}\,du = 1/S$$

(ii) In the MC process, let P_k be the probability that the next event will occur at the step k. For $k = 1 : P_1 = \sum_{\text{all } i} \Pr(\text{choose the spin } \sigma i) \times \Pr(\text{flip th spin } i)$

$$\Pr(\text{choose the spin } \sigma i) = 1/N$$

$$\Pr(\text{flip the spin } \sigma i) = Pi = \min(1, \exp(\Delta Ei/T))$$

$P_1 = S/N$, then $P_k = (1 - S/N)^{k-1}S/N$

$$\tau \equiv \sum_k^\infty kP_k = N/S \text{ (in MSC unit)} = \frac{1}{S} \text{ (in MSC/spin)}$$

by identification, we get

$$1 \text{ unit of time BKL} = 1 \text{ MCS/spin}$$

Note that $\tau = N/S$ is independent from N (because $S \sim N$).

Summary. We chose a random number D with an exponential probability (parameter 1). The duration of the present state is D/S in MCS/spin unit.

(c) Choice of the Spin. To each spin σ_i is associated an interval I_i with $I_i \subset [0, 1]$;

$$\bigcup_{\text{all } i} I_i = [0, 1], \qquad I_i \cap I_j = \emptyset$$

and the $\Delta(I_i)$ the length of I_i is proportional to the probability P_i of flip of the spin σi:

$$\Delta(I_i) = P_i \Big/ \sum_{\text{all } j} P_j$$

Now a random number R with uniform probability in [0, 1] is chosen. It identifies an internal I_i by $R \in I_i$ and the spin i.

(d) Calculation of the New S. The flip of σ_i changes only the value of P_i and the fourth P_j where j label the nearest-neighbors spins of σ_i.

For both these processes, the sequence of configurations of spins is the same; but the time of computation to build these sequences can be very different: Let us define the efficiency ratio $\gamma = t/t'$, where t is the mean elapsed time in simulation for a given sequence (for example, the mean time between two successive flips of spins) and t' the related time of computation. At high temperature γ is the same for both these processes because each trial provides a flip in Monte Carlo method as in BKL. At low temperature, the situation is different. In Monte Carlo kinetics t' is proportional to t and γ does not change from its high-temperature value. On the contrary, in BKL, t increases strongly for constant t'. For instance if the sequence is defined by[2] successive flips, $t = \tau$ the mean persistence time equal to S^{-1} which diverges exponentially as $T \to 0$. In the critical regime of the Ising model, we have typically found an efficiency ratio larger by a factor 4.5 in favor of BKL. We have checked that this factor can reach a very high value ($\sim 10^3$ to 10^6) at lower temperature.

3. FINITE-SIZE SCALING FOR THE CRITICAL DYNAMICS

The static critical behavior of finite systems has been discussed by Fisher[1] in terms of scaling functions involving the infinite lattice critical exponents. The basic assumption is that the thermodynamic functions for finite systems of $N = L^d$ spins and of linear size L with periodic boundary conditions are universal functions of the ratio L/ξ, where ξ is the characteristic correlation length $\xi = \xi_0 \epsilon^{-\nu}$ at temperature $\epsilon = [T - T_c(\infty)]/T_c(\infty)$. Here ξ_0 is an atomic distance for the system considered while $T_c(\infty)$ is the infinite-lattice transition temperature. For finite size (and specified boundary conditions) there is a shift in the "pseudoordering" temperature $T_c(N)$ (Landau[2]) defined by the maximum in the specific heat, given by

$$\delta\epsilon = \left[1 - T_c(N)/T_c(\infty)\right] \sim aL^{-\lambda} \tag{3.1}$$

according to scaling theory. This fundamental hypothesis leads to the following relations for the intensive variables such as the susceptibility $\chi(\epsilon, L)$ and the specific heat $C(\epsilon, L)$ (per spin)

$$\begin{aligned} \chi T &= L^{\gamma/\nu} Y^0(\epsilon L^{1/\nu}) \\ C &= L^{\alpha/\nu} Z^0(\epsilon L^{1/\nu}) \end{aligned} \tag{3.2}$$

