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LETTER TO THE EDITOR

The role of droplet fluctuations in kinetic Ising models

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Abstract. We examine, by Monte Carlo simulation and the damage algorithm, the late time behaviour of fluctuations in the low-temperature ordered phase of the two-dimensional kinetic Ising model. It has been suggested that at late times correlations could be dominated by long-lived droplet fluctuations of the other ordered phase, giving rise to stretched-exponential decays of the spin autocorrelation function. Over the time regimes we have studied, we see no evidence for anomalous long-lived droplets and find that the probability distribution for droplet lifetimes decays by an ordinary exponential.

Assumptions about the nature of long-time correlations in systems close to equilibrium provide the basis for important aspects of non-equilibrium statistical mechanics. For example, linear-response theory requires the existence of a perturbative regime sufficiently close to equilibrium. In particular, let us consider the non-conserved kinetic Ising model (called [1,2] model A) in one of its two equivalent ordered states below the critical temperature T_c, where the average spin $\langle S \rangle \approx \pm 1$. If one considers only the system's linear response, equivalent in this case to the Langevin equation linearized about the equilibrium state, the autocorrelation function $C(t) = \langle S(0)S(t) \rangle - \langle S \rangle^2$ obeys

$$C(t) \sim \mathrm{e}^{-t/\tau} \tag{1}$$

for late times, when the system is prepared in equilibrium at $t = 0$, where τ is the correlation time. Recently, however, independent phenomenological studies by Huse and Fisher [3], and Takano *et al* [4] have suggested that late time behaviour can be dominated by stretched exponentials of the form

$$C(t) \sim \mathrm{e}^{-(t/\tau)^{\phi}} \tag{2}$$

where $\phi < 1$, which is inconsistent with the above prediction of linear response.

In this letter we present a numerical investigation of these predictions. We use Monte Carlo simulation and damage dynamics [5–10] to study the close-to-equilibrium fluctuations in the two-dimensional spin-flip kinetic Ising model. Over the time regimes we have studied, we find behaviour consistent with ordinary exponential decay.

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To obtain the time correlation function, one can naively argue as follows. Spatial correlations fall off as $C(r) \sim e^{-r/\xi}$ with position $r \to \infty$, where ξ is the correlation length. It is straightforward to establish this by, for example, Ornstein–Zernicke theory. If correlations build up at a constant rate (ballistically) on small length scales, i.e. $r \propto t$, then one has $C(t) \sim e^{-t/\tau}$. This growth law for $r \leqslant \xi$ is natural to expect when growth is limited by causality ($r \propto t$ is as fast as clusters can grow) and not by thermodynamics, which might affect $r \gg \xi$.

However, this argument does not explicitly consider the possible effect of large droplets. Huse and Fisher have argued that the correlation function $C(t)$ is an analytic function of the probability $p(t)$ of a droplet living to time t, namely $C(t) \sim p(t) + O(p^2)$. If cluster fluctuations within the ordered phase $\langle S \rangle \approx +1$ are well-defined droplets of the other ordered phase $\langle S \rangle \approx -1$, only the droplet's surface energy contributes to suppressing such a fluctuation. Since that surface energy is proportional to the surface area, $p \sim e^{-r^{d-1}}$, in d dimensions. Furthermore, from studies of the kinetics of first-order phase transitions [2], large droplets of size r are known to decay via $r \sim t^n$, where n is $1/2$ for processes involving no conserved modes, or $1/3$ for processes controlled by a conserved variable (which need not be the order parameter). The argument then implies $C(t) \sim e^{-(t/\tau)^\phi}$ as $t \to \infty$, where the exponent for stretched-exponential decay is $\phi = (d-1)n$. When $\phi > 1$ the decay will be exponential, since the large droplets will be irrelevant. Independently, Takano *et al* have given a similar argument, with the additional assumption that the large droplets satisfy a self-similar scaling form as they do in first-order transitions. This derivation yields [12] $1/\phi = 1 + 1/[(d-1)n]$. These treatments [13] yield strong predictions for the two-dimensional kinetic Ising model: for example, the Huse–Fisher scenario with $n = 1/2$ implies $C(t) \sim e^{-t^{1/2}}$; experimental representations include chemisorbed systems undergoing order–disorder transitions. If a non-conserved order parameter's dynamics is controlled by a coupled conserved field (called [1,2] model C, with an asymmetric coupling to the order parameter) so that $n = 1/3$, the Huse–Fisher picture implies $C(t) \sim e^{-t^{2/3}}$ in three dimensions; experimental systems include binary alloys prepared off stoichiometry undergoing order–disorder transitions.

