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# Monte Carlo study of Griffiths phase dynamics in dilute ferromagnets

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**Abstract.** The asymptotic dynamics of the spin autocorrelation function is studied in the Griffiths phase of bond-dilute Ising and Heisenberg ferromagnets by Monte Carlo simulation, for simple relaxational dynamics (model A). Systems above, at and below the percolation threshold are studied. Relaxation is non-exponential in all cases. Agreement with theoretical predictions based on clustering arguments is excellent for the Heisenberg systems, less so for the Ising systems.

## 1. Introduction

The dynamics of random magnetic systems in the 'Griffiths phase' have attracted much recent attention [1-10]. The Griffiths phase is the name given to the temperature regime between the transition temperature for magnetic long-range order in the random system and the highest possible transition temperature allowed in principle by a rare statistical fluctuation of the disorder over the whole system. The latter temperature we term the 'Griffiths temperature' $T_G$. Figure 1 shows a schematic phase diagram for a ferromagnet with site or bond dilution. The Griffiths phase G is the region

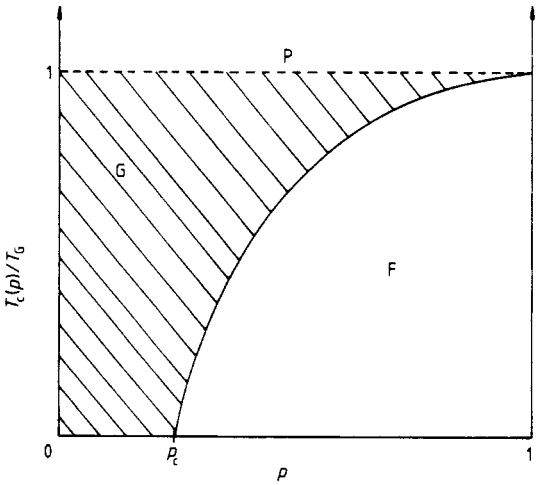


**Figure 1.** Schematic phase diagram for a dilute ferromagnet, showing paramagnetic (P), ferromagnetic (F) and Griffiths (G) phases. All simulations in this paper were performed in region G.

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between the horizontal broken line and the phase boundary for the onset of ferromagnetism. The latter boundary meets the zero-temperature axis at the percolation threshold $p_c$. The Griffiths temperature $T_G = T_c(1)$ is the critical temperature of the undiluted system.

For a random ferromagnet consisting of classical $n$-dimensional spins, with short-ranged interactions and simple relaxational ('model A' [11]) dynamics, the results

$$C(t) \sim \exp\{-A(\ln t)^{d/(d-1)}\} \qquad n = 1 \tag{1}$$

$$\sim \exp\{-Bt^{1/2}\} \qquad n \geq 2 \tag{2}$$

have been obtained for the asymptotic behaviour of the spin autocorrelation functions, defined by

$$C(t) = [\langle \boldsymbol{S}_i(0) \cdot \boldsymbol{S}_i(t) \rangle] \tag{3}$$

of Ising and vector spin systems in the Griffiths phase [1, 3-7]. In (1) and (2), $d$ is the spatial dimension, and the amplitudes $A$, $B$ depend on the system parameters (temperature, concentration of missing sites or bonds, etc). In (3), $\langle \ldots \rangle$ and $[\ldots]$ represent thermal and disorder averages respectively.

The physics behind (1) and (2) concerns the dominance, as $t \to \infty$, of large regions which, due to rare statistical fluctuations in the disorder, resemble locally a system which, in the bulk, would be in its ordered phase at the given temperature. Because these regions are finite they do relax, but only slowly due to their large size. As a result, the relaxation is *non-exponential* throughout the Griffiths phase, i.e. *above* the critical temperature $T_c(p)$ for the onset of magnetic long-range order. In other words a kind of 'dynamical phase transition' (from exponential to non-exponential relaxation) occurs at $T_G = T_c(1)$.

The arguments for (1) and (2) are physically appealing, but non-rigorous. For Ising spins, however, a result of the form (1) has been shown [5] to give a lower bound on $C(t)$, while very recently it has been shown that, provided $p < p_c$, the forms (1) and (2) provide both upper and lower bounds, thereby establishing them as the correct asymptotic forms in at least part of the Griffiths phase [7]. Simple variational arguments [3, 4, 6] lead us to expect that the forms (1) and (2) should hold throughout the Griffiths phase and for more general kinds of disorder than simple dilution.

A most important question, which has so far received little attention, is over what time domain the *asymptotic* behaviour will be observed. The question is probably best phrased in terms of how small $C(t)$ has become when the asymptotic behaviour sets in. This is a difficult question to address from a purely theoretical standpoint. We believe, however, that valuable insights can be obtained from numerical simulations, and in this paper we present the results of extensive Monte Carlo simulations of bond-diluted Ising and Heisenberg ferromagnets.

For Heisenberg systems, the asymptotic behaviour is found to set in rather quickly: equation (2) fits the data well over most of the decay of $C(t)$, failing only at very short times; for Ising systems, (1) fits the data much less well, although the data are consistent with the asymptotic correctness of (1). The data are somewhat better described, over the relevant timescales, by a phenomenological 'stretched exponential' dependence of the form $C(t) \sim \exp\{-(t/\tau)^{\beta}\}$, with a *temperature-dependent* stretched exponent $\beta$, in agreement with the conclusions of Jain [8] and Ogielski [9].

Finally, data for the non-equilibrium decay of the magnetisation $M(t)$, from an aligned start, are obtained as a by-product of the simulation, and are potentially revealing. The same clustering arguments which lead to (1) and (2) for $C(t)$ predict

*identical* asymptotic behaviour for $M(t)$. For the Heisenberg systems, we indeed find that $M(t)$ is well described by (2), with apparently the same values of $B$ as those obtained from the $C(t)$ data. For the Ising systems, however, a stretched exponential form again fits the data better than (1), but with (at least for $d=2$) a different stretched exponent $\beta$ from that extracted from the $C(t)$ data. The implications of this result are discussed in § 4.

## 2. Monte Carlo procedure

Simulations were carried out on three-dimensional ($d=3$), simple cubic, bond-diluted Heisenberg (i.e. $n=3$) ferromagnets and on bond-diluted Ising ferromagnets for $d=2$ (square lattice) and $d=3$ (simple cubic). The restriction to $d=3$ for the Heisenberg systems is necessary since $d=2$ systems order only at $T=0$, i.e. $T_G=0$ for $d=2$.

The bond percolation thresholds for simple cubic and square lattices are $p_c \simeq 0.247$ and $p_c=0.5$ respectively. For the $d=3$ Heisenberg system, bond occupation probabilities $p=0.2$ and 0.3 were used, being below and above $p_c$ respectively. For the Ising systems, $p=0.2$ and 0.5 were used for $d=3$ and 2 respectively.

Since, at the timescales of interest, the length scales involved (i.e. the sizes of the dominant clusters) are not particularly large, it was not thought important to simulate large systems. For $d=3$, all systems were of size $10^3$; for $d=2$, systems of size $32^2$ were used. Periodic boundary conditions were employed throughout.

