TEMPERATURE DEPENDENCE OF SPATIAL AND DYNAMIC HETEROGENEITIES ABOVE THE ISING SPIN GLASS TRANSITION

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ABSTRACT

The temperature dependence of the microstructure and local dynamics in the paramagnetic phase of the $d = 2$ and $d = 3$ $\pm J$ Ising spin glass model is examined by comparing the equilibrium distributions of local flip-rates and local energies calculated in large-scale Monte Carlo simulations. The emergence in this model of fast processes as the glass transition is approached corresponds with recent experimental results.

INTRODUCTION

An open question in the quest to understand the glass transition [1] and the relationship between microstructure, local dynamics, and global relaxation in glass-forming materials, is that of the homogeneity of the material as it is cooled. A number of recent experiments on supercooled liquids and polymers have detected dynamic spatial heterogeneities above the glass transition [2], fueling arguments put forth by numerous groups on the presence of clusters, cooperatively rearranging domains, or coexisting fluids, in such systems [3]. It has been known for some time that the global relaxation in equilibrium glass-forming materials above their glass transition temperature is poorly described by a simple exponential, and better described by a stretched exponential at long times. However, it is still not generally known whether individual subdomains relax homogeneously, that is, with each region associated with the same relaxation time and the same stretching exponent, or heterogeneously, that is, with each region having a different relaxation time and/or a different stretching exponent. In systems where the frustration is self-induced, i.e. emerges upon cooling due to packing constraints between the molecules, the relationship between local structure and local dynamics even in computer simulations is difficult to assess due to the time-dependent nature of the local energies and relaxation times.

Recently, we have described a detailed computer simulation study of the high temperature, equilibrium phase of a glass-forming system with *quenched* disorder — the $\pm J$ Ising spin glass — in both two and three dimensions [4, 5]. This model affords us the opportunity to characterize the temperature dependence of spatial heterogeneities that we know *a priori* exist in the system due to the quenched disorder. Heterogeneities in such quantities as the local site energy, local flip-rates, local relaxation times, local fields, etc. — which are absent in the pure Ising ferromagnet — give rise to complex behavior in the spin glass. For example, we recently reported the emergence of a subset of high-frequency, high-energy excitations that *increase* in magnitude as temperature T *decreases* toward the spin glass transition temperature T_{sg}. This phenomenon is a direct consequence of the frustration, and is similar to results of recent measurements of the magnetic susceptibility of an insulating spin glass in which the approach to the glass transition on cooling could be detected from the behavior of the *fastest* dynamics in the system [6].

In this proceedings, we focus on the role of frustration and disorder in producing the wide spectra of energies and dynamics in the high T, paramagnetic phase of the Ising spin glass, and discuss the temperature dependence of the correlation between these two distributions as the spin glass transition is approached from high temperature.

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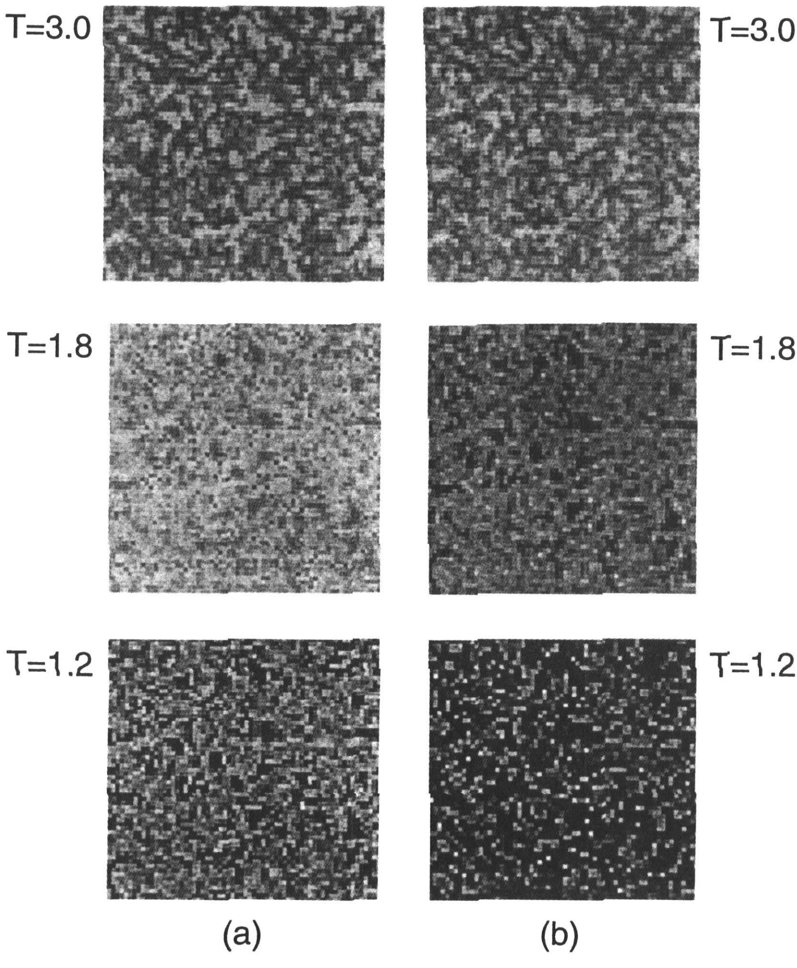

Figure 1: Equilibrium spatial distributions of the (a) local site energy ϵ_i and (b) local flip-rate ν_i in $d = 2$. High values of ϵ_i and ν_i are shown in white, low values in black. The lowest and highest values of ϵ_i possible for T ranging between zero and infinity are -4.0 and 0.0, respectively. The lowest and highest values of ν_i possible are 0.0 and 0.5, respectively.

