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A Monte Carlo study of the dynamics of the Ising SK model

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Abstract. The ergodic and short-time dynamics of the Ising Sherrington-Kirkpatrick model have been studied using the Monte Carlo method. The ergodic time associated with each bond configuration has been numerically calculated using an order parameter that is only sensitive to global spin flips. Assuming that the mean ergodic barrier height diverges with system size N as N^{λ} we find $\lambda = 0.25 \pm 0.05$. For the short-time dynamics the relaxation of order parameters that are insensitive to ergodic fluctuations are controlled by a spectrum of barriers. The largest of these diverges as N^{μ} where $0.25 < \mu < 0.45$.

1. Introduction

At the present time it is widely believed that Parisi's solution of the Sherrington-Kirkpatrick (SK) model (Parisi 1979, 1980a, b, c, d, e) is correct. This solution breaks the permutation symmetry between replicas and is intimately connected with the existence of many thermodynamic states. Parisi's solution cures both the negative-entropy problem and the de Almeida-Thouless (1978) instability that are features of the original replica symmetric solution. Young (1983) has found numerical evidence for many thermodynamic states by using a microscopic definition for the probability distribution of overlaps $P_N(q)$. Above the de Almeida and Thouless (AT) line in the limit of $N \to \infty$, $P_N(q)$ becomes a delta function, confirming that there is only one thermodynamic state in this regime. However, below the AT line, $P_N(q)$ is a broad distribution consistent with the picture of many states.

In an alternative approach to the SK model Thouless, Anderson and Palmer (TAP) (Thouless *et al* 1977) have studied the local mean field for the site magnetisations of a given bond configuration. Including the Onsager reaction field term in the naive mean-field equations yields the TAP equations. Bray and Moore (1980a), de Dominicis *et al* (1980), and Tanaka and Edwards (1980) have shown that there are an exponentially large number of solutions to the TAP equations below the AT line. These solutions may be interpreted as thermodynamic states separated by infinite free-energy barriers. Sompolinski and Zippelius (1982) have investigated the dynamics below the AT line starting from the Langevin equations for the relaxation of spin fluctuations. They conclude that the spin glass order parameters are time-persistent terms rather than purely static quantities. The central idea of this theory is that a large but finite system possesses a spectrum of relaxation times that diverge in the thermodynamic limit.

It is interesting to investigate numerically the divergence of the barrier heights and relaxation times that correspond to the many thermodynamic states of the SK model.

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Mackenzie and Young (1982, 1983) (hereafter referred to as MY) have investigated such properties in the Ising version of the SK model using the Monte Carlo method. The simulations were conducted below the AT line ($H=0$, $T=0.6$) and suggest a spectrum of relaxation times, the largest of which, ξ, diverges as:

$$\ln\{\xi_N\} \propto N^{\mu} \tag{1.1}$$

where $\mu = 0.27 \pm 0.1$. This implies non-ergodic behaviour in the thermodynamic limit. There is a single longer time, the ergodic time, arising from the symmetry of the Hamiltonian under the simultaneous flipping of all the spins. MY have suggested that the ergodic time $\tau(N)$ diverges as:

$$\ln\{\tau_N\} \propto N^{\lambda} \tag{1.2}$$

where $\lambda \simeq \frac{1}{2}$, although uncertainties in their data prevent an accurate determination of λ.

We have conducted an extensive Monte Carlo simulation of the Ising version of the SK model below the AT line ($H=0$, $T=0.5$) in order to determine the exponent λ more precisely. The divergence of the ergodic time was calculated by considering an order parameter that is sensitive only to global spin flips and we find that $\lambda = 0.25 \pm 0.05$. We also find a spectrum of times associated with the relaxation of order parameters that are *insensitive* to the ergodic fluctuations. The largest time, ξ_N, of this spectrum is the time taken for the order parameters to relax to their equilibrium statistical mechanics values. It is found that $\ln\{\xi_N\}$ diverges as N^{μ}, where $0.25 < \mu < 0.45$. If we could determine μ more accurately we would naively expect that $\mu < \lambda$, although the ergodic free-energy barrier does not necessarily have to be the largest barrier in the system. This paper is organised in the following way. In section 2 we introduce the various order parameters. Section 3 is concerned with a brief description of our Monte Carlo method. Sections 4 and 5 are, respectively, concerned with our results for the ergodic and short-time dynamics. Our conclusions are presented in section 6.