It *is* important, however, to average over a sufficiently large number of samples. Firstly, as the anomalous relaxation in the Griffiths phase is associated with regions of higher than average coordination, it is important to generate sufficiently many samples that such regions occur in reasonable numbers in the total set of samples. The number of samples required will in principle increase with the timescale probed. Secondly, a large number of samples is needed to reduce statistical errors to acceptable levels. It is convenient (see below) to evaluate both the time average (which replaces the thermal average $\langle \ldots \rangle$ in a Monte Carlo calculation) and the disorder average $[\ldots]$ by an average over samples, i.e. no *explicit* time average is performed.

Standard 'heat-bath' Monte Carlo algorithms were employed, efficient vectorisation being achieved by a 'red-black' splitting of the lattice into two sublattices which are updated alternately. For the Heisenberg systems, the basic move was to re-orient each spin to a new direction chosen randomly from the sphere of possible directions. In the heat-bath algorithm, the move is accepted with probability $\{\exp(\Delta E/T)+1\}^{-1}$, where $\Delta E$ is the energy change due to the move and $T$ is the temperature.

The spin autocorrelation function is given by

$$C(t) = N^{-1} \sum_{i=1}^{N} [\langle \boldsymbol{S}_i(t_0) \cdot \boldsymbol{S}_i(t_0+t) \rangle].$$

The thermal average for a given bond configuration should be performed in principle by averaging over many separate uncorrelated Monte Carlo runs. Carrying out this process separately for each bond configuration is very time consuming. Instead, therefore, we carry out the thermal and configuration averages together, using

$$C(t) = N^{-1} \sum_{i=1}^{N} \left( B^{-1} \sum_{n=1}^{B} \boldsymbol{S}_{i,n}(t_0) \cdot \boldsymbol{S}_{i,n}(t_0+t) \right)$$

**Table 1.** Simulation details and Griffiths temperatures for the four systems studied. Equilibration times are measured in Monte Carlo steps per spin. (*a*) 3D Heisenberg model ($T_G \simeq 1.45$), $p = 0.2$. (*b*) 3D Heisenberg model ($T_G \simeq 1.45$), $p = 0.3$. (*c*) 3D Ising model ($T_G \simeq 4.51$), $p = 0.2$. (*d*) 2D Ising model ($T_G \simeq 2.27$), $p = 0.5$.

| | Temperature | Equilibration time | Number of samples |
|---|---|---|---|
| (*a*) | 0.3 | 2000 | 3 991 |
| | 0.4 | 484 | 14 370 |
| | 0.5 | 289 | 5 015 |
| | 0.6 | 196 | 35 541 |
| (*b*) | 0.4 | 2300 | 3 254 |
| | 0.5 | 676 | 11 470 |
| | 0.6 | 400 | 17 892 |
| | 0.7 | 256 | 29 777 |
| (*c*) | 0.7 | 1000 | 22 665 |
| | 0.8 | 400 | 37 214 |
| | 0.9 | 300 | 41 639 |
| | 1.0 | 200 | 47 276 |
| (*d*) | 1.2 | 800 | 39 402 |
| | 1.3 | 500 | 58 231 |
| | 1.4 | 300 | 102 854 |
| | 1.5 | 200 | 134 479 |
| | 1.6 | 200 | 134 469 |
| | 1.7 | 200 | 153 675 |
| | 1.8 | 150 | 153 732 |
| | 1.9 | 100 | 134 623 |

where the subscript $n$ specifies the bond configuration, and $B$ is the total number of bond configurations used.

To ensure that the system is in equilibrium before sampling begins, the simulation is started from a completely aligned state. Equilibrium is taken to have been established when the component of magnetisation along the original alignment direction has decayed to a value smaller than that due to thermal fluctuations.

Data concerning equilibration times, numbers of samples (bond configurations) employed, the temperatures and bond concentrations studied, and the critical temperatures of the pure systems, are presented in table 1.

## 3. Results

### *3.1. 3D Heisenberg model*

In order to compare the results with the prediction (2), the data are plotted as $\ln C(t)$ against $\sqrt{t}$. If (2) is correct, such plots should yield straight lines, with temperature-dependent slope $B(T)$. The data are presented in figures 2 and 3. Apart from some initial curvature at short times, the data are remarkably linear (until statistical noise sets in at later times), and allows a reasonably precise determination of $B(T)$.

The values of $B(T)$ extracted from figures 2 and 3 are presented in figure 4. Over the temperature range considered, $B(T)$ is roughly linear in $T$, with a similar slope

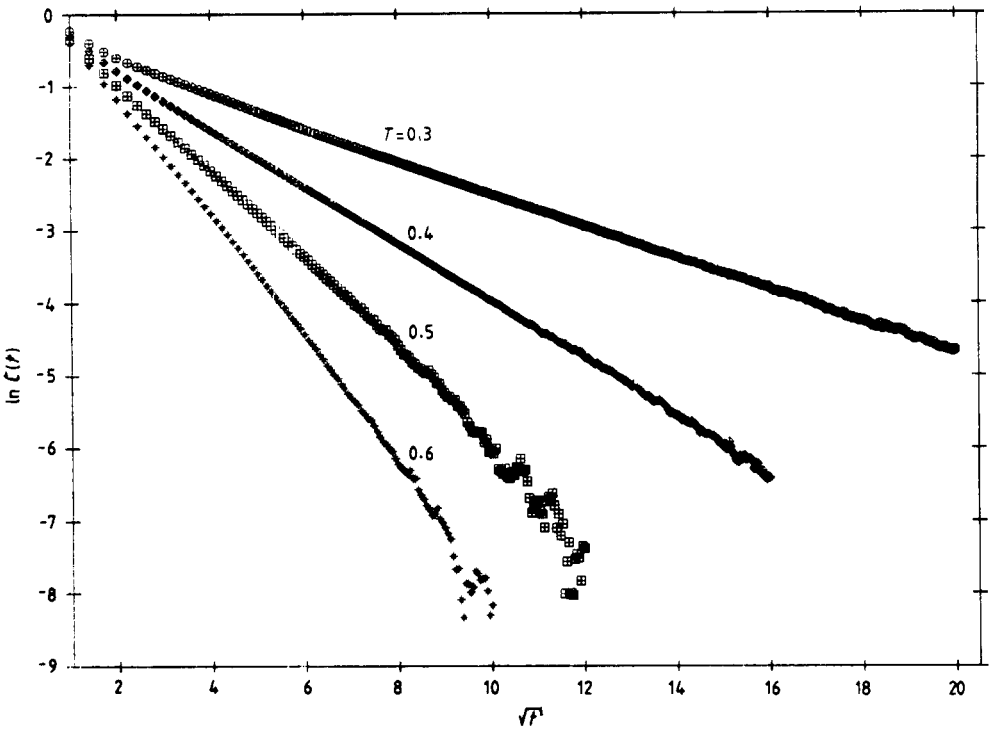


**Figure 2.** ln $C(t)$ against $t^{1/2}$ for the Heisenberg model with $p = 0.2$. According to (2), asymptotically the data should lie on straight lines.