METHOD

The Ising spin glass model is described by the Hamiltonian $H = -\sum_{\langle ij \rangle} \sigma_i J_{ij} \sigma_j$. Square (dimension $d = 2$) and simple cubic ($d = 3$) lattices of size 64^2 and 16^3 were prepared by randomly assigning exchange interactions $J_{ij} = \pm J$ to the edges of the lattice, and placing on the vertices (sites) Ising spins σ with values $\sigma = \pm 1$. The transition temperature $kT_{sg}/J = 0$ and 1.1 in d=2 and d=3, respectively [7], where k is Boltzmann's constant. Monte Carlo computer simulations were performed in zero magnetic field using heat bath dynamics with periodic boundary conditions. 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 temperatures ranging from $kT/J = 1.2$ to 3.0 in $d = 2$, and from $kT/J = 1.6$ to 6.0 in $d = 3$. Individual on-site magnetizations and spin autocorrelation functions were carefully monitored to ensure equilibration before commencing the evaluation of the quantities presented below. Time averages for all quantities were evaluated for up to 2×10^7 MCS following equilibration. Simulations with different random bond configurations for the quenched disorder confirm that all distributions are converged to their asymptotic, equilibrium form; that is, our conclusions are independent of the particular choice of random $\{J_{ij}\}$.

RESULTS

The spatial arrangement of local energies and local flip-rates in the $d = 2$ Ising spin glass at selected temperatures is shown in Figure 1. 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 induces the time average of E_i in equilibrium, ϵ_i, to vary from site to site as shown in Fig. 1a. That is, the local site energy is spatially heterogeneous [8]. 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. For example, we see from Fig. 1a that in most instances spins which have low energy at high T continue to decrease their energy with decreasing T, while spins which have high energy at high T may also have high energy at lower T. As shown elsewhere [4, 5], these highest energy spins actually first decrease, and then increase in energy with decreasing T.

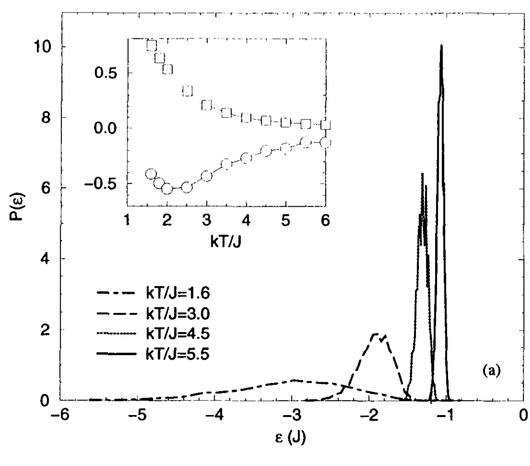

Figure 2: $P(\epsilon)$ versus ϵ for various T in $d = 3$.INSET: Skewness γ and standard deviation σ of the distribution versus T.

Next we define the local flip-rate ν_i to be the number of flips observed for spin i, divided by the total observation time in equilibrium. ν_i is therefore the equilibrium probability, per MCS, for spin i to flip. Like ϵ_i, ν_i is also spatially heterogeneous (Fig. 1b) [8]. Again the effect of the quenched disorder on the behavior of the system changes strongly with T. For example, we see from Fig. 1b that in most instances spins which have low flip-rate at high T continue to decrease their flip-rate with decreasing T, while spins which have high flip-rate at high T may also have high flip-rate at lower T. As shown elsewhere [4, 5], these highest flip-rate spins actually first decrease, and then increase, their flip-rate with decreasing T.

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 [4] and shown for $d = 3$ in Figs. 2 and 3, we observe that the shape of these distributions changes substantially even for T well above T_{sg}, becoming increasingly broad, and in particular developing long tails with decreasing T. As shown in the insets of Figs. 2 and 3, both the standard deviation σ and skewness γ characterizing the distributions are increasing as $T \to T_{sg}$ [9].

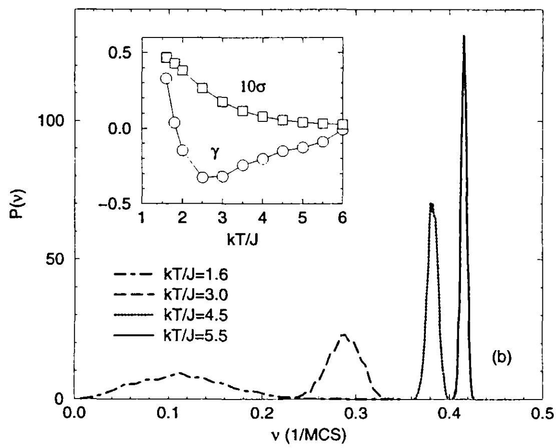

Figure 3: $P(\nu)$ versus ν for various T in $d = 3$. INSET: Skewness γ and standard deviation σ of the distribution versus T.

