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Dynamics of fluctuations in the ordered phase of kinetic Ising models

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Correlation functions $q(t)=\langle S_x(0)S_x(t)\rangle-\langle S_x\rangle^2$ and their momentum space expansions are studied in computer simulations of d-dimensional Glauber models below T_c ($d=2$, 3, and 4). For $d\geq 3$ the functions $\langle\tilde{S}_k(0)\tilde{S}_{-k}(t)\rangle_c$ decay exponentially and the relaxation-time spectrum is bounded, implying the asymptotically exponential $q(t)$, but that asymptotic form is far beyond any observable regime. For $d=2$, $\langle\tilde{S}_k(0)\tilde{S}_{-k}(t)\rangle_c$ decays nonexponentially for all $\mathbf{k}$ indicating a nonexponential asymptotic form of $q(t)$. In all cases the observable preasymptotic form of $q(t)$ can be approximated by Kohlrausch decay $\exp[-(\lambda t)^\beta]$, $0<\beta<1$.

Recent phenomenological theories searching to explain the nonexponential relaxation in complex disordered systems such as glasses, random magnetic materials, etc., concentrated on the approximate identification of simple dynamic modes with physically appealing substructures (such as clusters or droplet excitations) together with scaling *Ansätze* relating the appropriately defined "size" and distribution of substructures to their characteristic times, either in a straightforward fashion in position space[1,2] or more abstractly in terms of hierarchies of metastable states.[3]

Quite surprisingly, in two recent reports[2,4] it was proposed that droplet fluctuations could also lead to nonexponential asymptotic decay of Kohlrausch (stretched exponential) form even in ordinary (nonrandom) ferromagnetic Ising models in the ordered phase. The possibility of Kohlrausch decay in simple realistic models without disorder or activated dynamics is intriguing enough to warrant a thorough investigation which could give new insights into relaxation of truly glassy materials.

The subject of this Rapid Communication is the analysis of numerical solutions for the fundamental dynamic correlation functions in kinetic Ising models in zero field with stochastic dynamics of the Glauber type[5] below the critical temperature T_c in two, three, and four spatial dimensions. I obtain and study the autocorrelation function

$$q(t)=\langle S_x(0)S_x(t)\rangle-\langle S_x\rangle^2 \tag{1}$$

and correlations of the Fourier-transformed spin variables $\tilde{S}_k=\sum_x e^{ikx}S_x$,

$$G(\mathbf{k},t)=\frac{1}{V}[\langle\tilde{S}_{\mathbf{k}}(0)\tilde{S}_{-\mathbf{k}}(t)\rangle-|\langle\tilde{S}_{\mathbf{k}}\rangle|^2] \ . \tag{2}$$

The objective is to examine the validity and usefulness of the simple dynamic droplet models, and to establish the range of asymptotic behavior: While phenomenological scaling models lead to definite predictions for the asymptotic decay of $q(t)$, they are unable to produce estimates of the magnitude of correlation functions at the onset of asymptotic behavior.

The main results are as follows.

(1) In dimension three and higher ($d\geq 3$) the analysis of the expansion

$$q(t)=\frac{1}{V}\sum_k G(\mathbf{k},t)\rightarrow\frac{1}{(2\pi)^d}\int d\mathbf{k}\,G(\mathbf{k},t) \tag{3}$$

(the last expression corresponds to the thermodynamic limit $V\rightarrow\infty$) demonstrates that (i) $G(\mathbf{k},t)$ decays exponentially with minor corrections at short times

$$G(\mathbf{k},t)\approx G(\mathbf{k},t=0)e^{-\lambda(\mathbf{k})t} \ ; \tag{4}$$