2. Order parameters

The Hamiltonian of the SK model in the absence of an external magnetic field is

$$H = -\tfrac{1}{2}\sum_{ij} J_{ij} S_i S_j. \tag{2.1}$$

The S_i are Ising spins interacting, via bonds J_{ij} chosen from a Gaussian distribution, with all the other spins in the system. The mean of this distribution is zero and the standard deviation is $(N-1)^{-1/2}$, where N is the total number of spins. Boltzmann's constant is set equal to unity so that in the thermodynamic limit the critical temperature is unity in zero magnetic field. Given that the phase space is a many-valley structure it is necessary to distinguish between single and many-valley order parameters. Only the latter corresponds to the complete Gibbs average. Consider the spin self-correlation function $q_N(t)$ as an order parameter:

$$q_N(t) = \frac{1}{N}\left\langle \left\langle \sum_{i=1}^{N} S_i(t_0) S_i(t_0+t) \right\rangle_T \right\rangle_J. \tag{2.2}$$

The $\langle\ \rangle_J$ represents averaging over different bond configurations and the $\langle\ \rangle_T$ represents the Gibbs average. For finite systems the average $\langle\ \rangle_T$ is correct because all of the

accessible phase space can be sampled. To obtain the full Gibbs average the thermodynamic limit must be applied carefully. For example, taking the limit $N \to \infty$ first, followed by $t \to \infty$, localises the system in a single valley yielding the Edwards–Anderson (1975) order parameter q_{EA}:

$$\lim_{t\to\infty} \lim_{N\to\infty} q_N(t) = q_{EA}. \tag{2.3}$$

For the Gibbs average q these limits are reversed:

$$\lim_{h\to\infty} \lim_{N\to\infty} \lim_{t\to\infty} q_N(t) = q. \tag{2.4}$$

This reversal allows all of the accessible phase space to be sampled. The uniform magnetic field h breaks the spin inversion symmetry of the Hamiltonian. Young and Kirkpatrick (1982) have pointed out that the limit $h \to 0$ is difficult to apply to finite systems because h must satisfy the inequality:

$$h \gg T/\sqrt{N} \tag{2.5}$$

where T is the temperature. This difficulty can be avoided by defining order parameters that are insensitive to the spin inversion symmetry of the Hamiltonian. Thus, throughout this study, we work without an applied magnetic field. Following MY we define:

$$q_N^{(2)}(t) = \frac{1}{N(N-1)} \sum_{i\neq j} \langle\langle S_i(t_0) S_j(t_0) S_i(t_0+t) S_j(t_0+t)\rangle_T\rangle_J \tag{2.6}$$

and

$$q_N^{\mathrm{mod}}(t) = \frac{1}{N} \left\langle \left\langle \left| \sum_{i=1}^{N} S_i(t_0) S_i(t_0+t) \right| \right\rangle_T \right\rangle_J. \tag{2.7}$$

The Gibbs averages are defined as:

$$\lim_{N\to\infty} \lim_{t\to\infty} q_N^{(2)}(t) = q^{(2)} \tag{2.8}$$

and

$$\lim_{N\to\infty} \lim_{t\to\infty} q_N^{\mathrm{mod}}(t) = q. \tag{2.9}$$

For a Monte Carlo simulation the previous definitions are impractical because we are restricted to finite systems and computing times. The limit $t \to \infty$ is replaced by the condition $t > t_{eq}$, where t_{eq} is the longest relevant relaxation time. The infinite limit $N \to \infty$ is dropped and instead we deal with finite-size statistical mechanics averages. These extrapolate to Parisi's predictions for $q^{(2)}$ and q in the thermodynamic limit (Mackenzie and Young 1982, 1983).