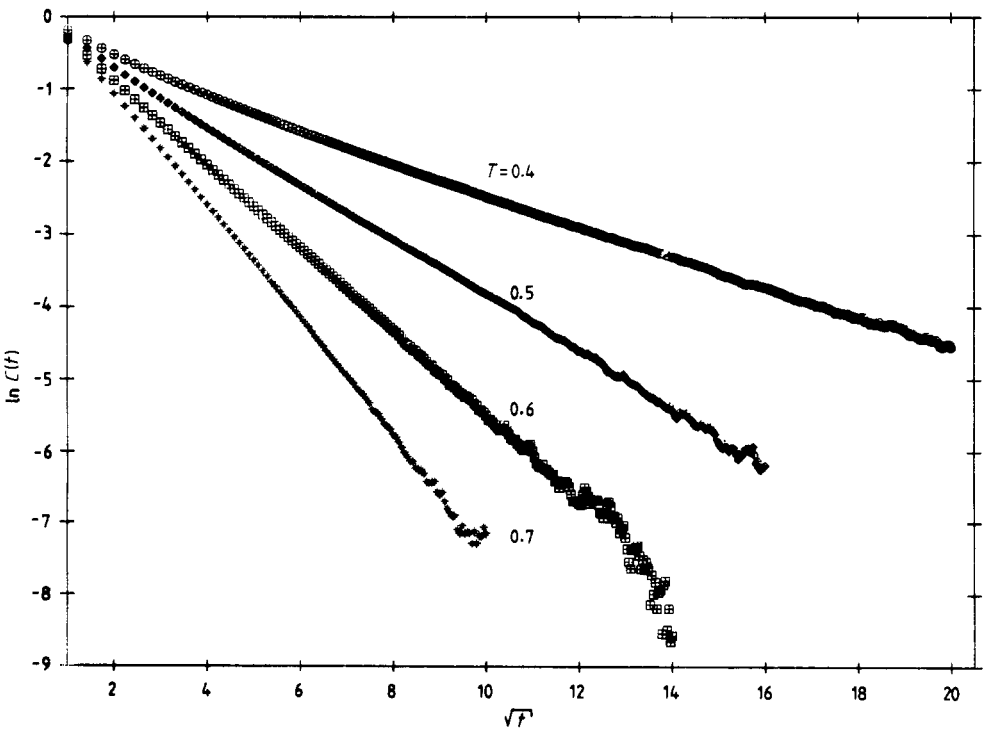


**Figure 3.** ln $C$ against $t^{1/2}$ for the Heisenberg model with $p = 0.3$.

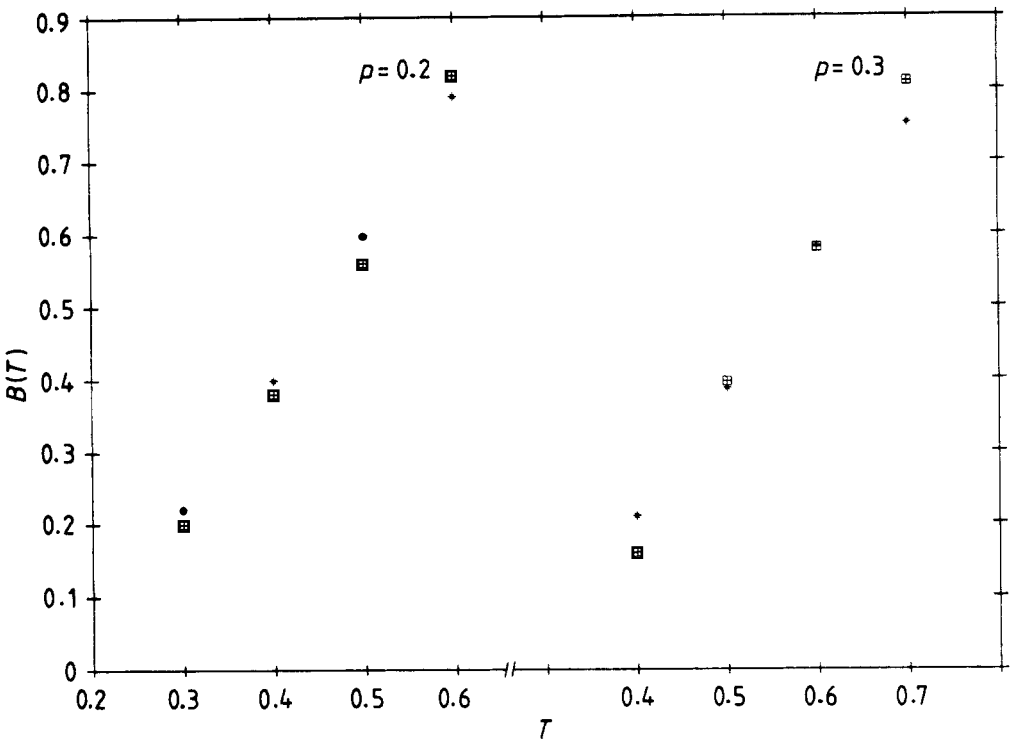


**Figure 4.** $B(T)$ against $T$ for the Heisenberg models with $p = 0.2$ and 0.3, extracted from the $C(t)$ data (⊞) in figures 2 and 3. Also shown are the corresponding data (*) extracted from the decay of the magnetisation $M(t)$.

($\sim$1.8-1.9) for both concentrations. On theoretical grounds [4], we expect $B$ to vanish at $T = 0$ (if $p < p_c$) or at $T = T_c(p)$ (if $p > p_c$), when long-range order becomes established, and to diverge at $T = T_G \equiv T_c(1)$, above which temperature simple exponential relaxation should apply. Therefore the linear behaviour suggested by figure 4 must be strongly modified for $T \to T_G \simeq 1.445$. Similarly, for $p = 0.2 (< p_c)$ the linear fit suggests that $B(T)$ vanishes at a non-zero temperature $T \sim 0.2$, so modifications must also occur for small $T$.

### 3.2. 3D *Ising model*

The interpretation of the Ising data is much more problematical. In order to compare with the prediction (1), a number of ways of presenting the data were tried, none very successfully. The obvious plot of $\ln C(t)$ against $(\ln t)^{3/2}$ yields substantial curvature, with no really convincing linear regime for the timescales studied.

Significant straightening of the data *can* be achieved by plotting $\ln C$ against $\{\ln(t/\tau)\}^{3/2}$, with $\tau(T)$ a fitting parameter which depends on temperature. Such a timescale does, in fact, emerge naturally from the clustering arguments [4] which lead to (1): for $T$ near $T_G$ the dependence $\tau \propto \xi^{d+z}$ is predicted [4] (where $\xi$ and $z$ are the correlation length and dynamical exponent respectively of the *pure* system), i.e. we expect $\tau$ to be an increasing function of temperature. Figure 5 shows the 3D Ising data