For large values of the variable $\epsilon L^{1/\nu}$, these functions must reproduce the infinite-lattice critical behavior in such a way that $Y^0(x) \sim x^{-\gamma}$ and

$Z^0(x) \sim x^{-\alpha}$. On the contrary, in the "rounded" regime, $x \to 0$, $Y^0(x)$ and $Z^0(x)$ go to constant values. These assumptions have been tested successfully by various authors and particularly by numerical Monte Carlo simulations.[2] It is indeed a predilection field for numerical experiments since the size dependence is much easier to study than by true experiments and leads very directly to the fundamental exponents of infinite systems. In this article, we use the same method to study the dynamics of the Ising system in the very critical regime $T = T_c(N)$, in view of verifying the basic hypothesis of the critical dynamics.

Our study is devoted to the autocorrelation functions of the total magnetization $M(t)$ and total energy $E(t)$ of the Ising square lattice of spins (with periodic boundary conditions). These functions are defined by the following expressions:

$$\begin{aligned} C_M(t) &= \langle \delta M(0)\, \delta M(t) \rangle \\ C_E(t) &= \langle \delta E(0)\, \delta E(t) \rangle \end{aligned} \tag{3.3}$$

Here the brackets represent the ensemble average (calculated by a time average as described in the following paragraph), $\delta M(t) = M(t) - \langle M \rangle$ the deviation of the magnetization from its average value $\langle M \rangle$, and $\delta E(t) = E(t) - \langle E \rangle$ the fluctuations of the energy around the mean value $\langle E \rangle$. The power spectrum of these functions are defined by a Fourier transform

$$\begin{aligned} S_m(\omega) &= 2 \int_0^\infty (\cos \omega t) C_M(t)\, dt \\ S_E(\omega) &= 2 \int_0^\infty (\cos \omega t) C_E(t)\, dt \end{aligned} \tag{3.4}$$

where it has been taken into account that the correlation function is even. By analogy with static scaling, the dynamical scaling assumption consists in assuming the existence of a characteristic correlation time τ_L depending on the size $\tau_L \sim L^z$, where z is the bulk critical exponent like ν in the spatial problem. This hypothesis is supported by renormalization group arguments developed by Suzuki[4] on the time-dependent Ginzburg–Landau model or the Glauber kinetics for Ising models. Then, the time dependence of the dynamical variables like the correlation functions is embedded in the scaled variables t/τ_L or tL^{-z} for samples of various sizes. More precisely, it is assumed that

$$\begin{aligned} C_M(t) &= C_M(0) f_M(tL^{-z}) \\ C_E(t) &= C_E(0) f_E(tL^{-z}) \end{aligned} \tag{3.5}$$

It is expected that the same z appears in the magnetization as well as the energy since one single characteristic time τ_L is present in this model.

From (3.5) and (3.4), the spectrum power takes the scaled invariant form:

$$\begin{aligned} S_M(\omega) &= C_M(0) L^z \Psi_M(\omega L^z) \\ S_E(\omega) &= C_E(0) L^z \Psi_E(\omega L^z) \end{aligned} \tag{3.6}$$

The fluctuations of the extensive magnetization $C_M(0)$ and of the energy $C_E(0)$ are proportional, respectively to the intensive magnetic susceptibility and specific heat by the relations

$$\begin{aligned} C_M(0) &= \langle \delta M^2 \rangle = L^d \chi T \\ C_E(0) &= \langle \delta E^2 \rangle = L^d C T^2 \end{aligned} \tag{3.7}$$

In the very critical regime $T = T_c(N)$, $\epsilon = \delta\epsilon \ll 1$ and $\epsilon L^{1/\nu} \ll 1$. The functions Y^0 and Z^0 of (3.2) reach a constant value, where the unique size dependence is contained in the functions $\Psi_M(tL^{-z})$, $\Psi_E(tL^{-z})$ and the prefactors. This "rounded" regime in temperature is very convenient for studying the dynamical exponent z revealed directly by the size dependence of the scaled functions Ψ.