3. Simulation method

The Monte Carlo method is a Markov process and is therefore governed by the master equation:

$$\frac{\mathrm{d}P(x,t)}{\mathrm{d}t} = -\sum_{x} W(x \to x') P(x,t) + \sum_{x'} W(x' \to x) P(x',t). \tag{3.1}$$

Here x is a state vector representing a particular spin configuration of the system. $W(x \to x')$ is the transition probability, per unit time, of the move $x \to x'$. The equilibrium probability distribution $P_{eq}(x)$ is a stationary solution of (3.1) provided the detailed-balance condition is satisfied:

$$P_{eq}(x)\, W(x \to x') = P_{eq}(x')\, W(x' \to x). \tag{3.2}$$

We use the Glauber (1963) dynamics in which

$$W(x' \to x) = \frac{1}{2\tau_0}(1 - \tanh\{[H(x') - H(x)]/2T\}). \tag{3.3}$$

This choice of $W(x' \to x)$ yields a Boltzmann equilibrium probability distribution. The spins are updated sequentially using single spin-flip moves.

The three order parameters that we calculate, namely $q_N(t)$, $q_N^{\mathrm{mod}}(t)$ and $q_N^{(2)}(t)$, all involve a thermal average followed by a disorder average. The correct way to perform the thermal average for a given bond configuration is to perform many separate uncorrelated Monte Carlo runs. Hence:

$$\langle S_i(t_0) S_i(t_0 + t)\rangle_T = \frac{1}{R} \sum_{n=1}^{R} S_{i,n}(t_0) S_{i,n}(t_0 + t) \tag{3.4}$$

where R is the number of runs and the summation is over each of the n separate runs. This process must be carried out for each bond configuration and is therefore very time consuming. This is exactly what we do in our study of the ergodic dynamics. MY have pointed out that the short-time dynamics can be more efficiently studied by performing the bond and thermal averages together. For every bond configuration only a single Monte Carlo run is performed. The averaging is now given by:

$$\langle\langle S_i(t_0) S_i(t_0 + t)\rangle_T\rangle_J = \frac{1}{B} \sum_{n=1}^{B} S_{i,n}(t_0) S_{i,n}(t_0 + t). \tag{3.5}$$

One of the main difficulties of any Monte Carlo simulation is ensuring that the system is in equilibrium before sampling takes place. Bray and Moore (1980b) have shown that the following convenient relation holds in equilibrium:

$$q^{(2)} = 1 - 2T|U(T)|. \tag{3.6}$$

$U(T)$ is the internal energy per spin and is calculated at the end of the equilibration period. Hence prior to sampling for $q^{(2)}$, we already know what it should relax to. If the equilibration period is too short, then the out-of-equilibrium values $|U(T)|$ and $q^{(2)}$ only satisfy the following inequality:

$$q^{(2)} < 1 - 2T|U(T)|. \tag{3.7}$$

In this case the calculations were repeated until equation (3.6) was satisfied. The data concerning the Monte Carlo statistics are presented in table 1. The values quoted for q_N^{mod}, $|U(T)|$ and $q_N^{(2)}$ are the equilibrium values. If the equilibrium values of $|U(T)|$ are inserted into equation (3.6), then the predicted values of $q_N^{(2)}$ agree, to four decimal places, with the equilibrium data in table 1.

Note that some of the systems have identical equilibration times. This is not an error. We used too many equilibration steps for the smaller systems.

Table 1. Monte Carlo statistics data.