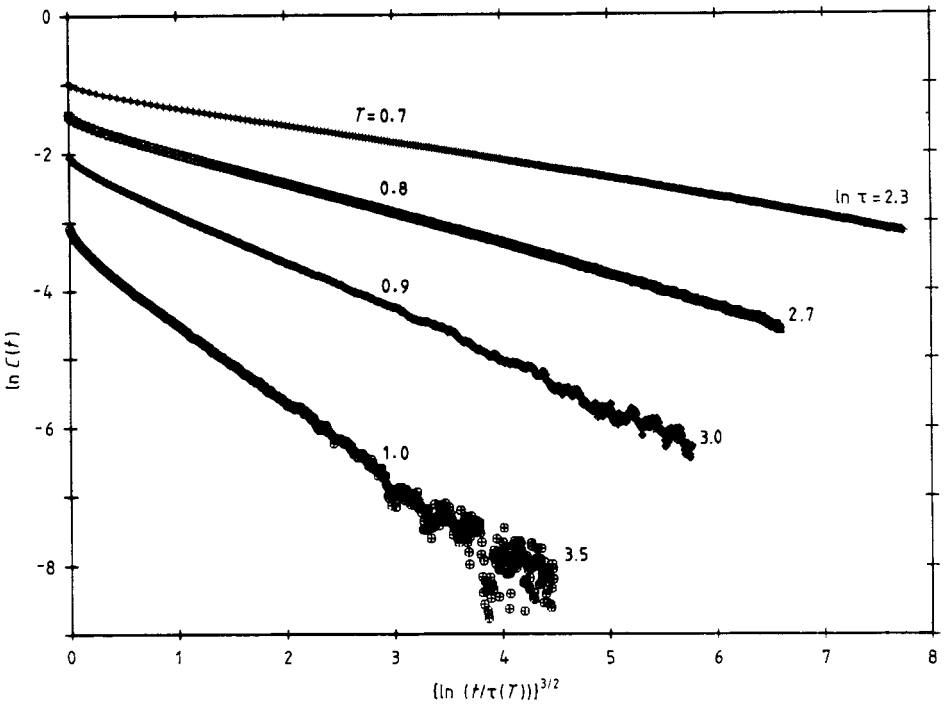


**Figure 5.** ln $C$ against $\{\ln(t/\tau)\}^{3/2}$ for the 3D Ising model with $p = 0.2$. The values of ln $\tau$, which was adjusted until a reasonable straightening of the data was obtained, are shown in the figure.

plotted in this form, with the values of ln $\tau$ indicated. The values of $\tau$ were adjusted 'by hand' until reasonable linearity was obtained: no systematic fitting was attempted. The required values of $\tau$ do increase with $T$ as expected, although the temperatures are too far from $T_G$ to test the prediction $\tau \propto \xi^{d+z}$.

A somewhat more convincing fit (in that no adjustable parameters are required) is to the stretched exponential (or 'Kohlrausch') form $C(t) \sim \exp\{-(t/\tau)^{\beta}\}$. In figure 6 we plot $\ln(-\ln C(t))$ against $\ln t$. A stretched exponential decay would appear as a straight line with slope $\beta$. For all temperatures, there appear to be two linear regimes (this is particularly marked for the lowest temperature), the 'long-time' linear regime covering about three 'e-cades' of time. The values of the exponent $\beta$ extracted from these plots are given in figure 7. Note that they depend on $T$, with $\beta$ an increasing function of $T$.

Since $p = 0.2$ is below the percolation threshold for the simple cubic lattice, the arguments [7] that (1) is asymptotically exact apply to these data. In an attempt to reveal the asymptotic behaviour described by (1) we finally plot $\ln(-\ln C(t))$ versus $\ln \ln t$. According to (1), this should asymptotically yield straight lines with slope $d/(d-1)$, i.e. slope $\frac{3}{2}$ for $d = 3$. The data are presented in figure 8, with lines of slope $\frac{3}{2}$ added as guides to the eye. Clearly the data are consistent with the asymptotic correctness of (1), though there is a worrying hint that the slopes may be just starting to exceed $\frac{3}{2}$ at the longest times.

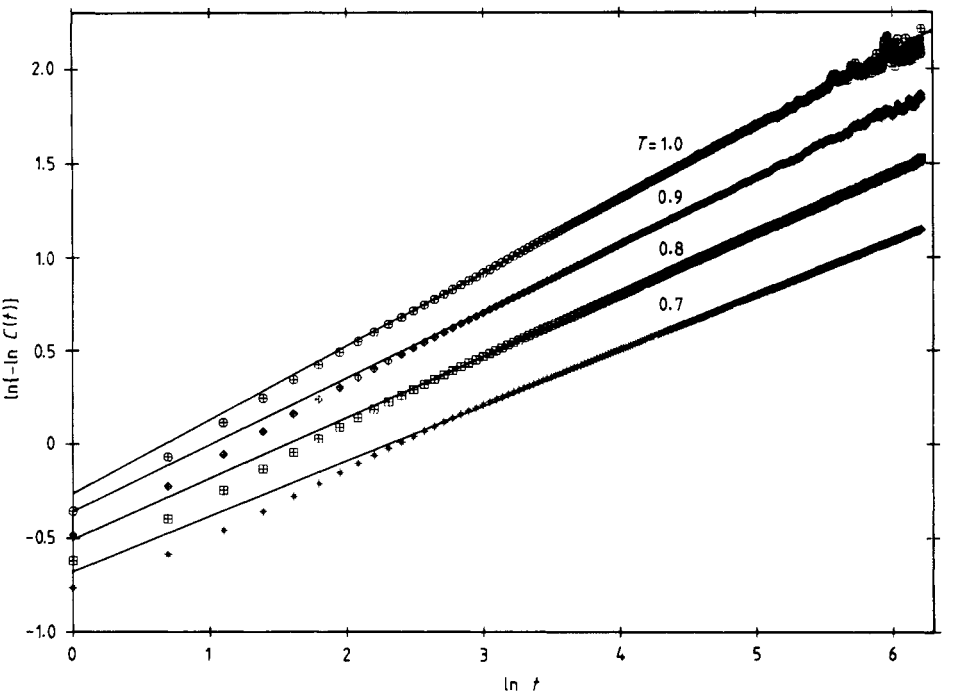


**Figure 6.** $\ln(-\ln C)$ against $\ln t$ for the 3D Ising model with $p = 0.2$. The straight lines, included as guides to the eye, suggest a good fit to the stretched exponential form $C(t) \sim \exp\{-(t/\tau)^{\beta}\}$.

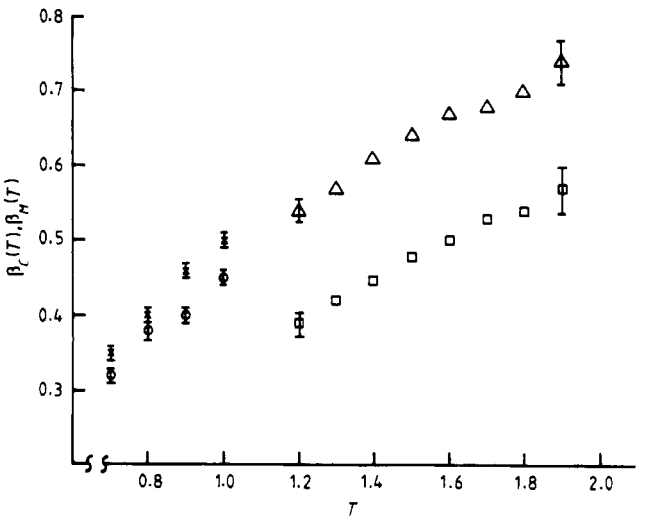


**Figure 7.** The stretched exponents $\beta(T)$ for the 3D Ising model with $p = 0.2$ ($\times$) and the 2D Ising model with $p = 0.5$ ($\square$), obtained from the asymptotic slopes of the data in figures 6 and 10. Also shown are the exponents $\beta(T)$ obtained from the data for the magnetisation $M(t)$ shown in figures 13 and 14, for the 3D ($\bigcirc$) and 2D ($\triangle$) Ising models.