(ii) at small momenta (relevant for long-time behavior) the rate is

$$\lambda(\mathbf{k})=\lambda_0+c\mathbf{k}^2+o(k^4) \ . \tag{5}$$

(iii) The existence of the gap $\lambda_0>0$ at $T<T_c$ implies that the autocorrelation function $q(t)$ must asymptotically approach the exponential decay

$$q(t)\rightarrow Ae^{-\lambda_0 t} \text{ as } t\rightarrow\infty \ . \tag{6}$$

This is the expected decay law, in agreement with the droplet model of Fisher and Huse[2] who use the Langevin equation for dynamical evolution of large droplets. (iv) A striking new result is that the asymptotic formula (6) is really *irrelevant* for the analysis of any conceivable experimental or numerical data for $q(t)$: The magnitude of $q(t)$ at the onset of the asymptotic behavior is extremely small, for instance, in $d=3$ below T_c when the correlation length ξ is about four lattice spacings the asymptotic form (6) will not be seen until the time when $q(t)\approx 10^{-200}$. In contrast, the functional form of the preasymptotic $q(t)$ is well approximated by the stretched exponential

$$q(t)\approx e^{-(t/\tau)^{\beta(T)}}, \ t<t_{\text{crossover}} \tag{7}$$

with weakly temperature-dependent exponent β in the range 0.3–0.5. It should be strongly stressed that (7) does *not* represent the analytic approximation which can be obtained from Eq. (10) below, but merely a convenient and acceptably accurate fit to the data.

(2) Dynamics in dimension $d=2$ is very different from that described above for $d\geq 3$. (i) In marked contrast to $d\geq 3$, here the momentum modes $\tilde{S}_k$ are not simply relat-

ed to exponentially relaxing eigenmodes of the evolution operator, that is the functions $G(\mathbf{k},t)$ display a nonexponential decay and cannot be approximated by (4) in the observable range $[G(\mathbf{k},t)>10^{-4}]$ even if one allows for power-law corrections at shorter times. (ii) The observable decay of $q(t)$ is very nonexponential. Again, it can be reasonably well approximated by a stretched exponential function (7), this time with a smaller exponent $\beta(T)$, $\beta(T)\approx 0.3$, for temperatures corresponding to the correlation length ξ between a few to a few tens of lattice spacings, although deviations from this phenomenological form indicate a slightly faster asymptotic decay. Similar behavior was observed in numerical simulations reported in Ref. 4.

The above-mentioned analysis of droplet fluctuation by Fisher and Huse[2] predicts the asymptotic behavior with $\beta=\frac{1}{2}$, which is not observed in computer simulations. By the same reasoning as in (iv) above it *might* be indeed the correct asymptotic behavior, but it cannot be seen nor verified with experimental or computer-generated data in any reasonable range of $q(t)$.

The analysis of the representation (3) of $q(t)$ by Takano, Nakanishi, and Miyashita,[4] suggests the *asymptotic* stretched exponential decay in every dimension d with $\beta=(d-1)/(d+1)$. Their analysis essentially depends on the assumption that in every dimension one can approximate (3) by $\int d\mathbf{k}\exp(-ck^{-(d-1)}-\mathbf{k}^2t)$, which is not consistent with our results nor with the known momentum dependence of correlation functions.

Ising models discussed in this Rapid Communication are defined by the standard nearest-neighbor Hamiltonian

$$H=-\sum_{xy}S_xS_y\ , \qquad (8)$$

with spin variables $S_x=\pm 1$ populating the sites of the square ($d=2$), simple cubic ($d=3$), or hypercubic ($d\geq 4$) lattice. The dynamics is introduced in terms of a Markovian stochastic process on the space of spin configurations $\sigma=\{S_x\}$

$$\frac{\partial}{\partial t}P(\sigma,t)=\sum_{\sigma'}\Gamma(\sigma|\sigma')P(\sigma',t)\ , \qquad (9)$$

where $P(\sigma,t)$ is the probability of spin configuration σ at time t.

I consider the rate matrix Γ of the type introduced by Glauber,[5] where $\Gamma(\sigma|\sigma')=0$ unless configurations σ and σ' differ by at most one spin. In the latter case the transition rates are chosen to satisfy the detailed balance condition. With these definitions the stochastic process is Markovian, ergodic, and converges to the Boltzmann distribution in the stationary state.