Nevertheless, the analysis leading to either value of the growth exponent n requires a full nonlinear treatment of the Langevin equation describing the dynamics of the system [2]. Thus the droplet arguments are not consistent with linear response theory [17]: for example, on linearizing the nonlinear Langevin equation for model A [1,2] around the ordered state one obtains $C(t) \sim e^{-t/\tau} + O(e^{-t/\tau})^2$. So there is no obvious source for the breakdown of linear response. It is also worth noting that previous analytic work by Binder, Stauffer and Müller-Krumbhaar [14] on cluster dynamics found exponential decay below T_c.

It is natural to test the predictions of the phenomenological droplet theories by computer simulation. This was first attempted by Takano *et al* [4] and Ogielski [15] who used standard Monte Carlo methods to evaluate the spin correlation function $C(t)$ and the correlation function of the Fourier-transformed spin variables. In two dimensions, Takano *et al* reported $\phi = 1/3$, while Ogielski found inconclusive results, and noted that long transients played an important role in the time regime investigated: both groups were limited to times $t \leqslant 50$–100 Monte Carlo steps (MCS). More recently Stauffer [16] used standard Monte Carlo to directly examine the growth and decay of equilibrium droplets and found evidence supporting a stretched-exponential decay. However the results were also restricted to short droplet lifetimes

($t \leqslant 40$ MCS), owing to the difficulty of locating and analysing individual droplets.

We use damage dynamics [5–10] to evaluate the late time behaviour of close-to-equilibrium fluctuations in the two-dimensional spin-flip kinetic Ising model [18]. This method, which involves the explicit introduction and monitoring of microscopic fluctuations in replica lattices, has recently been used to study equilibrium response and spatial correlation functions [8,9], as well as time-dependent correlations functions and dynamic critical exponents [10] in a variety of systems. The advantage of the technique comes from its ability to track the evolution of the induced microscopic fluctuation independent of those thermal fluctuations common to the two replica lattices. In our case this allows us to look at the behaviour of fluctuations out to significantly later times, $t \leqslant 500$–1000 MCS, than in previous studies.

Starting with two Ising lattices with identical spin configurations we introduce a microscopic fluctuation by taking one of these lattices and flipping a single, randomly chosen spin. We then evolve the two systems, including the damaged site, according to the same Metropolis Monte Carlo dynamics, by using the same sequence of random numbers for both lattices. The damage $M(t)$, which measures the magnitude of this fluctuation (the cluster size) as a function of Monte Carlo time, t, can be defined by $M(t) = \sum_i |S_i(t) - S_i^d(t)|$, where $S_i(t)$ is the spin at site i in the undamaged lattice, $S_i^d(t)$ is the state of the corresponding site in the damaged lattice, and where for convenience we take the spin states to be 1 or 0. For temperatures $T < T_c$, damage can on the average only occur over length scales given by the correlation length: damage grows to a length of order ξ and then decreases and disappears in a time proportional to τ.

We use the algorithm to estimate two quantities. The first quantity is $N(t)$, the ensemble-averaged number of clusters which live until time t. This measures the probability that a system damaged at time $t = 0$ will lose memory of this at time t, so the integral $\int_t^\infty N(t)\,dt$ is just the probability that a droplet still exists at time t. As noted by Huse and Fisher [3] the correlation function $C(t)$ is proportional, to lowest order, to this probability. Thus if $C(t)$ takes on a non-exponential form at late times $N(t)$ should also do so [11]. We also measure the ensemble-averaged size $M(t', t)$ of those clusters which vanish at some fixed time t, as a function of time t'. Damage can only become large if the initial damage causes a large anti-domain fluctuation in one system, but not the other. Therefore monitoring the dynamics of damage cluster evolution for long-lived events is equivalent to monitoring the dynamics of droplet growth and decay. This allows us to check whether large, long-lived droplets behave differently from small, short-lived ones.

