Non-Monotonic Temperature Dependence of Local Dynamics and Local Energy upon Cooling toward the Ising Spin Glass Transition

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We have performed a detailed analysis of the local dynamics and local energies of the equilibrium, paramagnetic phase of the $d = 2$ and $d = 3$ $\pm J$ Ising spin glass model. Here we discuss our recently reported observations[1)] that while the average flip rate and average energy decrease monotonically with decreasing temperature, both the flip rate and energy of an increasing fraction of spins *increase* as the glass transition is approached on cooling. These findings are consistent with recent experimental results for the frequency-dependent magnetic susceptibility of an insulating spin glass, which showed that the approach to the glass transition could be detected from the high frequency behavior.

In an effort to better understand the effects of frustration as the glass transition is approached, and to elucidate recent claims of the presence and ramifications of dynamic heterogeneities significantly above the glass transition temperature T_g in glass-forming materials with self-induced frustration,[2)-7)] we are currently exploring the relationship between microstructure and local dynamics in a variety of systems, including supercooled liquids with self-induced disorder[8)] and paramagnets with random, quenched disorder.[1)]

In particular, we have recently performed a detailed Monte Carlo simulation study of the paramagnetic phase of the Ising spin glass to characterize the heterogeneities induced in this system by the quenched disorder, and to test the model for the emergence of fast processes recently reported in an experimental study of an Ising-like spin glass.[4)] In the Ising spin glass model, exchange interactions $J_{ij} = \pm J$ are fixed randomly to the edges of a lattice, and Ising spins with values $\sigma_i = \pm 1$ are placed on the vertices (sites). Quenched disorder exists in this system due to the random configuration of fixed exchange interactions $\{J_{ij}\}$. Because of the presence of frustrated plaquettes (loops along the edges of the lattice in which the product of the exchange interactions around the loop is negative), all the spins cannot satisfy all the interactions simultaneously at any temperature. A glass transition results at temperature $T = 1.1$ in dimension $d = 3$ and $T = 0$ in $d = 2$.[9)]

Our simulations are performed using the heat-bath Monte Carlo algorithm with periodic boundary conditions for lattices of size 64^2 in $d = 2$ and 16^3 in $d = 3$. Depending on T, between 3×10^5 and 2×10^7 Monte Carlo Steps (MCS) were used to

equilibrate the system. Simulations were performed for T ranging from $kT/J = 1.2$ to 3.0 in $d = 2$, and from $kT/J = 1.6$ to 6.0 in $d = 3$, where k is Boltzmann's constant.

Equilibration of each lattice was carefully monitored before commencing the evaluation of the quantities presented below. Time averages for all quantities were then evaluated for up to 2×10^7 MCS following equilibration. The results shown here were performed for one configuration of quenched disorder. Simulations with different disorder configurations confirm that our conclusions are not affected by the particular choice of random disorder configuration.

At each site i, the instantaneous energy $E_i = -\sum_j \sigma_i J_{ij} \sigma_j$, where j labels the nearest neighbors (nn's) of i. Quenched disorder causes the time average of E_i in equilibrium, ϵ_i, to vary from site to site; thus the local energy is spatially heterogeneous. The length scale of the heterogeneity is presumably set by the intrinsic length scale of the random quenched disorder, which is present at all T. The effect of the quenched disorder on the behavior of the system, however, changes strongly with T as discussed below. A number of different measures of the local dynamics exist. Here we define the local spin-flip rate ν_i to be the fraction of flips observed in a chosen observation time for spin i in equilibrium. Thus ν_i is the equilibrium probability, per MCS, for spin i to flip. Like ϵ_i, ν_i is a function of position in the system, i.e., it is spatially heterogeneous.

We calculated both the normalized probability density $P(\epsilon)$ for a given site to have an average energy ϵ, as well as the probability density $P(\nu)$ for a given site to have an average flip rate ν, for several $T > T_{sg}$. As reported elsewhere,[1] we observe

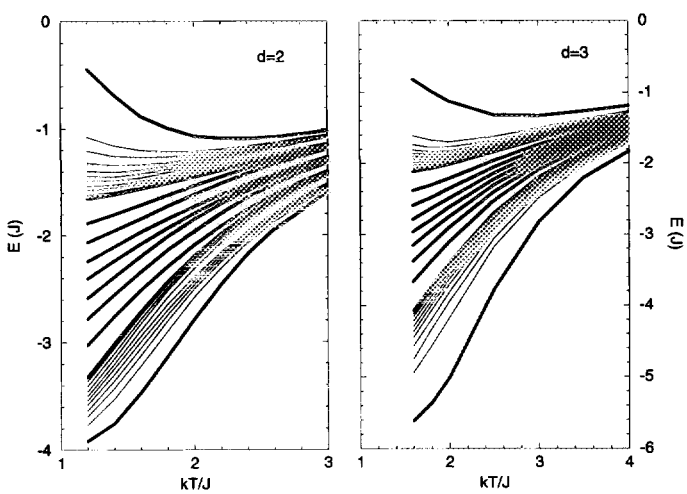

Fig. 1. Plot of ϵ^* for fixed f as a function of T in (a) $d = 2$ and (b) $d = 3$. The thick lines show ϵ^* for $f = 0$ (lowest curve), $f = 0.10$ (next lowest curve), and so on up to $f = 1.0$ (highest curve). The two highest thick lines therefore delimit the range of the top 10% of all ϵ values. The thin lines show ϵ^* curves within the top 10% of ϵ values with a resolution in f of 0.01. The top 1% of ϵ values therefore lie between the highest thin line and the highest thick line.