The correlation functions (1) and (2) were obtained in large-scale, discrete-time Monte Carlo simulations performed on a special purpose computer.[6] Discrete time does not present any conceptual difficulties since we may consider it as an embedded Markov process with the same time dependence as (9) at integral values of time. Single-spin transitions were chosen according to the "heat-bath" algorithm.[6] Simulations were performed on lattices of size 512^2, 64^3, and 16^4 with periodic boundary conditions. Spin variables were selected for updates according to a preassigned sequence, with consecutive sites x separated by at least several lattice spacings, not along any lattice axis. The updating sequence could be varied, and as in related study of spin-glass dynamics[7] it did not seem to affect the shape of correlation functions. The statistical errors in estimates of correlation functions were reduced below one part in a thousand by averaging over 10^5 or more processes with distinct initial states drawn from the stationary Boltzmann distribution. At each temperature where $q(t)$ was recorded the correlation length was also estimated and found to be significantly smaller than the lattice size, thus guaranteeing no bias due to finite-size effects. Large lattice size excluded the transitions between oppositely magnetized ordered states, allowing for unbiased estimates of $\langle S_x\rangle$. In $d=2$ these were found in agreement with the Onsager's solution, viz., $\langle S_x\rangle=[1-\sinh^{-4}(2\beta)]^{1/8}$.

Figure 1 shows the numerical solutions for $q(t)$ at selected temperatures below T_c in two, three, and four dimensions. The usual coordinates in these plots, $\log_{10}q(t)$ vs t^β, and the values of β were chosen with the purpose of enhancing their similarity to the stretched exponential function (7). The time unit (MCS) denotes the number of Monte Carlo updates per spin.

Naively, it looks as if the recorded $q(t)$ decay asymptotically as stretched exponential function. Let us test the validity of this statement by employing the Fourier expansion (3), and by analyzing the time dependence of numerical solutions for $G(\mathbf{k},t)$ for a range of momenta $\mathbf{k}$.

A typical behavior observed in three dimensions is shown in Fig. 2. The method of plotting, log-log plot of $-t/\ln f(t)$ vs t, gives equal space to each decade of time, and enlarges the errors and deviations of $f(t)$ from purely exponential decay at long times. It is clearly seen that for all momenta the decay is almost purely exponential, and

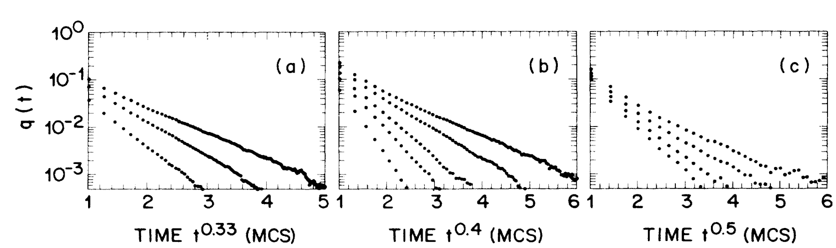

FIG. 1. Numerical solutions for the autocorrelation function $q(t)$. (a) $d=2$, at temperatures $T=2.15$ (top), 2.10, and 2.00 (bottom). (b) $d=3$, $T=4.45$ (top), 4.40, 4.30, 4.20, and 4.00 (bottom). (c) $d=4$, $T=6.60$ (top), 6.50, 6.40, and 6.30 (bottom). The critical temperatures are $T_c=2.27$, 4.51, and 6.7 for $d=2$, 3, and 4, respectively.

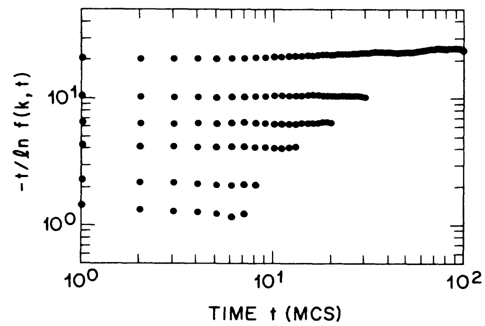

FIG. 2. Normalized correlation function $f(k,t)=G(\mathbf{k},t)/G(\mathbf{k},0)$ for several momenta $\mathbf{k}=(2\pi/L)(0,0,q)$ at $T=4.40$, $L=64$ in three dimensions. The log-log plot displays $-t/\ln f(k,t)$ vs time t for the wave number $q=0$ (top), 4, 6, 8, 12, and 16 (bottom).