More precisely, by replacing the size dependence of χ and C from (3.2) in (3.7), then finally in (3.6) we obtain

$$\begin{aligned} S_M(\omega, L) &= L^{d+z+\gamma/\nu} \Psi_M(\omega L^z) \\ S_E(\omega, L) &= L^{d+z+\alpha/\nu} \Psi_E(\omega L^z) \end{aligned} \tag{3.8}$$

The expressions (3.8) can be developed in two different ways which will be described in next section:

(1) The correlation times for the linear dynamics:

$$\begin{aligned} \tau_M(L) &= \frac{S_M(0, L)}{C_M(0)} \\ \tau_E(L) &= \frac{S_E(0, L)}{C_M(0)} \end{aligned} \tag{3.9}$$

These correlations explore the scaling function in a regime of very long time or low frequency where we expect the rounding effects: $\lim_{x \to 0} \Psi_M(x) = \text{const.}$ and $\lim_{x \to 0} \Psi_E(x) = \text{const.}$ These "rounding effects" are understandable for finite systems in a regime where the time of fluctuation is longer than the longest correlation time ($\sim \tau_M$ or τ_E). No correlation exists here and the power spectrum appears white. These correlation times have a size dependence given by (3.8) and (3.7) that reflects the fundamental

assumption

$$\tau_M(L) = AL^z$$
$$\tau_E(L) = A'L^z \tag{3.10}$$

(2) The spectrum power analysis of these fluctuations which defines the exponent μ in the asymptotic regime where the bulk behavior is expected[7] at $(T > T_c)$:

$$\lim_{L\to\infty} S_M(\omega) = \frac{L^d}{\omega^{\mu_M}} \qquad (T > T_c)$$
$$\lim_{L\to\infty} S_E(\omega) = \frac{L^d}{\omega^{\mu_E}} \tag{3.11}$$

The asymptotic behavior of $S_M(\omega)$ is in L^d instead of L^{2d} since the average magnetization is vanishing for $T > T_c$. These relations take into account the extensivity of the thermodynamic variables M and E and define the critical exponent of the power spectrum at T_c. The exponents μ_M and μ_E are related to z and to the other static exponents γ, α, ν by imposing the asymptotic variation (3.11) to the scaling functions Ψ of (3.8):

$$\lim_{x\to\infty} \Psi_M(x) \sim \frac{1}{x^{\mu_M}}$$
$$\lim_{x\to\infty} \Psi_E(x) \sim \frac{1}{x^{\mu_E}} \tag{3.12}$$

By combining (3.12), (3.11), and (3.8) we obtain

$$\mu_M = 1 + \frac{\gamma}{\nu z}$$
$$\mu_E = 1 + \frac{\alpha}{\nu z}$$

For an Ising system in two dimensions $d = 2$, we know that $\nu = 1$, $\gamma/\nu = 7/4$, $\alpha = 0$. From the numerical determination of the correlation time described in next section we shall get $z = 2(\pm 0.1)$ and $\mu_M = 15/8$ and $\mu_E = 1$. These values as well as the scaling invariance will be compared to the numerical experimentation in next section. The expression for μ_M differs from the one given in Ref. 7 because here we study the total magnetization or energy instead of the magnetization or energy per spin.

The correspondence between the exponents μ_M or μ_E with μ_M^1 or μ_E^1 the analogous one for the extensive variable (per spin) is

$$\mu_M = 1 + \mu_M^1$$
$$\mu_E = 1 + \mu_E^1$$

At lower temperature $T < T_c$ one would find: $\mu_M = \mu_M^1$.