N	No of bond configurations	No of equilibration steps	q_N^{mod}	$\lvert U(T)\rvert$	$q_N^{(2)}$
16	10 000	1 000	0.590	0.6064	0.3936
32	10 000	1 000	0.560	0.6391	0.3608
64	7 105	5 000	0.540	0.6637	0.3362
128	1 000	10 000	0.531	0.6813	0.3186
256	240	10 000	0.522	0.6919	0.3080

4. Ergodic dynamics

In this section we shall only be concerned with the dynamics of global spin flips that preserve the spin inversion symmetry of the Hamiltonian. Ergodic fluctuations are most easily examined by considering the following combination of order parameters:

$$R_N(t,\{J\}) = \frac{q_N(t,\{J\})}{q_N^{\mathrm{mod}}(t,\{J\})}. \tag{4.1}$$

The notation $(t,\{J\})$ denotes that $q_N(t)$ and $q_N^{\mathrm{mod}}(t)$ have been calculated for a given bond configuration. $q_N(t,\{J\})$ relaxes as a result of short-time and ergodic dynamics, whereas $q_N^{\mathrm{mod}}(t,\{J\})$ relaxes only via short-time dynamics. Therefore, the short-time dynamics are factored out of the ratio $R_N(t,\{J\})$, which is unity for times much less than the ergodic time. For ergodic timescales, $R_N(t,\{J\})$ decays to zero as shown schematically in figure 1. For each system size N we have calculated $R_N(t,\{J\})$ for a large number of bond configurations and find that on ergodic timescales it decays exponentially:

$$R_N(t,\{J\}) = \exp(-t/\tau_N(\{J\})) \tag{4.2}$$

$\tau_N(\{J\})$ is the ergodic time for a given bond configuration. Some typical examples of this behaviour for $N=8$ are shown in figure 2. Such exponential decay implies that a single barrier separates a pure state and its globally spin-flipped counterpart in *a given*

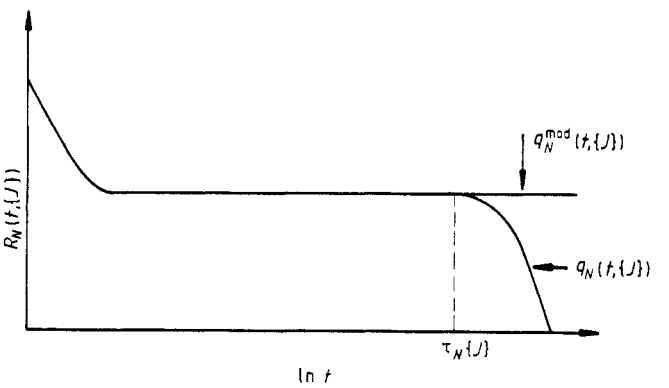

Figure 1. The schematic decay of $R_N(t,\{J\})$. Note that $q_N^{\mathrm{mod}}(t,\{J\})$ and $q_N(t,\{J\})$ are equal for times $t \ll \tau_N\{J\}$. For $t \sim \tau_N$, $R_N(t,\{J\})$ decays to zero purely exponentially.

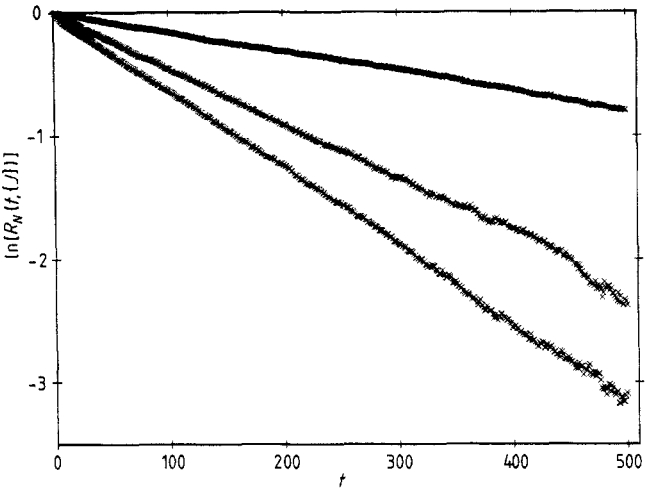

Figure 2. This figure shows $\ln(R_N(t,\{J\}))$ plotted as a function of time t for different bond configurations. The straight lines indicate that $R_N(t,\{J\})$ decays purely exponentially on ergodic timescales. This data was obtained using the system size $N=8$.