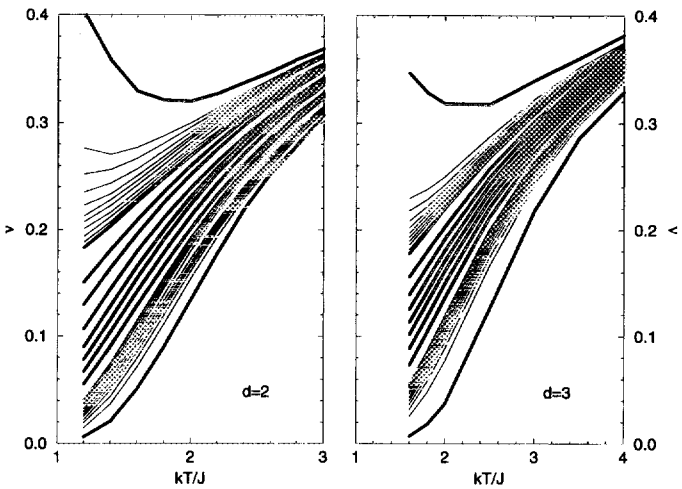

Fig. 2. Plot of ν^* as a function of T in (a) $d = 2$ and (b) $d = 3$. The thick lines show ν^* for $f = 0$ (lowest curve), $f = 0.10$ (next lowest curve), and so on up to $f = 1.0$ (highest curve). The thin lines show ν^* with a resolution of 0.01 for the top 10% (as in Fig. 1).

that the shape of these distributions change substantially even for T well above T_{sg}, becoming increasingly broad, and in particular developing long tails with decreasing T.

To highlight this behavior, we evaluate the function $\epsilon^*(f)$, implicitly defined by $f = \int_{-\infty}^{\epsilon^*} P(\epsilon)d\epsilon$. Hence, a fraction f of the sites will have a value $\epsilon \leq \epsilon^*$. We define a similar function $\nu^*(f)$ via $f = \int_0^{\nu^*} P(\nu)d\nu$.

In Figs. 1 and 2 we plot $\epsilon^*(f)$ and $\nu^*(f)$ as functions of T for specific values of f. From Fig. 1 we find that for the range of T simulated here, $\epsilon^*(f)$ is a non-monotonic function of T for $f > 0.92$ in both $d = 2$ and $d = 3$. That is, at the lowest T we simulate, the top 8% of local energy values in the system are increasing in value as T decreases. That is, though the average energy of most spins decreases as T decreases, surprisingly, for a fraction of spins it increases. Note also that the trend of the curves suggests that an even greater fraction will show this behavior as $T \to T_{sg}$.

The corresponding behavior for local flip rates is shown in Fig. 2. In the T-range of our simulations we find that $\nu^*(f)$ is a non-monotonic function of T for $f > 0.98$ in $d = 2$ and for $f > 0.99$ in $d = 3$. Hence the largest 1%–2% of ν values increase as T decreases. The data also suggest that the fraction of ν values with this behavior will grow as $T \to T_{sg}$. That is, *as the glass transition is approached from above there is a subset of sites in the Ising spin glass that exhibit an increasingly fast dynamics, despite the fact that the global relaxation of the system is becoming increasingly slow.* [10]

We see that the fast dynamics that emerge upon cooling in this system are intimately coupled to the local energetic environment, or microstructure. As one example, a site will have a high flip-rate at low T if (i) its nn sites each have a very

low flip rate (which will occur if the average energy of those sites is low), and (ii) half of the interactions with the nn sites are satisfied and half are unsatisfied. Thus the system appears to "partition" the local energies in such a way as to "focus" the frustration on a subset of sites in the system, raising the energy and flip-rate of those sites. This "focusing" allows other spins to locally order and thus lower their energy, while keeping the entire system in equilibrium.

Recently,[4] the frequency-dependent magnetic susceptibility $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$ was measured on the insulating Ising spin glass, $LiHo_{0.167}Y_{0.833}F_4$. The results showed that the approach to the glass transition upon cooling could be detected from the high frequency behavior of the complex part of the susceptibility. Recent experiments on liquids attach a similar importance to fast processes in these systems.[11),12)] In the Ising spin glass model, we too can detect the approach to T_{sg} upon cooling from the high frequency behavior.

In summary, the Ising spin glass model – the fruitfly glass-forming spin model of statistical mechanics – affords us the opportunity to study in great detail the effects of disorder and frustration on local equilibrium thermodynamic and dynamic quantities as the system is cooled toward its glass transition. In this paper, we have focused on our recent findings that the approach to the transition can be detected already at high temperature by either the dynamic or energetic behavior of the fastest or highest energy spins alone, in agreement with findings reported in recent experiments.

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