Emergence of Fast Local Dynamics on Cooling toward the Ising Spin Glass Transition

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We present a detailed Monte Carlo evaluation of the equilibrium distribution of local spin-flip rates and local energies in the paramagnetic phase of the $d = 2$ and $d = 3 \pm J$ Ising spin glass. Both quantities are spatially heterogeneous, and we find that the shapes of the distributions change dramatically with decreasing temperature. In particular as temperature decreases we find that for an increasing fraction of spins the local spin-flip rate and local energy *increase* as the glass transition is approached.
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Despite ongoing efforts to understand the glass transition—both in liquids with self-induced frustration, and in spin glasses with quenched disorder—the relationship between local structure, local dynamics, and global relaxation is still poorly understood [1]. A number of recent studies have reported the observation of anomalous fast relaxation processes which appear as the glass transition is approached. For example, spatially heterogeneous, enhanced rotational and/or translational diffusion has been reported just above the glass transition temperature in supercooled orthoterphenyl [2], polystyrene [3], and polyvinylacetate [4]. Also, the emergence of high frequency modes has been observed in experiments on supercooled liquids [5–7] and in the paramagnetic phase of an insulating spin glass [8]. Both the microscopic origin of these fast processes, in particular, and in general the relationship between glass-forming systems with annealed (self-induced) and quenched disorder are currently topics of intense research.

One of the most commonly studied models of a system with quenched disorder is the Ising spin glass [9]. In this Letter, we use Monte Carlo computer simulations of the Ising spin glass to test if this model exhibits any anomalous fast relaxation processes as temperature T decreases toward the spin glass transition temperature T_{sg}. To this end, we show how the quenched disorder of this system gives rise to spatial heterogeneities in the local energy and local dynamics, and we evaluate the distribution of values characterizing these heterogeneities. Although the average spin-flip rate and average energy of the system decrease as $T \to T_{\mathrm{sg}}$ from above, we observe the emergence of local regions in the paramagnetic phase of the Ising spin glass for which the local spin-flip rate and energy *increase* as $T \to T_{\mathrm{sg}}$ from above.

We use Monte Carlo computer simulations to study the Ising spin glass, described by the Hamiltonian $H = -\sum_{\langle ij\rangle} s_i J_{ij} s_j$, on a square (dimension $d = 2$) and simple cubic ($d = 3$) lattice. (The external magnetic field is zero.) Lattices are prepared by randomly assigning exchange interactions $J_{ij} = \pm J$ to the edges of the lattice, and placing on the vertices (sites) Ising spins s with values $s = \pm 1$. The sum in H is taken over all nearest-neighbor (nn) pairs of sites.

For this model the transition temperature $kT_{\mathrm{sg}}/J = 0$ and $\simeq 1.1$ in $d = 2$ and $d = 3$, respectively [10]. Our simulations are performed using the heat-bath Monte Carlo algorithm [11] with periodic boundary conditions for lattices of size 64^2 ($d = 2$) and 16^3 ($d = 3$). Individual spins are updated in random order. Simulations are 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. The results presented here are obtained for one particular random $\{J_{ij}\}$ configuration for the quenched disorder. Simulations using different random $\{J_{ij}\}$ configurations confirm that the quantities evaluated here are not affected by the particular choice of $\{J_{ij}\}$.

For the present study, ensuring equilibration at all T simulated is particularly important, both globally and microscopically. Depending on T, between 3×10^5 and 2×10^7 Monte Carlo steps (MCS) are used for equilibration. Time averages for all quantities are evaluated for up to 2×10^7 MCS following equilibration. We confirm in the following ways that these run times are sufficient to establish equilibrium and to evaluate equilibrium properties. First, we evaluate the equilibrium time average of s_i at each site i, $\langle s_i\rangle$, and require that the run time be sufficiently long so that $|\langle s_i\rangle| < 0.04$ for *all* i. Second, we evaluate the spin autocorrelation function $q(t) \equiv (1/N)\sum_i \langle s_i(0)s_i(t)\rangle$, where N is the total number of sites and t is the time [9]. We ensure that our run times are at least 3 orders of magnitude longer than the time taken for $q(t)$ to decay to less than 0.01 [12].