We used a multi-spin coding metropolis algorithm, and studied temperatures relatively close to the critical temperature T_c, $0.9\,T_c$ and $0.95\,T_c$, to minimize non-universal differences between the Langevin model A and the kinetic Ising model. The correlation lengths at these two temperatures are $\xi \approx 3$ and 5, respectively, in units of the lattice spacing. Since we damage only a single site the perturbation is small on the scale of the correlation length, ensuring that the induced fluctuation is microscopic and essentially thermal. Systems examined were square lattices of sizes 32^2 and 64^2. We ensured there were no appreciable finite-size effects by undertaking test runs on a larger system, and also by observing that a negligible fraction of damage spread through the entire system during the course of the simulations. Approximately 10^7 trials were performed at each temperature. As can be seen from figure 1, we have observed rather large cluster fluctuations. This is a cluster roughly three correlation lengths in diameter. The largest clusters which appreciably contribute to our results

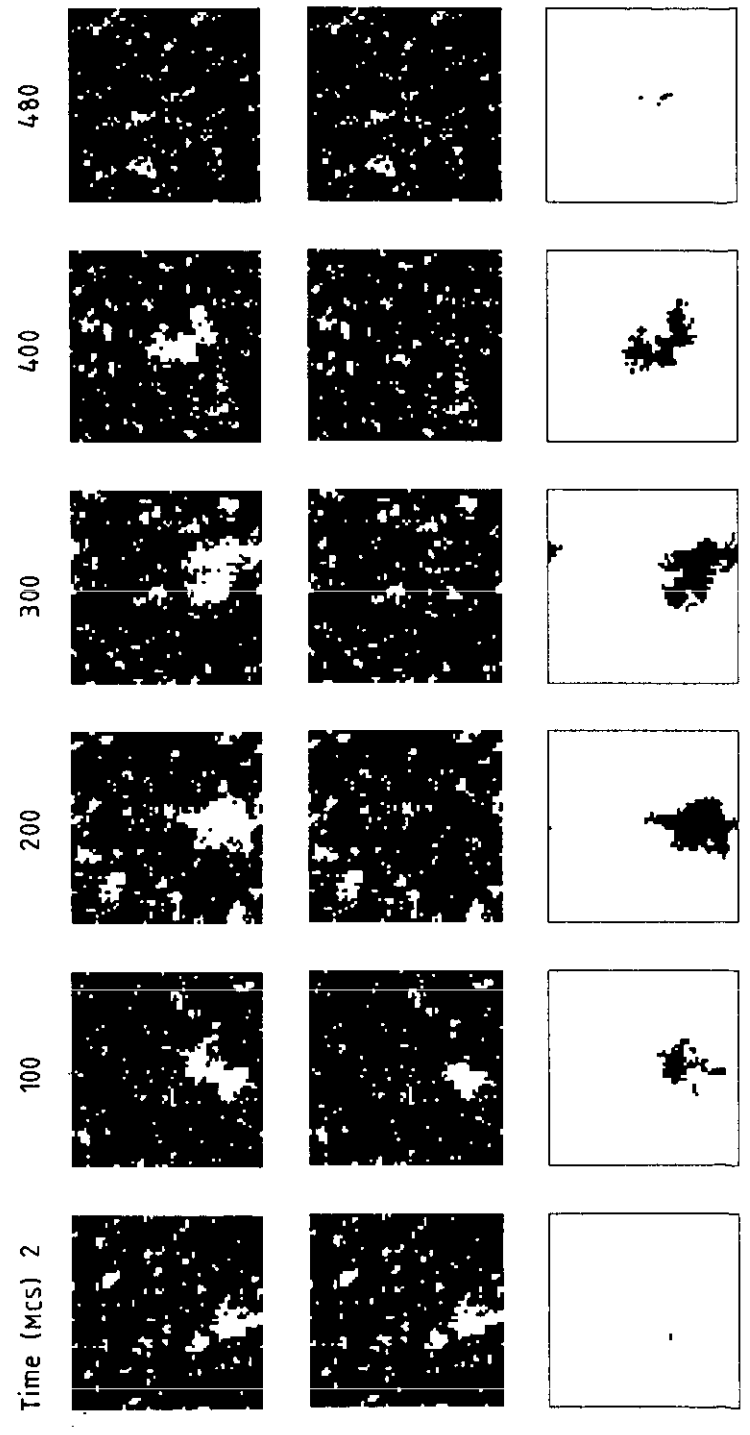

Figure 1. Snapshots in time, for a system of size $L = 64$, of the undamaged (A) and damaged (B) lattices, as well as a map (C) of the damaged sites, for the case of a large improbable cluster fluctuation at $0.95\,T_c$ which lasted 500 MCS. Times shown are 2, 100, 200, 300, 400, and 480 MCS, from left to right. Note the cluster does not have a well-defined surface.

are of diameter 3–7 correlation lengths. Nevertheless, these very large droplets we observe are fuzzy and are not well-formed compact droplets.