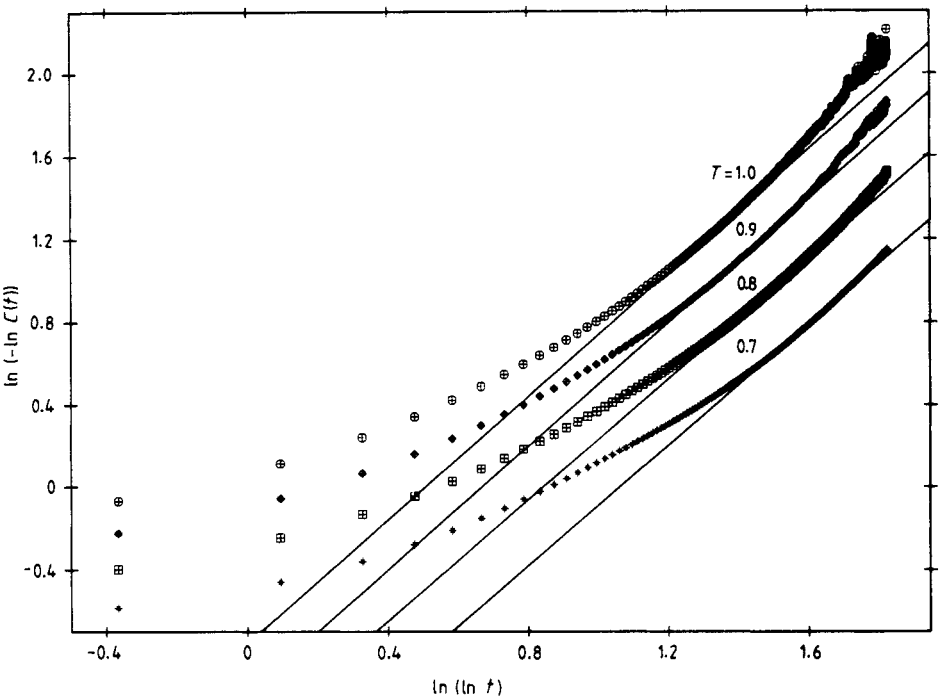


**Figure 8.** $\ln(-\ln C)$ against $\ln\ln t$ for the 3D Ising model with $p = 0.2$. The straight lines, included as guides to the eye, have slope $\frac{3}{2}$.

### *3.3. 2D Ising model*

The two-dimensional Ising simulations were carried out at the percolation threshold, $p = \frac{1}{2}$, and therefore provide an independent check of the results of Jain [8]. The data were analysed in a similar manner to the 3D data, and the results are presented in figures 9-11. In figure 11, the straight lines, drawn as guides to the eye, have slope $d/(d-1) = 2$. Again, the data are consistent (figure 9) with the asymptotic correctness of (1), but the most convincing fit is to the stretched exponential form (figure 10). The values of $\beta$ extracted from figure 10 are given in figure 7. These results are completely consistent with those of Jain [8].

### *3.4. Non-equilibrium decay of the magnetisation*

Since the equilibration process was monitored by following the decay of the magnetisation $M(t)$, from a completely aligned start ($M(0) = 1$), data for $M(t)$ were obtained as a bonus. (For Heisenberg spins, we mean by $M(t)$ the projection of the magnetisation onto its direction at $t = 0$.)

The clustering arguments which lead to (1) and (2) can also be used to calculate the asymptotic decay of $M(t)$: the same large regions, locally resembling a system in its ordered phase, which are responsible for the slow decay of $C(t)$ also lead to slow decay of $M(t)$. Although the decay of $M$ is a non-equilibrium process, at the (asymptotic) timescales of interest all modes will have equilibrated except those associated with the re-orientation of the cluster magnetisation as a whole. The timescale

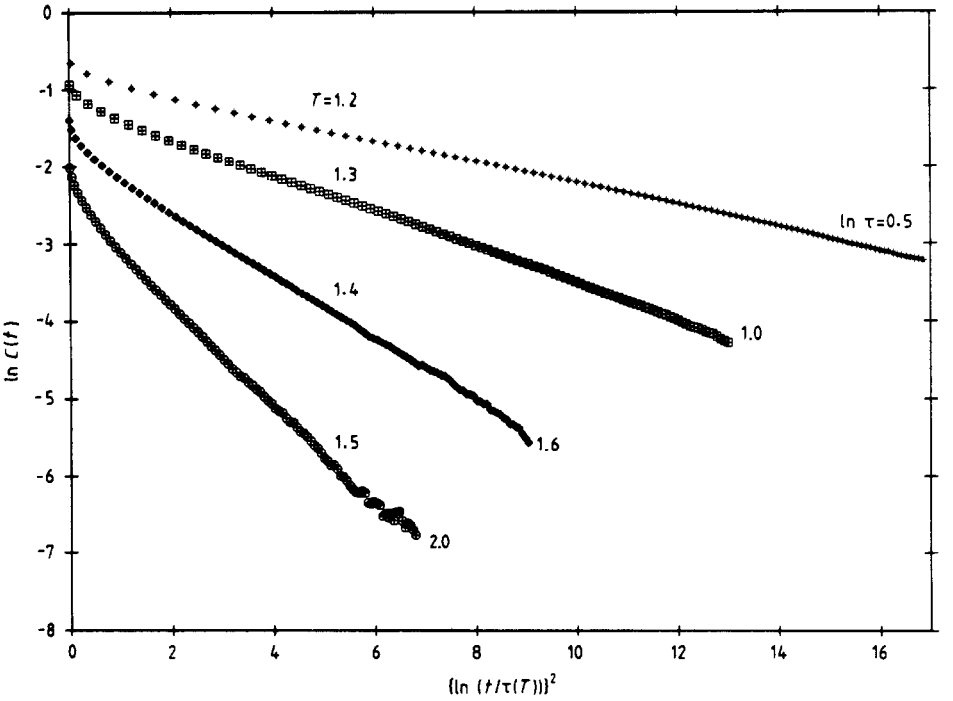


**Figure 9.** ln $C$ against $\{\ln(t/\tau)\}^2$ for the 2D Ising model with $p = 0.5$. The values of ln $\tau$, which was adjusted to 'straighten out' the data, are shown in the figure.

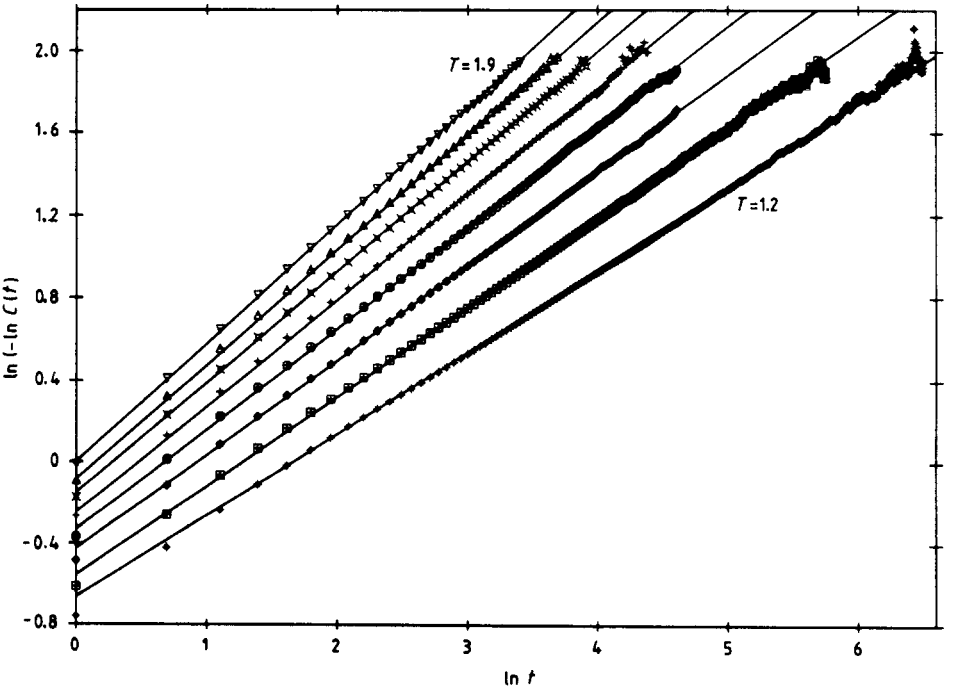


**Figure 10.** ln($-\ln C$) against ln $t$ for the 2D Ising model with $p = 0.5$, for the temperature listed in table 1. Figure 7 gives the values of the stretched exponent $\beta$ extracted from these data.