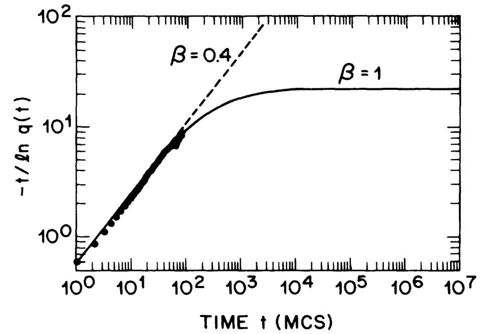

FIG. 4. Plot of $-t/\ln q(t)$ vs t at $T=4.40$ in three dimensions. Continuous curve represents the values of the integral representation of Eq. (10). Note the crossover to asymptotic exponential decay at $t\approx 10^4$. The dashed line extrapolating the short-time behavior (where data points are displayed) corresponds to a stretched exponential with $\beta=0.4$.

can be written in form (4), with the decay rate $\lambda(k)$ given by (5) (cf. Fig. 3). The existence of the gap λ_0 in the spectrum of relaxation rates as $\mathbf{k}\to 0$ is crucial: From the expansion (3) we see that $q(t)$ *must* asymptotically decay as $\exp(-\lambda_0 t)$.

In order to reconcile these statements with behavior shown in Fig. 1(b), I use the integral representation (3) for $q(t)$, and the numerically established formula (4) and the Lorentzian approximation to $G(\mathbf{k},t=0)$, which indeed is valid for numerical solutions at small momenta.

In this way I obtain the representation

$$q(t)\approx\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{B}{k^2+\kappa^2}\exp[-(\lambda_0+ck^2)t] . \quad (10)$$

The long-time behavior is dominated by small momentum behavior of the integrand, and the approximations for $G(\mathbf{k},t=0)$ and $\lambda(k)$ become exact in this limit.

The integral (10) can be evaluated numerically with parameters B, κ, λ_0, and c extracted from the correlation functions $G(\mathbf{k},t)$ estimated in the simulation. In Fig. 4 it is plotted together with independently recorded data for $q(t)$ at temperature $T=4.40$. As noted above, the choice of plotting coordinates is suitable for displaying the stretched exponential decay, which would appear as a straight line in the plot; exponential decay would correspond to a horizontal line.

It is immediately seen that the recorded values for $q(t)$ never reach the asymptotic regime. It is instructive to compute from (10) the value of $q(t)$ at time $t=10^4$ corresponding to the onset of the asymptotic decay: It is found to be of order 10^{-196}, and as such the asymptotic decay could *never* be observed in practice.

Analysis in four dimensions closely parallels that conducted above and will not be presented here. We have good reasons to believe that there are no surprises in still higher dimensional systems ($d>4$), and that formulas (4)-(7) and (10), and the behavior illustrated in Fig. 2, 3, and 4 remain valid.

In two dimensions, however, the dynamics of fluctuations in the ordered phase is very different. Typical time dependence of the correlation functions below T_c is shown in Fig. 5. The nonexponential decay of $G(\mathbf{k},t)$ is clearly seen, moreover one observes that the approximation

$$G(\mathbf{k},t)\approx G(\mathbf{k},0)\exp\{-[\lambda(k)t]^\beta\}$$

is not as good as in three dimensions (where $\beta=1$), even if one allows for power-law prefactors in the time dependence and fits the best value of β.