Figure 2 shows a log–log plot of the distribution $N(t)$ as a function of time t. Results are shown for $T = 0.95\,T_c$; similar results were observed at the lower temperature. The distributions have been normalized so that $N(1) = 50$. For early times there is a clear $1/t^2$ dependence. This can be understood as follows. Consider a system of size L^d. The probability of a fluctuation of size ℓ will be $\sim (L/\ell)^d \mathrm{e}^{-kt^{d-1}}$, where the first term is proportional to the available volume in phase space (i.e. the number of ways of making clusters of size ℓ) while the second term arises from the free energy of the fluctuation, and will be negligible at early times. If we assume that the early-time size is proportional to the lifetime, $\ell \sim t$, we get the limiting form $N(t) \propto 1/t^d$. We can therefore usefully present the data by estimating the form of $t^2N(t)$.

In figure 3 we plot $t^2N(t)$ as a function of time. This semi-log plot yields good straight-line fits to the late time data, implying ordinary exponential decay at late times rather than a stretched exponential. From this, and other more complicated fits, we conclude that simple exponential decay provides the best representation of the data over the time regimes we have studied.

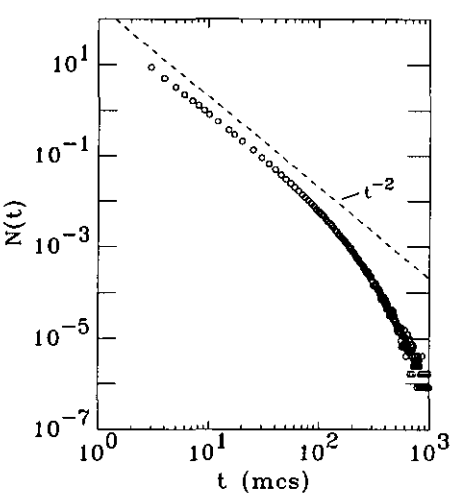

Figure 2. Log–log plot of the cluster lifetime distribution $N(t)$ as a function of time t for $T = 0.95\,T_c$. The early-time $1/t^2$ dependence is clearly evident.

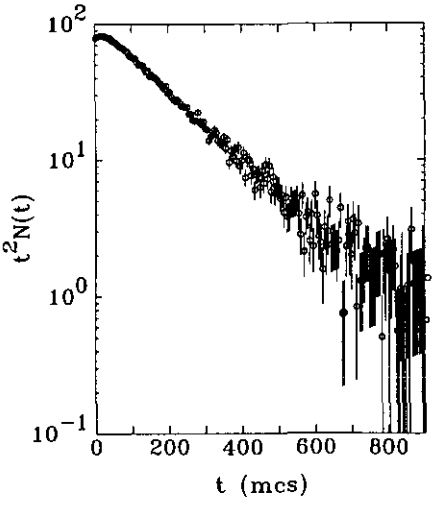

Figure 3. Log–linear plot of the quantity $t^2N(t)$ as a function of t, showing the late time exponential decay.

In figure 4 we plot the average evolution in time t' of the size $M(t, t')$ of clusters which grow, decay and then disappear at times $t = 61$–500. According to the droplet models the time evolution of long-lived large droplets should be quite different from that of short-lived smaller ones. However, it is straightforward to see that there is no qualitative difference between the clusters on the time scales $t = 61$–500: indeed the similarity in the shapes of the $M(t, t')$ versus t' suggests one should scale the data via the ansatz $m^*(t^*) = M(t', t)/M_{\max}(t)$, where $t^* = t'/t$ and $M_{\max}(t)$ is

the maximum value of M for a given lifetime t [19]. The transformed data collapse onto a single universal curve, as shown in figure 4, demonstrating that large and small clusters behave in the same fashion, over the time scales we have investigated.

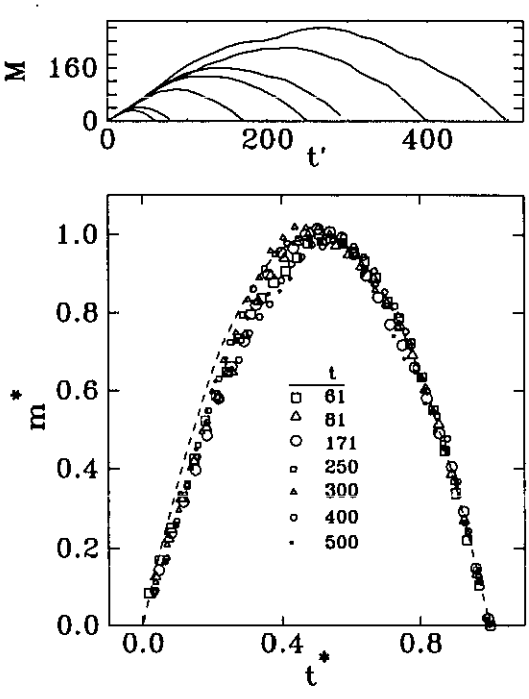

Figure 4. The top shows the average size $M(t', t)$ for clusters which disapear at times $t = 61$, 81, 171, 250, 300, 400 and 500, from left to right. The bottom shows that scaled size m^* versus scaled time t^* is independent of time t. The scaled size is $m^* = M(t', t)/M_{\max}(t)$, while $t^* = t'/t$, where $M_{\max}(t)$ is the maximum M for a given t. The dashed parabola is the shape for a ballistic growth law, as discussed in the text.