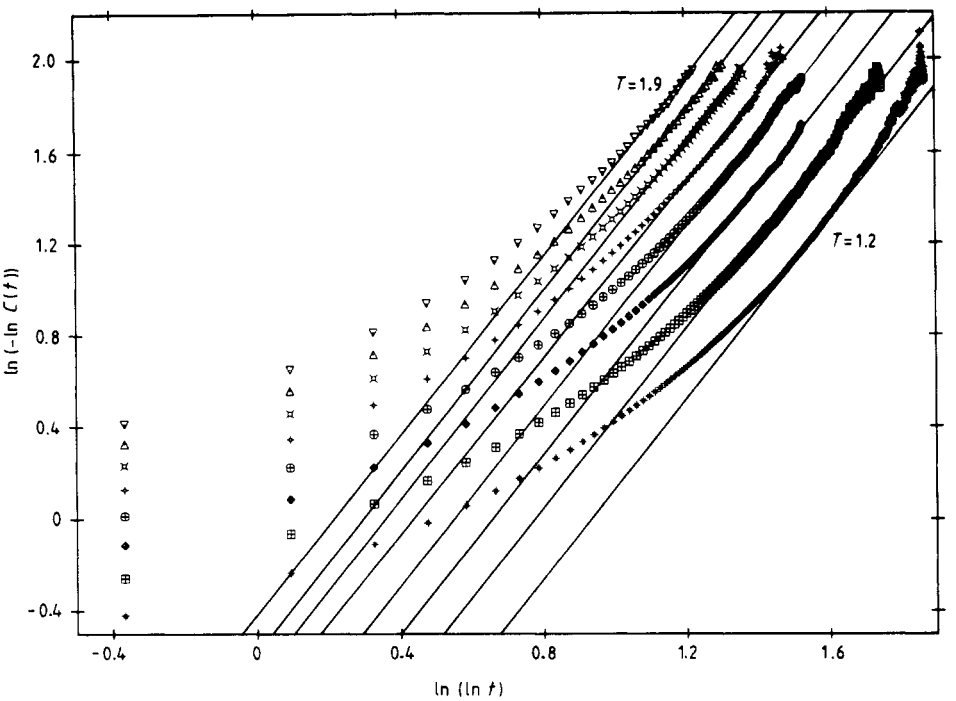


**Figure 11.** $\ln(-\ln C)$ against $\ln\ln t$ for the 2D Ising model with $p = 0.5$, for the temperatures listed in table 1. The straight lines, included as guides to the eye, have slope 2.

for this last process is the same as it would be in the calculation of $C(t)$, i.e. the important clusters are effectively in equilibrium, so the asymptotic decay of $M(t)$ should also be described by (1) and (2).

For the Heisenberg systems, an analysis similar to that used for $C(t)$ yields similar results. Specifically, a plot of $\ln M(t)$ against $\sqrt{t}$ yields reasonably straight lines at longer times. However, the transient 'short-time' region before the linear regime sets in is generally larger in the $M(t)$ data than in the $C(t)$ data, except at the lowest temperatures. Data from the lowest-temperature run at each concentration are shown in figure 12. The linearity of the data indicates consistency with the asymptotic form (2), in agreement with the clustering arguments. A more rigorous test is provided by extracting values of $B(T)$ from the $M(t)$ data. According to the clustering arguments, $B(T)$ for the magnetisation should be the *same* as for the autocorrelation function. The results for $B(T)$ are included in figure 4, and confirm that, for given $p$, and within the uncertainty of the data, the same results are indeed obtained from the $C(t)$ and $M(t)$ data. This is powerful evidence in support of the validity of (2).

For the Ising systems, the $M(t)$ data yield some intriguing results. Plots of $\ln(-\ln M(t))$ against $\ln t$, designed to reveal any stretched exponential behaviour, are presented in figures 13 and 14. The data are reasonably linear, after an initial transient period, consistent with a stretched exponential decay $M(t) \sim \exp\{-(t/\tau)^{\beta}\}$. The values of $\beta$ extracted are, however, at least for $d = 2$, convincingly different from the corresponding values extracted from the $C(t)$ data. This is surprising, as one expects the same microscopic processes to be responsible for the decay of both quantities. Further surprises are in store: the values of $\beta$ presented in figure 7 are, for $d = 2$, *larger* for

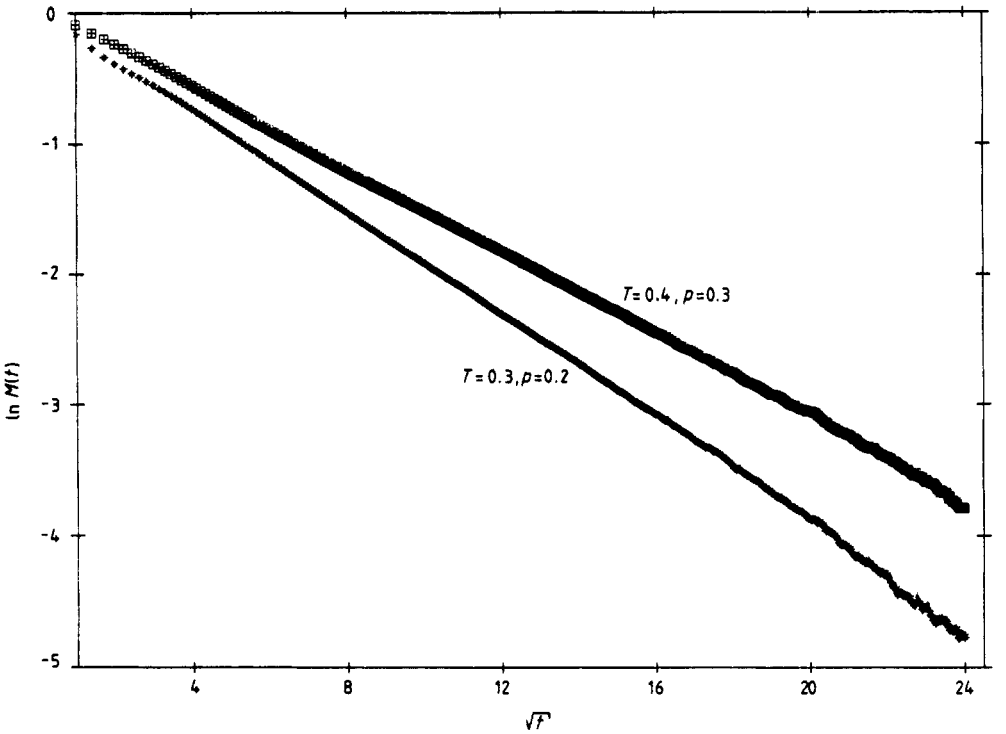


**Figure 12.** $\ln M(t)$ against $t^{1/2}$ for the 3D Heisenberg model, for the temperatures and concentrations indicated. The linearity of the data implies a good fit to (2). The values of $B(T)$ obtained from the slopes are shown in figure 4.