bond configuration. The barrier height $B_N\{J\}$ and the relaxation time $\tau_N\{J\}$ are related by the Arrenhius law:

$$\ln(\tau_N\{J\}) \propto B_N\{J\}/T. \tag{4.3}$$

Averaging over a large number of bond configurations introduces a distribution of ergodic barrier heights such as the one shown in figure 3. This was obtained by calculating $\ln(R_N(t,\{J\}))$ for each bond configuration and performing a least-squares fit for $\tau_N\{J\}$. We are interested in how the mean and variance of these distributions

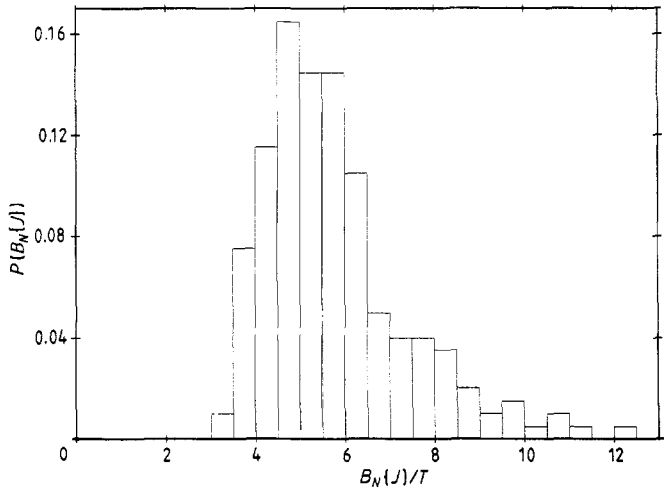

Figure 3. The distribution of ergodic barriers $p(B_N\{J\}))$ plotted as a function of $B_N\{J\}/T$. This was obtained by calculating $\ln(R_N(t,\{J\}))$ for each bond configuration and performing a least-squares fit for the ergodic time $\tau_N\{J\}$.

depend on the system size N. Assuming that the mean barrier height diverges as:

$$\langle B_N\{J\}\rangle_J \propto N^{\lambda} \tag{4.4}$$

we find that $\lambda = 0.25 \pm 0.05$ as shown in figure 4.

Note that Mackenzie and Young (1982, 1983) have suggested that $\lambda \simeq \frac{1}{2}$. We suggest that our value is correct because the method we have used is more accurate than MY. First let us review our method. An accurate determination of λ depends upon an accurate determination of the mean barrier height $\langle B_N\{J\}\rangle_J$ (see equation (4.4)). This has been determined by calculating the distribution of ergodic barrier heights from the purely exponential decay of $R_N(t, \{J\})$. The determination of the single barrier height $B_N\{J\}$ associated with a given bond configuration results from least squares fitting a straight line to $\ln R_N(t, \{J\})$. The linear plots shown in figure 2 imply that an accurate determination of $B_N\{J\}$ is possible. MY determined λ using a different method. They determined the mean barrier height $\langle B_N\{J\}\rangle_J$ by averaging the ergodic fluctuations in $q_N(t, \{J\})$. This process involves recording the ergodic fluctuations of $q_N(t, \{J\})$ for a bond configuration and averaging them to obtain an estimate of the single barrier height $B_N\{J\}$ associated with this bond configuration. This process is very computationally expensive and limited MY to sampling over a small number of bond configurations. We have used a much greater number of bond configurations and have therefore found that $\lambda = 0.25 \pm 0.05$ rather than the MY estimate of $\lambda \sim \frac{1}{2}$.

The system sizes 8 to 10 are clearly not asymptotic and have been disregarded. The self-averaging of the barrier height distributions can be investigated by calculating the normalised variance:

$$\sigma_N^2 = \frac{\langle B_N\{J\}^2\rangle_J - \langle B_N\{J\}\rangle_J^2}{\langle B_N\{J\}\rangle_J^2}. \tag{4.5}$$

We define self-averaging to be $\lim_{N\to\infty}(\sigma_N^2) = 0$. This property is interesting because self-averaging implies that in the thermodynamic limit a single barrier separates all