To examine the correlation between ν and ϵ, in Fig. 4 we plot the value of ν against ϵ for each site in the system, for various T in $d = 2$ and $d = 3$ [10]. As expected from the distributions in Figs. 2 and 3, Fig. 4 shows an increasing spread in the range of both ν and ϵ as T decreases. Also, we find that at high T, a given value of ν correlates well to a specific value ϵ. As T decreases, the lowest and highest values of ν and ϵ remain strongly correlated. However, at intermediate values of ϵ, a given ϵ corresponds to a broad spectrum of ν values, which widens further with decreasing T. This last effect occurs because the correlation length is increasing as T decreases toward T_{sg}, causing local relaxation rates to be influenced by interactions beyond the nn interactions quantified by ϵ.

Despite the fact that the global relaxation of the system is becoming increasingly slow [7], we see in Fig. 4 the surprising emergence of spins whose flip-rate and energy are higher than that observed at higher T for the range of T simulated. In fact, we showed elsewhere [4, 5] that both the energy and flip-rates of those spins actually first decrease, and then increase, with decreaing T.

The approach to the glass transition in this system upon cooling can thus be detected by observing the behavior of the *fastest* dynamics. In a recent experiment by Bitko, et al. [6], the magnetic susceptibility was measured over 8 decades of frequency for an insulating Ising spin glass $LiHo_{0.167}Y_{0.833}F_4$. The results showed that the approach to T_{sg} upon cooling could be detected from the high frequency behavior alone, similar to that observed here and in several other recent experimental studies [11]-[13].

We see that the complex dynamics that emerge upon cooling in this system [7] is intimately coupled to the local energetic environment, or microstructure. For example, consider the following extreme case: an individual 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 time-averaged energy of each of those sites is low), and (ii) half of the interactions with the nn sites are satisfied and half are unsatisfied. On the other hand, a site with an intermediate energy at low T may have one of many different flip-rates, depending on the environment around the spin beyond the nn's but within the correlation length at that T. Thus as the system cools, it 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 as much as environmentally allowed, while keeping the system globally in equilibrium.

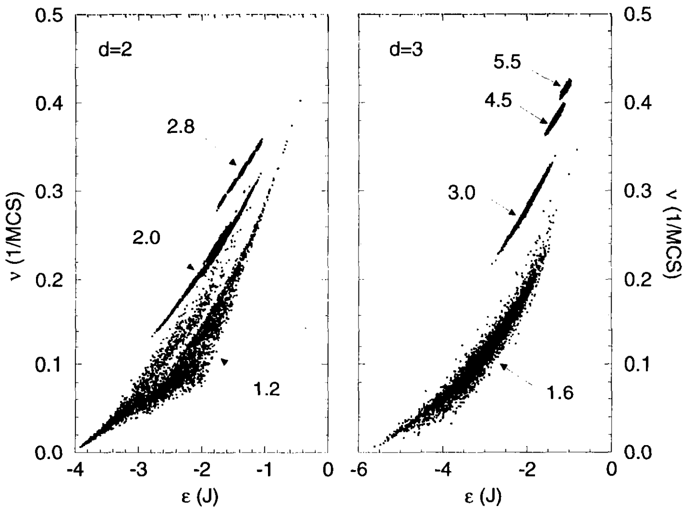

Figure 4: Scatter plot of local fliprate ν versus local energy ϵ for all sites at various kT/J (a) in $d=2$, and (b) in $d=3$.

CONCLUSIONS

In summary, the much-studied "fruitfly" glass-forming spin model of statistical mechanics — the nn Ising spin glass — has much to teach us about the effects of frustration and disorder on equilibrium thermodynamic and dynamic properties as a glass transition is approached. The fact that in this model the disorder is quenched to the lattice — and not annealed, or self-induced as in liquids — provides us with a unique opportunity to measure and characterize the frustration and disorder-induced heterogeneities in such quantities as the local energies and local flip-rates, in a system where we know *a priori* that heterogeneities exist. It is our hope that such a study will provide a useful approach and benchmark by which to investigate frustration-induced heterogeneities in a wider class of glass-forming materials.

Acknowledgements

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[8] For comparison, note that for a ferromagnetic Ising model ϵ_i would approach the same value for all sites. The same is true for ν_i.

[9] If $P(x)$ describes the distribution of a set of N values $\{x_i\}$, then the standard deviation σ of $P(x)$ is given by $\sigma^2 = [1/(N-1)]\sum_{i=1}^{N}(x_i - \langle x\rangle)^2$ where $\langle x\rangle$ is the average value of x. The skewness γ of $P(x)$ is given by $\gamma = (1/N)\sum_{i=1}^{N}[(x_i - \langle x\rangle)/\sigma]^3$.

[10] A similar plot for the ferromagnetic Ising model would display a single point for each temperature.

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