The spatial arrangement of local energies and local spin-flip rates in the $d = 2$ Ising spin glass at $kT/J = 1.2$ is shown in Fig. 1. At each site i, the instantaneous energy $E_i = -\sum_j s_i J_{ij} s_j$, where j labels the nn's of

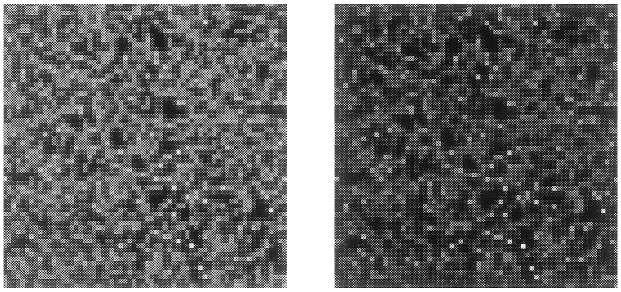

FIG. 1. Equilibrium spatial distributions of ϵ_i (left panel) and ν_i (right panel) in $d = 2$ for $kT/J = 1.2$. High values of ϵ_i and ν_i are shown in white, low values in black.

i. Quenched disorder induces the time average of E_i in equilibrium, ϵ_i, to be spatially heterogeneous as shown in Fig. 1(a) [13]. Next we define the local frequency or spin-flip rate ν_i to be the number of flips observed for spin i, divided by the total observation time. ν_i is therefore the equilibrium probability, per MCS, for spin i to flip. Like ϵ_i, ν_i is spatially heterogeneous, as shown in Fig. 1(b).

In Fig. 2 we show the normalized probability density $P(\epsilon)$ for a site to have an average energy ϵ, for several $T > T_{\mathrm{sg}}$. We find that $P(\epsilon)$ displays a rich set of behaviors as a function of T. For example, distinct peaks and shoulders are evident both in $d = 2$ and $d = 3$. These features are each associated with a particular type of local interaction environment generated on the lattice in any random $\{J_{ij}\}$ configuration [14]. Moreover, we observe that the shape of $P(\epsilon)$ changes significantly as T decreases, even for values of T well above T_{sg}. As shown in the insets of Fig. 2, both the standard deviation σ and skewness γ characterizing $P(\epsilon)$ are increasing as $T \to T_{\mathrm{sg}}$ [15].

In Fig. 3 we present the probability density $P(\nu)$ for a site to have an average spin-flip rate ν, for several $T > T_{\mathrm{sg}}$. As for $P(\epsilon)$, $P(\nu)$ also displays distinct peaks and shoulders [14]. The shape of $P(\nu)$ also changes dramatically for values of T well above T_{sg}, with σ and γ increasing as $T \to T_{\mathrm{sg}}$ (see insets).

To examine the correlation between ν and ϵ, in Fig. 4 we plot the value of ν against ϵ for each site in