4. RESULTS AND CONCLUSIONS

With the method described in Section 2, the fluctuations of the total magnetization and energy have been recorded over very long periods. These periods of recording time are reported in Table I: the longest periods correspond to 5×10^5 events of one single spin flip, therefore to 2×10^6 MC steps since the mean time between two consecutive events is always 4.6 MCS (a transitory regime of many 10^4 MCS is performed before each recording in order to enter into the equilibrium thermal regime). In this experimentation the factor 4.6 represents the gain in saving time by using the queuing process versus the standard Monte Carlo method. A concentration procedure is used where a set of many events (many L^2 events typically) is replaced by one single event of mean value at a mean date of the set. In Fig. 2 a typical record of the magnetization fluctuations is represented: it is shown that the magnetization reaches very frequently its maximum value where it fluctuates with small amplitude, then it jumps suddenly to its opposite value. This nonlinear behavior may be understood intuitively from the very strong increase of the spontaneous magnetization just below the critical domain. The autocorrelation function of the magnetization is obtained by a time averaging simulating the thermal averaging:

$$\langle \delta M(0)\, \delta M(t) \rangle = \frac{1}{t_f - t - t_i} \int_{t_i}^{t_f - t} \delta M(t')\, \delta M(t' + t)\, dt' \qquad (4.1)$$

and a similar expression for the energy $E(t)$.

The unit of time is one Monte Carlo step *per spin* and the related frequency unit for the Fourier transform is $(\text{MCS/spin})^{-1}$.

The average magnetization is very small as expected from this study at $T_c(L)$. The second moments $C_M(0)$ or $C_E(0)$ are proportional to the magnetic susceptibility or specific heat (3.7). The values of $C_M(0)$ for

Table I. Fluctuations of Magnetization: Numerical Simulation

L	T_c	Recording time (MCS/spin)	S (MCS)	$C(0)$ (MCS/spin)	$C(0)/L^{3.75}$	τ_c (MCS/spin)
2	2.68	19 739	6.58	12.056	0.896	31.02
4	2.47	22 984	4.597	94.51	0.522	56.56
5	2.43	23 387	4.677	269.46	0.6446	101.77
6	2.405	23 216	4.643	589.54	0.712	182.68
7	2.386	22 934	4.587	1090	0.74	224.17
8	2.371	13 868	4.623	1932	0.793	306.16
9	2.365	13 622	4.541	3787	0.716	232.5
10	2.36	22 944	4.57	4913	0.87	425
15	2.32	8 858	4.53	21571	0.838	652

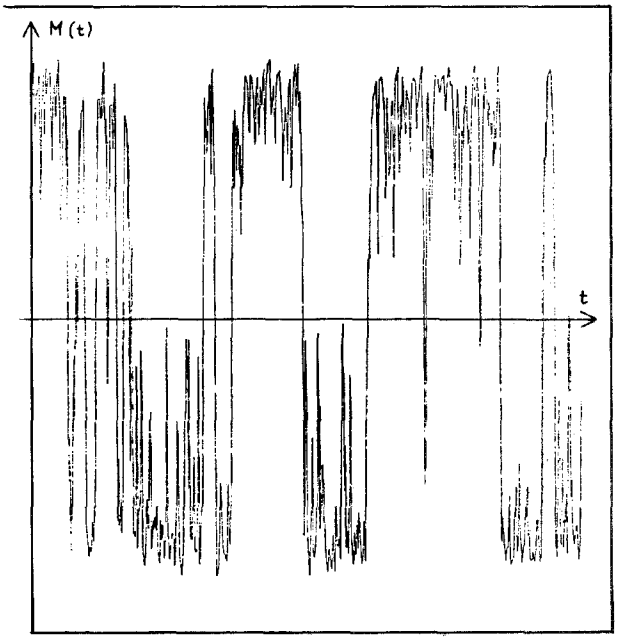

Fig. 2. Noise of magnetization recorded over a period of 10^3 MCS/spin for a small sample of size 6×6. The largest amplitude of the fluctuations corresponds to the saturated magnetization proportional to $L^2 = 36$.

various sizes L are indicated in Table I; the ratio of $C_M(0)/L^{3.75}$ gives precisely the value of the scaling function $Y^0(\epsilon L^{1/\nu})$:

$$\frac{C_M(0)}{L^{d+\gamma/\nu}} = Y^0(\epsilon L^{1/\nu}) \tag{4.2}$$

as defined by Landau.[2] These values are close to 1—except for the small-size samples—because our investigation is performed at $T = T_c(L)$ in the rounded critical regime ($\epsilon < 1$). The autocorrelation function is calculated by relation (4.1) over long periods where it falls down to 1% of the initial value; finally the Fourier transform is performed (fast Fourier transform algorithm of Eberhart[9]) leading to the functions $S_M(\omega)$ and $S_E(\omega)$ [cf. (3.4)].