The form of $m^*(t^*)$ is also indicative of the processes taking place. First note that the data are approximately symmetric about the maximum, as required by detailed balance. Furthermore, the shape of the scaling function determines the way clusters grow and decay. Since the scaled size of the two-dimensional clusters is $m^* \sim \ell^2$ ballistic growth and decay, with $\ell \sim t'$, implies that the scaling function $m^*(t^*) \sim t^{*2}$, i.e. the unique parabola shown by the dashed line in figure 4. The data are entirely consistent with ballistic growth, which again implies exponential decay over the time regimes we have investigated.

Finally, despite this numerical evidence, one must ask if the phenomenological droplet arguments are so compelling as to suggest that our work is only observing transients. Note that those theories assume fluctuations are well-defined droplets. In nucleation theory, where droplets in local equilibrium play an important role, the critical droplet is characterized by two length scales: the width of the interface, which is proportional to ξ, and the droplet radius, which is proportional to the reciprocal of the applied field. However, in phenomenological droplet theories only one length scale is assuredly present, the correlation length. It is therefore not apparent that

there will be a well-defined separation of length scales between the droplet's surface width and its radius, if both are proportional to ξ. Again note the fuzzy features of the typical large cluster in figure 1.

In conclusion, we find that our data are consistent with ordinary exponential decay. We cannot rule out the possibility of other behaviour on longer time scales than we have studied. Nevertheless, the consistency of our results for the cluster decay, the scaling of the size $M(t', t)$ of clusters, and the absence of an obvious length scale to set a fluctuating droplet size, lead us to believe that our results are indicative of the asymptotic time regime. Finally, as mentioned elsewhere, we believe a good candidate for an extensive experimental test, capable of probing time scales much larger than in a numerical study, would be a binary alloy such as β-CuZn prepared off stoichiometry.

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[11] Huse and Fisher [3] give a droplet argument for $C \sim p(1-p)$, where $p(t)$ is the probability that a droplet lasts until time t. In our case this implies $C(t) \sim \int_t^\infty N(t)\,dt$ at late times, when $C(t)$ is dominated by the lowest order term. We have checked this by comparing $C(t)$, evaluated by standard Monte Carlo methods, with the integral of $N(t)$. The two functions are nearly identical over the latest time regimes acessible to both simulation methods ($t \leqslant 160$ MCS).
[12] While the generalization of the Huse and Fisher argument to $n \neq 1/2$ is trivial, that to the work of Takano *et al* requires an assumption concerning the weighting of the droplet distribution in the spirit of the original work. This point is also discussed in [13].
[13] Tang C, Nakanishi H and Langer J S 1989 *Phys. Rev.* A **40** 995 have investigated some of the assumptions of the phenomenological approach, through a more rigorous theory. They introduce a model dynamical system wherein all fluctuations are assumed to be well-defined droplets. From this, they recover analytically the results of Huse and Fisher, but not those of Takano *et al* implying the former theory incorporates droplet fluctuations self-consistently. However, the larger issue of the behaviour of, say, model A cannot be tested through the approach of Tang *et al*.
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[17] Such a breakdown of transport theory has a precedent in two-dimensional hydrodynamics, where transport coefficients are renormalized by relevant logarithms in the long-time limit. This was found in the classic numerical study of Alder, Wainwright and co-workers, and is now understood

by both rigorous and phenomenological theory. A review is given by Pomeau Y and Résibois P 1975 *Phys. Rep.* **19** 63

[18] Further results, as well as a study of the kinetics of domain growth by this method, will be presented in a future paper by Graham I S, Roland C, and Grant M.

[19] We find $M_{max} \approx t$. This is consistent with slowing down near T_c, since we expect $M_{max} \sim t^{2/z}$, where z is the dynamical critical exponent defined through $\xi^z \sim t$ as $T \to T_c$. Many methods find $z \approx 2$, including earlier studies at $0.95T_c$, although the dynamical critical region is thought to be rather narrow in temperature, so we are presumably only seeing an effective z.