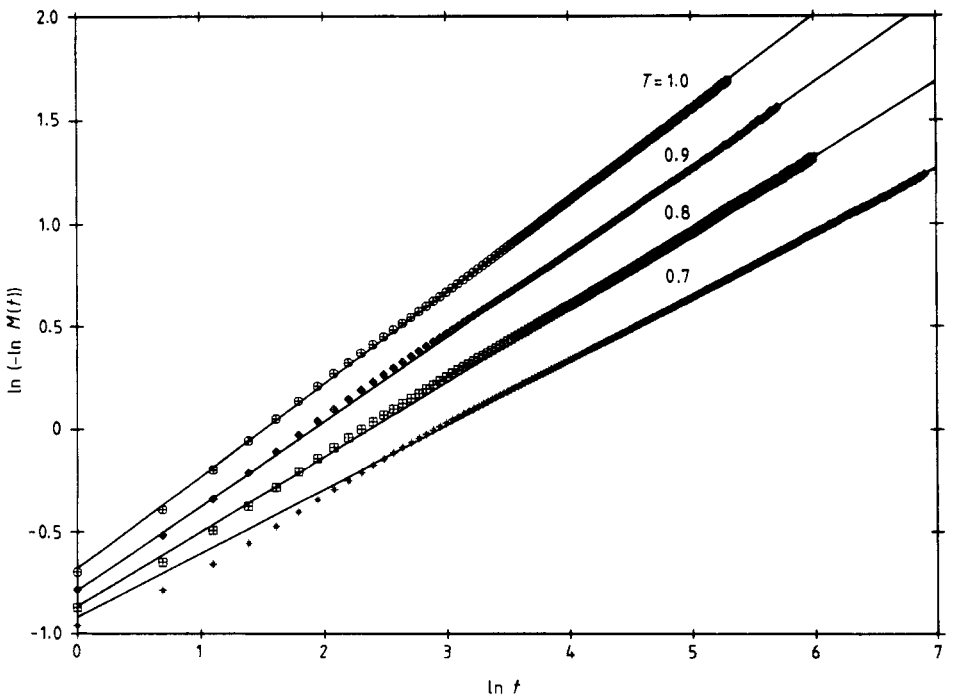


**Figure 13.** $\ln(-\ln M)$ against $\ln t$ for the 3D Ising model with $p = 0.2$. Figure 7 shows the values of $\beta$ extracted from this data.

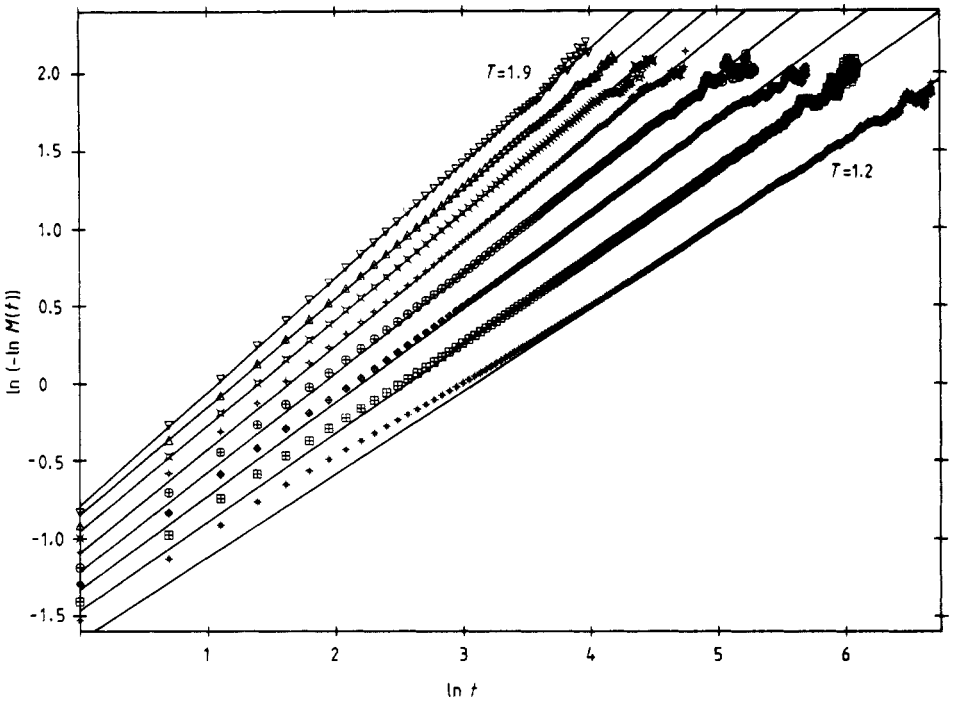


**Figure 14.** $\ln(-\ln M)$ against $\ln t$ for the 2D Ising model with $p = 0.5$, for the temperatures listed in table 1. Figure 7 shows the values of $\beta$ extracted from this data.

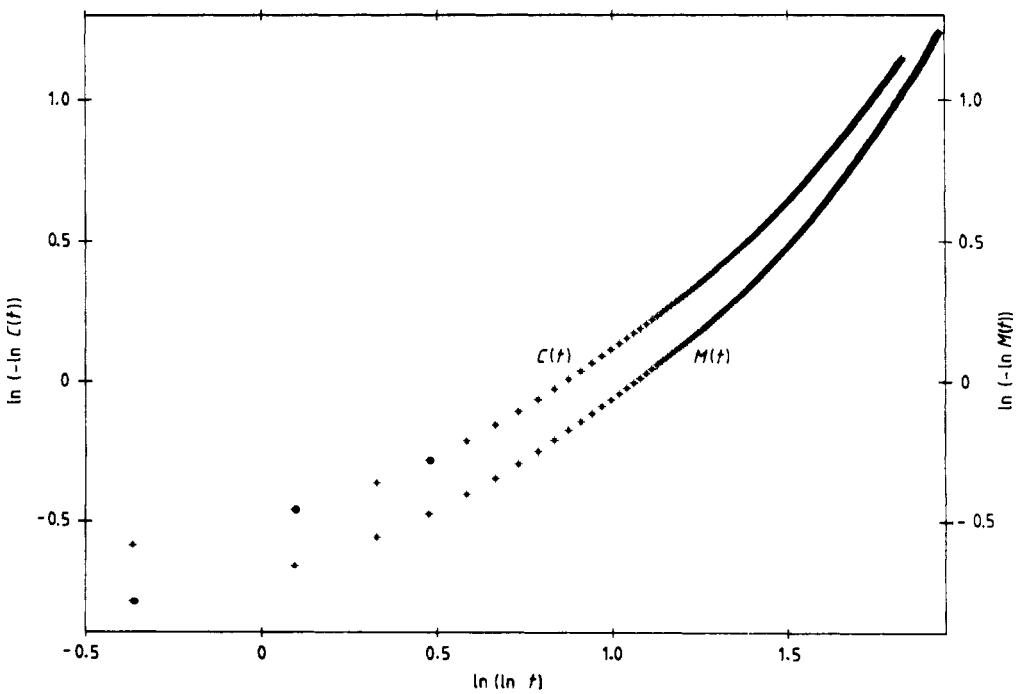


**Figure 15.** $\ln(-\ln M)$ and $\ln(-\ln C)$ against $\ln\ln t$ for the 3D Ising model with $p = 0.2$ at temperature $T = 0.7$.