4.1. Size Dependence: Determination of z

The correlation times for magnetization and energy are defined by the relations (3.9). Their numerical values are listed in Tables I and II and plotted in Fig. 3. The points for the magnetization are very well aligned

Table II. Fluctuations of Energy: Numerical Simulation

L	T_c	Recording time (MCS/spin)	S (MCS)	$C(0)$ (MCS/spin)	Average energy per spin	τ_c (MCS/spin)
6	2.405	4 600	4.59	176.9	−1.36	11.5
7	2.386	6 640	4.43	247.1	−1.34	15.5
8	2.371	3 030	4.85	372.57	−1.39	13.842
9	2.365	4 305	4.465	470.97	−1.414	18.28
10	2.36	3 519	4.4	631.9	−1.4	20.4
13	2.33	6 781	4.5	1 081.25	−1.35	35.89

except for the $L = 15$ sample, where the maximum time of recording the correlation function is probably too short for an accurate determination of z. The straight line corresponds to the law

$$\tau_M(L) = AL^z \text{ (MCS/spin)} \tag{4.3}$$

with $A = 4.5$ and $z = 2.0 \pm 0.1$. This value validates Suzuki's prediction and

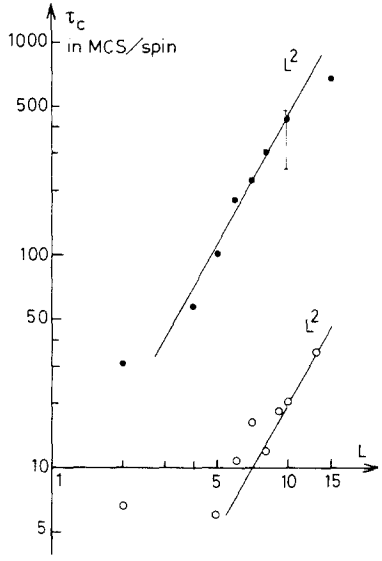

Fig. 3. Size variation of the correlation time at $T = T_c$. Black points are related to magnetization and circles to energy. The straight line among the circles corresponds to the L^2 law. For black points the straight line is obtained by a best fit with a L^2 law by a linear regression on data (except the 15×15 sample: see text). The bar reproduces the result of Ref. 3. The line through the white circles describes the correlation time for the energy obeying the equation $E = A'L^{z'}$ with $A' = 0.2$ and $z' = 2$. It does not fit all the points but only the largest size of our simulation, namely, $L = 9$, $L = 10$, $L = 13$. It is not the best fit of all our data because the smaller size gives values of τ_E too close to the paramagnetic cutoff of the relaxation time τ_0. See text.

gives a better determination of A than previous work. Previous determination of z by Stoll, Binder, and Schneider[10] has used the reduced temperature variable rather than the size length L. They have found $z = \Delta_{\delta\mu,\delta\mu} = 1.85 \pm 0.10$ instead of 2 ± 0.1 in this work.

For the energy, the points for large size define a straight line corresponding to

$$\tau_E = A' L^z \text{ (MCS/spin)} \tag{4.4}$$

where $A' = 0.2$ and $Z = 2$. This result confirms the scaling assumptions of one single characteristic time for the dynamics. However, the correlation times for the energy are shorter than those for the magnetization: for the smaller size $L < 7$, $\tau_E(L)$ deviates from the scaling variation and reaches a constant value τ_0 which belongs to the smallest sample $L = 2 : \tau_0 = 6.5$ (MCS/spin).

The time τ_0 represents the paramagnetic relaxation time that characterizes the correlation times (present) outside the critical regime: its value does not depend on the size L, but only on temperature ($\tau_0 = 1$ at $T \to \infty$). In the short-time behavior (below or near τ_0) the results depend on the details of the kinetics—Glauber and queuing process—and they do not have a universal character.