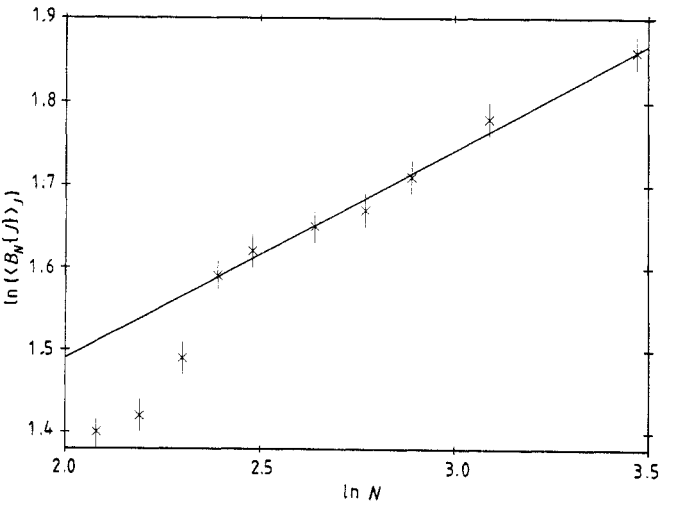

Figure 4. This figure shows $\ln(\langle B_N\{J\}\rangle_J)$ plotted as a function of $\ln N$. The straight-line fit indicates that the mean ergodic barrier height $\langle B_N\{J\}\rangle_J$ diverges as N^{λ}, where $\lambda = 0.25 \pm 0.05$. The system sizes 8 to 10 are clearly not asymptotic and have been ignored.

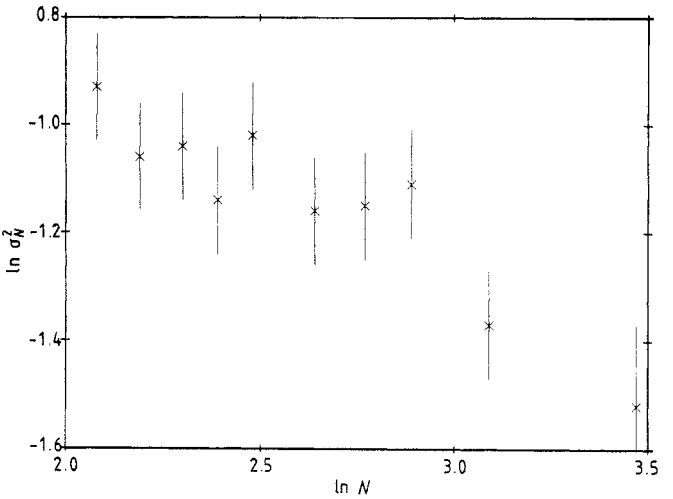

Figure 5. This figure shows $\ln \sigma_N^2$ plotted as a function of $\ln N$. Self-averaging of the distribution of ergodic barriers implies that $\lim_{N\to\infty} \sigma_N^2 = 0$. The scatter of the data points suggests a lack of self-averaging. However, the size of the error bars prevent a definite conclusion on this issue.

the pure phases from their globally spin-flipped neighbours. Our data for σ_N^2, presented in figure 5, suggest a lack of self-averaging. However, the error bars on the data prevent a definite conclusion from being made.

5. Short-time dynamics

In this section we determine the divergence of the free-energy barriers between the pure states residing in half of the accessible phase space. The other half of the phase space contains the globally spin-inverted counterparts of these pure states. We suppress the effects of fluctuations between each half of the phase space by using the order parameter $q_N^{(2)}(t)$, which is insensitive to ergodic fluctuations.