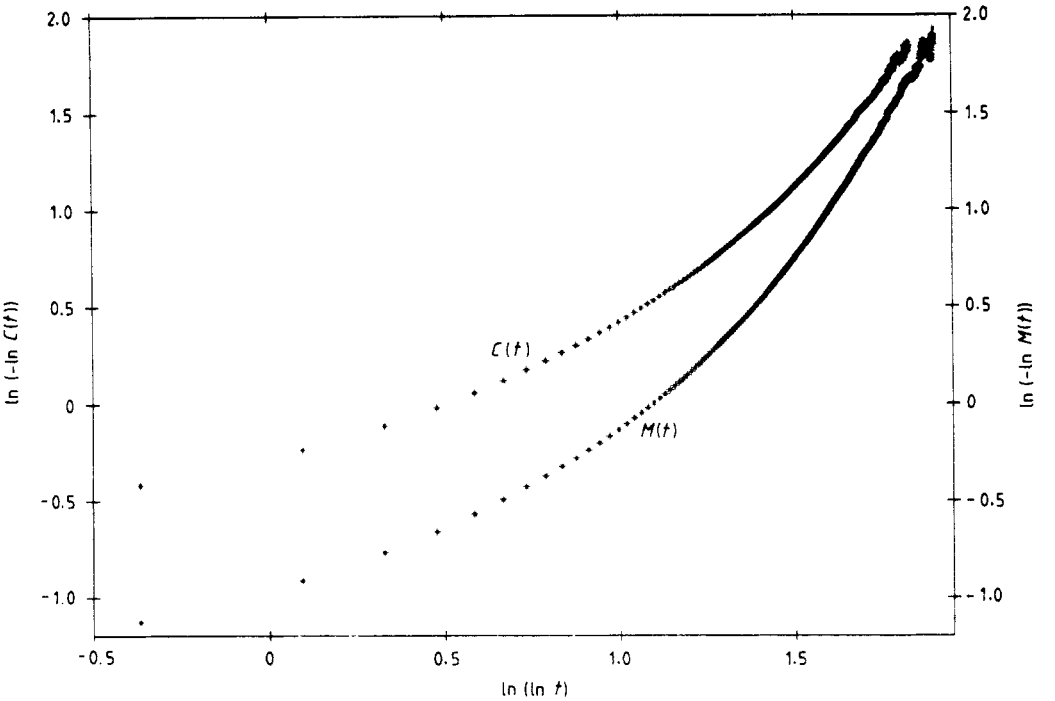


**Figure 16.** $\ln(-\ln M)$ and $\ln(-\ln C)$ against $\ln\ln t$ for the 2D Ising model with $p = 0.5$ at temperature $T = 1.2$.

$M(t)$ than for $C(t)$, implying that, if the stretched exponential decay is to be believed, $M(t)$ is asymptotically *smaller* than $C(t)$. On the other hand, direct comparison of $C(t)$ and $M(t)$ (see figures 15 and 16) shows that $M(t)$ is *larger* than $C(t)$ over the whole range of the simulation. Thus if $M(t)$ is asymptotically smaller than $C(t)$ for $d = 2$, the curves in figure 16 must eventually cross at some time which is beyond the range of the current simulations. For reasons which are discussed in the following section, we do not find this a very plausible scenario. Instead, it seems to us much more likely that the $C(t)$ and $M(t)$ data in both figures 15 and 16 will asymptotically run together, consistent with the form (1).

## 4. Discussion and summary

For Heisenberg ferromagnets in the Griffiths phase, with relaxational (model A) dynamics, the asymptotic form (2) is predicted to hold for the decay of both the equilibrium autocorrelation function $C(t)$ and the non-equilibrium decay, from an aligned start, of the magnetisation $M(t)$. The data are entirely consistent with this prediction: the data for $B(T)$ against $T$ (figure 4) show that $B(T)$ is indeed the same for the $C(t)$ and $M(t)$ data. Perhaps the most surprising feature of the data is that the asymptotic behaviour sets in so *quickly*.

By contrast, a convincing interpretation of the Ising data is much more problematical. Plots designed to reveal the form (1) are far from convincing, and it may well be that the true asymptotic regime is simply beyond the range of the current data.

Another puzzle is the rather good fit to the stretched exponential form, in agreement with Jain's $d = 2$ results [8] and Ogielski's data [9] for the $d = 3$ Ising spin glass, for which the form (1) has also been predicted [2]. There is a serious problem, however, with taking the stretched exponential form seriously as a candidate asymptotic form: it violates asymptotically an exact lower bound [5], which has the form (1). Furthermore, a temperature-dependent stretched exponent seems to us *a priori* unlikely. Finally, for reasons given above, we would expect $C(t)$ and $M(t)$ to have the *same* asymptotic forms. The fact that they are quite well described by stretched exponential forms with different (at least for $d = 2$) values of $\beta$ is therefore surprising.

Even more surprising is the inequality $\beta_M > \beta_C$ extracted from the $d = 2$ data (figure 7). Taken seriously, it implies $M(t) < C(t)$ for sufficiently large $t$. Over the entire range of the data, however, $M(t) > C(t)$. Do $M(t)$ and $C(t)$ cross at some time beyond the range of the current data? We think this unlikely, for the following reason.

Consider a generalised correlation function

$$F(t, t_0) = [\langle S_i(t_0) S_i(t_0 + t) \rangle]$$

computed with the initial condition $S_i(0) = 1$ for all $i$. Then $C(t)$ and $M(t)$ are limiting cases of $F$: $C(t) = F(t, \infty)$, $M(t) = F(t, 0)$. It seems extremely plausible that, for fixed $t$, $F(t, t_0)$ is a smooth, monotonic function of $t_0$. If we accept this hypothesis, it follows that if there exists a time $t^*$ such that $C(t^*) = M(t^*)$, then $F(t^*, t_0)$ is independent of $t_0$, an extremely unlikely result in our view. It seems to us much more likely that $M(t) > C(t)$ for all $t$. Then the pairs of curves in figures 15 and 16 would asymptotically run together for $t \to \infty$. The fact that they have not yet done so is further evidence that the true asymptotic regime has not yet been reached.

In conclusion, the simulation data rapidly approach, for Heisenberg systems, the asymptotic form (2). For Ising systems, it seems that we are not yet in the asymptotic regime. The reason for this may be the existence of additional long timescales in the Ising systems. In particular, it is known [12] that even in the *pure* Ising ferromagnet, relaxation is non-exponential below $T_c$ due to the slow relaxation of large thermally activated droplets of the 'wrong phase'. It may be that, to obtain a reasonable description of the Griffiths phase dynamics, one has to include the effects of such thermal droplets occurring within the quasi-ordered regions generated by statistical fluctuations.

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