4.2. Spectral Power: Determination of μ

The Fourier transform (3.4) defines $S_M(\omega)$ and $S_E(\omega)$, which are now calculated for various sizes $L = 5$ up to $L = 15$ and are plotted in Fig. 4.

In order to test the dynamical scaling hypothesis of finite-size behavior a plot of $S_M(\omega)/L^{5.75}$ and $S_E(\omega)/L^4$ as functions of ωL^2 is used. These exponents correspond to the dimensional analysis of the relations (3.8) for the following values: $z = 2$, $\gamma = 7/4$, $\alpha = 0$, $\nu = 1$. Under the assumption that scaling is satisfied, this plot has the advantage that it graphically defines the shape function $\Psi(\omega L^z)$. However, the validity of the bulk scaling law is reduced to a small range of frequency:

$$\frac{1}{\tau(L)} < \omega < \frac{1}{\tau_0} \tag{4.5}$$

Here $\tau(L)$ is the correlation time and τ_0 is the paramagnetic relaxation time defined above. Actually, at low frequency $\omega\tau(L) < 1$, a white spectrum $S(\omega) = \omega^0$ is expected since $\tau(L)$ has the meaning of the longest correlation time due to the finite-size cutoff. At high frequency $\omega\tau_0 > 1$, all fluctuations are indeed strongly correlated by the thermal fluctuations described by τ_0, leading to a Brownian power spectrum $S(\omega) \sim \omega^{-2}$. The necessity of large-size simulation appears clearly in long τ_L for opening the frequency