In figure 6 we present data showing how $q_N^{(2)}(t)$ relaxes to its finite-size statistical mechanics average value $q_N^{(2)}$ for $N = 32$. This data has the following obvious features. For times greater than some relaxation time ξ_N $q_N^{(2)}(t)$ is time independant. Such behaviour suggests that $q_N^{(2)}(t)$ relaxes by thermal activation over a spectrum of free-energy barriers. When activation over the entire spectrum has occurred $q_N^{(2)}(t)$ develops its statistical mechanics plateau value. We have obtained data similar to that shown in figure 6 for the system sizes $N = 16$, 64, 128, 256. If we assume that ξ_N diverges as $\ln(\xi_N) \propto N^{\mu}$, then μ can be determined from ξ_N. However, for the larger systems a precise determination of ξ_N from the onset of the statistical mechanics average plateau is difficult. Instead, we extract μ more accurately by collapsing the data for different system sizes onto a single universal curve using a dynamic scaling ansatz. The abrupt change of gradient in figure 6 when $q_N^{(2)}(t)$ becomes time independent suggests $\ln(t)/\ln(\xi_N)$ as a suitable scaling variable. Given that we assume that $\ln(\xi_N) \propto N^{\mu}$ this scaling ansatz becomes $\ln(t)/N^{\mu}$. The order parameter $q_N^{(2)}(t)$ decays to its size-dependent statistical mechanics value $q_N^{(2)}$. Hence, as well as the dynamic scaling ansatz, the static finite effects must be removed from the data. We have done this by

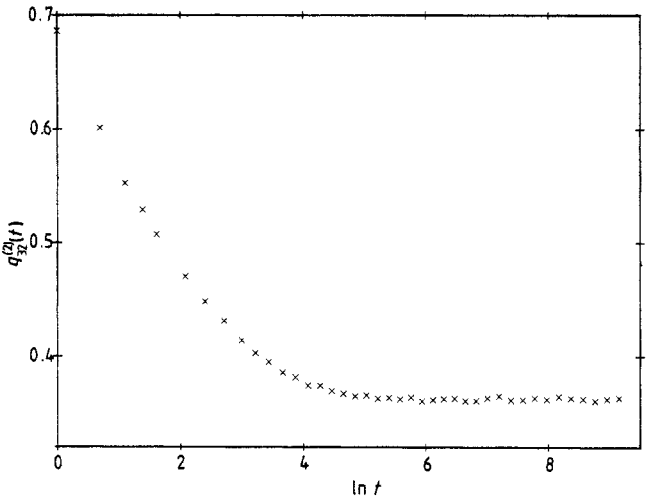

Figure 6. This figure shows $q_{32}^{(2)}(t)$ plotted as a function ln t; $q_{32}^{(2)}(t)$ is time independent for $t > \xi_{32}$ because it is insensitive to ergodic fluctuations.

choosing the dependent variable to be:

$$\frac{q_N^{(2)}(t) - q_N^{(2)}}{1 - q_N^{(2)}}. \tag{5.1}$$

let us call this variable $Y_N(t)$. For all N this variable is restricted to the interval $0 \leqslant Y_N(t) \leqslant 1$. We produced a range of plots of $Y_N(t)$ as a function of $\ln(t)/N^{\mu}$, each with a different value of μ. Only values of μ in the range $0.25 < \mu < 0.45$ yielded acceptable universal curves. A typical result using $\mu = 0.34$ is presented in figure 7. Our bounds for μ are consistent with the recent study of Vertechi and Virasoro (1989) in which they find $0.26 < \mu < 0.42$. The sensitivity of the scaling ansatz to variations

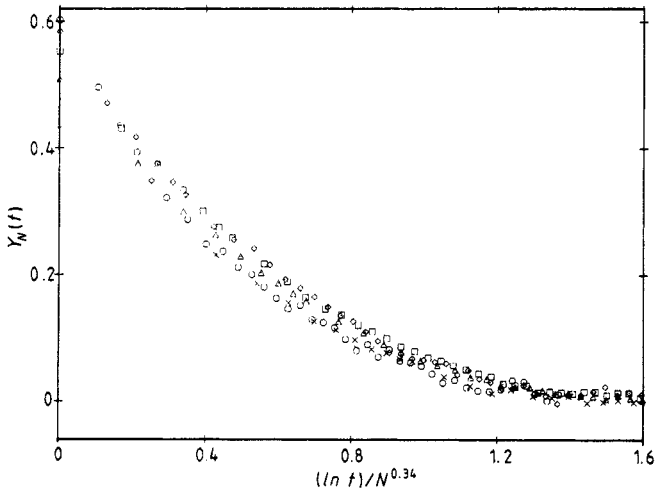

Figure 7. $Y_N(t)$ plotted as a function of $\ln(t)/N^{\mu}$ where $\mu = 0.34$. The data for the different system sizes fall on a universal curve. The system sizes (N) are represented as follows: ×, 16; △, 32; □, 64; ◇, 128; ⊙, 256.