From the momentum expansion (3) one finds again that

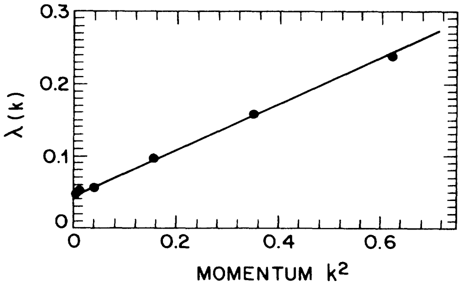

FIG. 3. Decay rate $\lambda(k)$ at $T=4.40$, $d=3$ plotted vs momentum squared k^2. Note the gap at $\mathbf{k}=0$.

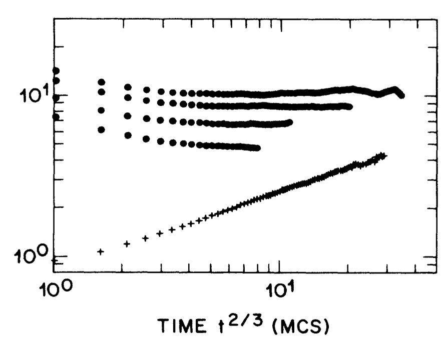

FIG. 5. Joint plot of normalized functions $-t^\beta/\ln[q(t)/q(0)]$ (crosses) and $-t^\beta/\ln f(k,t)$ (circles) in two dimensions at $T=2.15$, $L=512$, with $\beta=\frac{2}{3}$ and $f(k,t)=G(\mathbf{k},t)/G(\mathbf{k},0)$. In this plot Kohlrausch decay $f\sim\exp[-(\lambda t)^\beta]$ would appear as a straight line (horizontal for $\beta=\frac{2}{3}$). Nonexponential decay of $f(k,t)$ is clearly seen for selected values of $\mathbf{k}=(2\pi/L)(0,q)$ with wave number $q=0$ (top), 8, 16, and 24 (bottom).

the true asymptotic behavior of $q(t)$ in $d=2$ is the same as that of $G(\mathbf{k},t)$ for $\mathbf{k}\rightarrow 0$, since the static correlation function $G(\mathbf{k},t=0)$ is a rational function of $\mathbf{k}$, and cannot modify the long-time behavior. From numerical data such as that shown in Fig. 5, I cannot unambiguously extract the long-time behavior nor a meaningful, simple approximation to $G(\mathbf{k},t)$. Nevertheless, one can tentatively use the expansion analogous to (10), substituting the very accurate Fisher-Tarko approximation[8] for $G(\mathbf{k},t=0)$ in place of the Lorentzian, and replacing the exponential term in (10) by $\exp\{-[\lambda(k)t]^{\beta}\}$, with $\lambda(k)$ approximately given by (5) and a choice of $\beta=\frac{2}{3}$. The analysis similar to that described below Eq. (10) shows again that $q(t)$ would achieve its asymptotic behavior until it decays to a ridiculously small value. This exercise indicates that there is no basis to accept the approximate observed behavior $q(t)\sim\exp[-(t/\tau)^{1/3}]$ shown in Fig. 1(a) and in Ref. 4 as the true asymptotic behavior of $q(t)$. The analysis of droplet fluctuations in $d=2$ given in Ref. 2 predicts the asymptotic stretched exponential decay of $q(t)$ with $\beta=\frac{1}{2}$. The analysis given in Ref. 4 rests on the assumptions about the form of $G(k,t)$ which do not seem to be correct.

In any case, it is demonstrated in the present work that although simple phenomenological droplet theories of fluctuations in the ordered phase could *in principle* give correct asymptotic time dependence of correlation functions, they may be of very limited value in the analysis of *dominant* fluctuations governing the behavior of correlation functions in the range of times where they could be observed in practice. We believe that phenomenological theories should rather attempt to describe the dominant, observable phenomena. It is not clear at the moment if analogous droplet (or cluster) theories of fluctuations in disordered systems[1] suffer from the same limitations as in the simplest possible case of nonrandom Ising models, but it has been found already that the analogous arguments for Ising spin glasses above T_g lead to the predictions[9] for asymptotic decay which have not been observed in very accurate numerical solutions.[7]

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