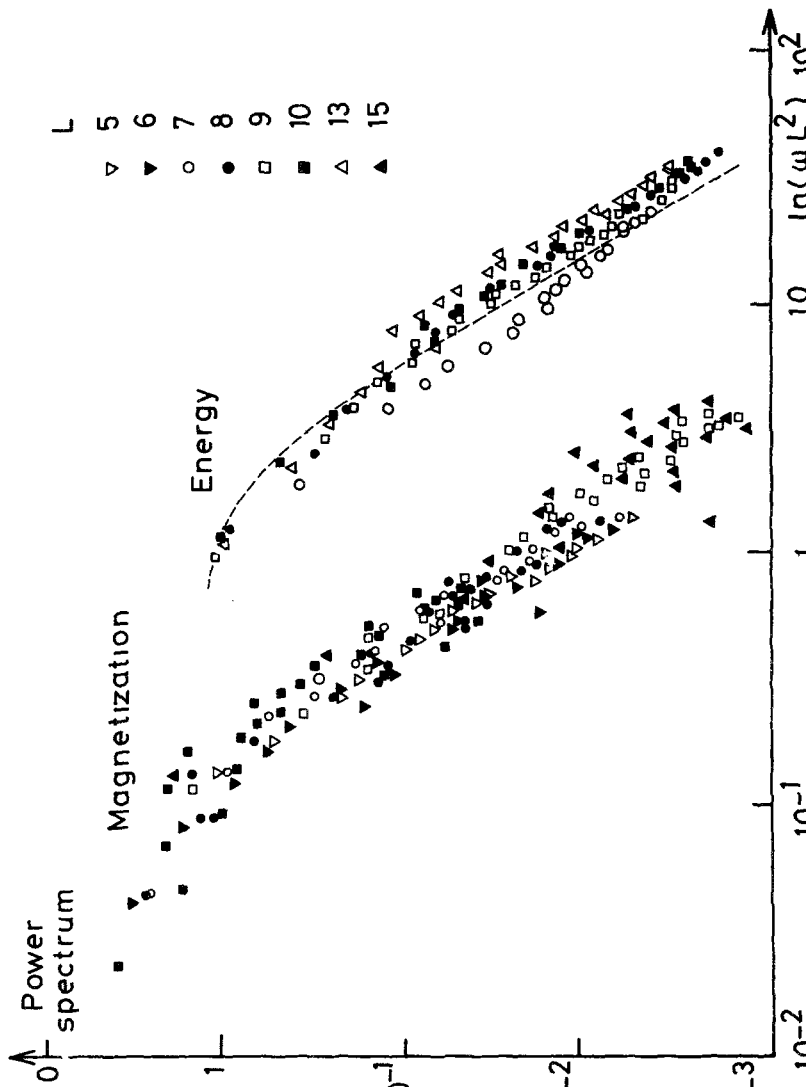

Fig. 4. Power spectrum for fluctuations of energy and magnetization. The various sizes are described by the list of symbols. The dashed line running into the points of energy is a fit to the expression 4.7 of the text with $\tau'_L/L^2 = 0.3$ and $\tau'_0/L^2 = 0.05$ (to be compared with $\tau_L/L^2 = A' = 0.2$ and $\tau_0/L^2 = 0.065$ for $L = 10$).

"window" (4.5). (For the scaling variable ωL^2 of Figs. 3 and 4 the low-frequency cutoff $L^2/\tau_L = A$ or A' is size independent while the upper cutoff varies as L^2/τ_0.) For $S_M(\omega)$ it is remarkable that the samples of different sizes contribute to a rather concentrated cloud of points, validating the finite-size scaling. The power law $\omega^{-\mu_M}$ variation of $S_M(\omega)$ in the "window" is determined from the slope: $\mu_M = 1.9 \pm 0.1$. This value is compatible with the prediction of the scaling hypothesis with $z = 2$ given in Section 3: $\mu_M = 1.875$.

Consider now the power spectrum of energy $S_E(\omega)$ of Fig. 4: the expected exponent is $\mu_E = 1$. This slope is not observed except perhaps at low frequency. We understand this result in terms of "window narrowing": $\tau_E(L)$ is at best only four times as long as τ_0 for $L = 13$, but only twice τ_0 for $L = 7$. Therefore, the scaling regime is mixed up with the white and Brownian regimes. A phenomenological way to understand this effect is to assume a distribution of independent correlation time $n(\tau_c) \sim \tau_c^{-a}$, the exponent of which must be fitted to μ. For a superposition of this correlation time τ_c given by $n(\tau_c)$, the autocorrelation is obtained by a Laplace transform of $n(\tau_c)$, while the power spectrum is given by

$$S(\omega) \sim \omega^{-\mu} \sim \int_{\tau_c}^{\infty} n(\tau_c) \frac{\tau_0 \, d\tau_c}{1 + \omega^2 \tau_c^2} \tag{4.6}$$

The condition of existence of (4.6) implies $a = 2 - \mu$ and $0 < a < 2$ when τ_c varies from 0 to ∞. This relaxation mode analysis can be generalized in a straightforward way to the case where a "window" (4.5) is now considered as a cutoff for the distribution $n(\tau_c)$:

$$S(\omega) \sim \int_{\tau_0}^{\tau_L} n(\tau_c) \frac{\tau_c}{1 + \omega^2 \tau_c^2} \, d\tau_c \tag{4.7}$$

This expression is easily handled in case of energy where $\mu_E = 1$, hence $a = 1$:

$$S(\omega) \sim \frac{1}{\omega} \left[\arctan(\omega \tau_L') - \arctan(\omega \tau' 0) \right] \tag{4.8}$$

The function (4.8) is plotted in Fig. 4 and shows that the scaling hypothesis combined with the "window" effect gives a good understanding of these results.

In conclusion, the method first proposed by Bortz, Kalos, and Lebowitz[6] has been used as the kinetics for the Ising model in two dimensions at the critical temperature. Under the conditions of critical slowing it permits accelerating the kinetics of the spins by a factor of 5. The finite-size scaling hypothesis has been verified both for magnetic and energetic fluctuations and the scaling shape functions have been determined. New

determinations of the dynamical exponent z and, for the first time, of the power spectrum $S_E(\omega)$ and $S_M(\omega)$ have been obtained and characterized by the critical exponents μ_E and μ_M which obey the expected scaling relations.

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