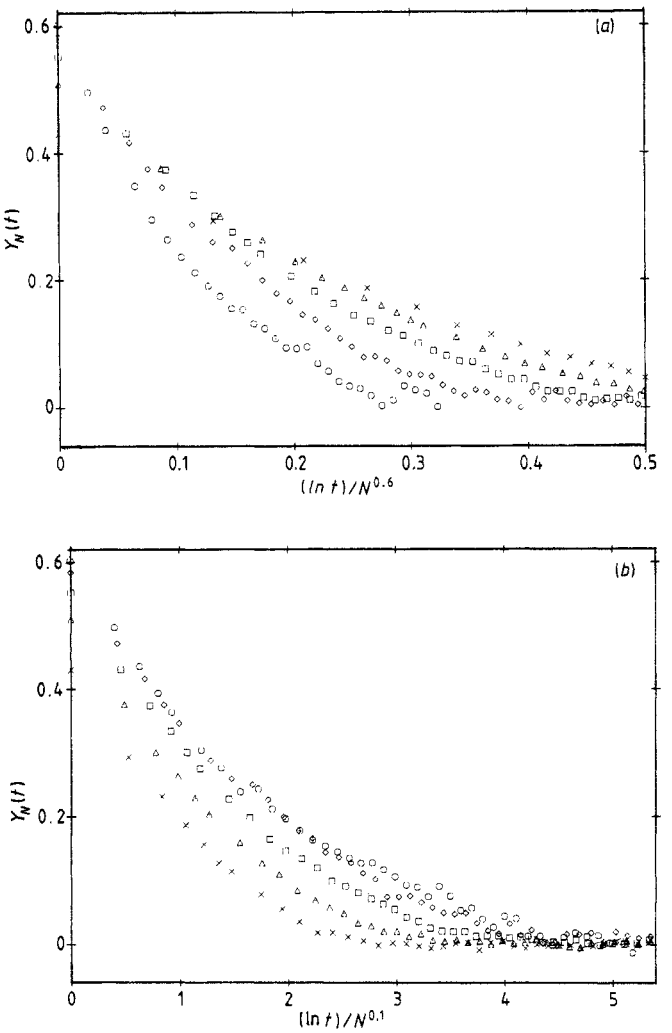

Figure 8. $Y_N(t)$ plotted as a function of $\ln(t)/N^{\mu}$ where (*a*) $\mu = 0.60$ and (*b*) $N = 0.10$. The data points do not fall on a universal curve because μ is unacceptably large. The system sizes are as represented in figure 7.

in μ is demonstrated in figures 8(a) and (b). These figures were obtained using values of μ outside the acceptable bounds.

The data from the previous section implies that the ergodic energy barrier(s?) diverges as N^{λ}, where $\lambda = 0.25 \pm 0.05$. We would naively expect that a more accurate determination of μ would yield $\mu < \lambda$. However, the ergodic free-energy barrier(s?) does not necessarily have to be the largest free-energy barrier in the system.

6. Conclusions

Extensive Monte Carlo simulations of the Ising model have been conducted below the AT line ($h = 0$, $T = 0.5$). Each bond configuration has an ergodic time that has been calculated by studying the decay of an order parameter that is only sensitive to ergodic

fluctuations. The mean ergodic time averaged over bond configurations diverges as N^{λ}, where $\lambda = 0.25 \pm 0.50$. The distribution of ergodic barriers associated with the different bond configurations may not be self-averaging. For the short-time dynamics we find a spectrum of barriers the largest of which diverges as N^{μ} where $0.25 < \mu < 0.45$.

Acknowledgments

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