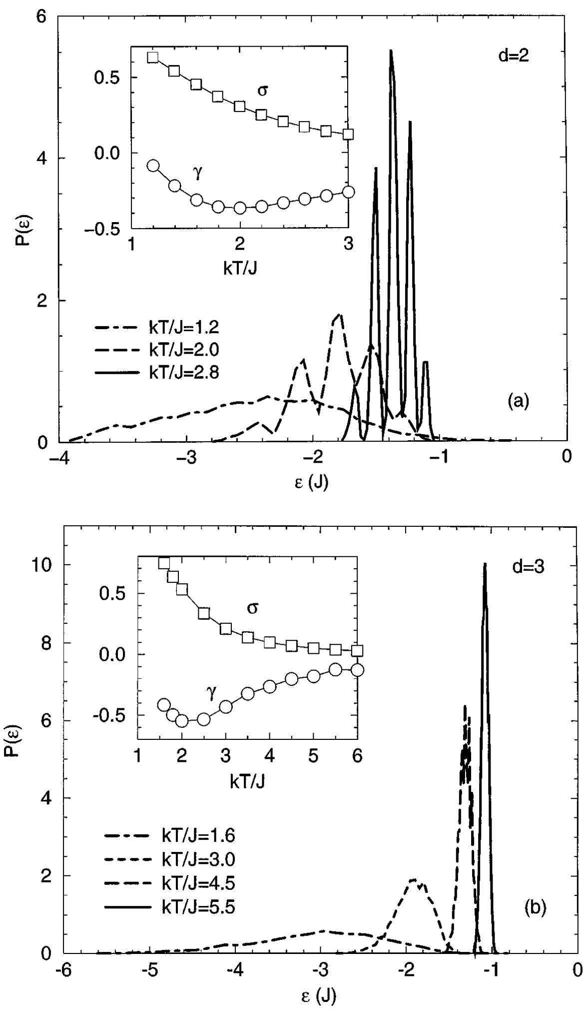

FIG. 2. $P(\epsilon)$ versus ϵ for various T (a) in $d = 2$, and (b) in $d = 3$. Insets: σ and γ for $P(\epsilon)$ plotted versus T for (a) $d = 2$ and (b) $d = 3$.

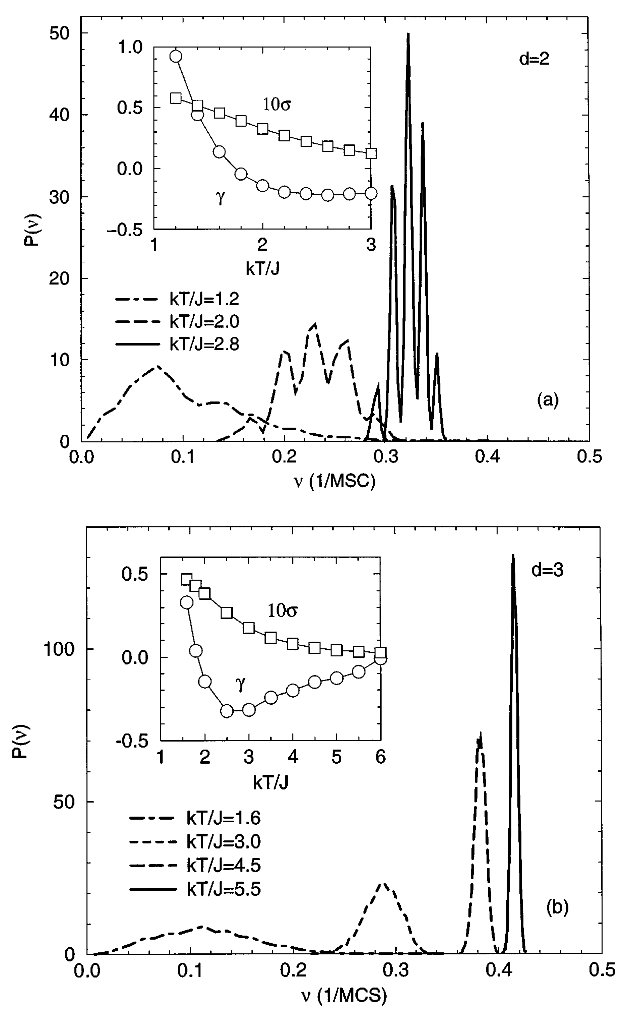

FIG. 3. $P(\nu)$ versus ν for various T (a) in $d = 2$, and (b) in $d = 3$. Insets: σ and γ for $P(\nu)$ versus T for (a) $d = 2$ and (b) $d = 3$.

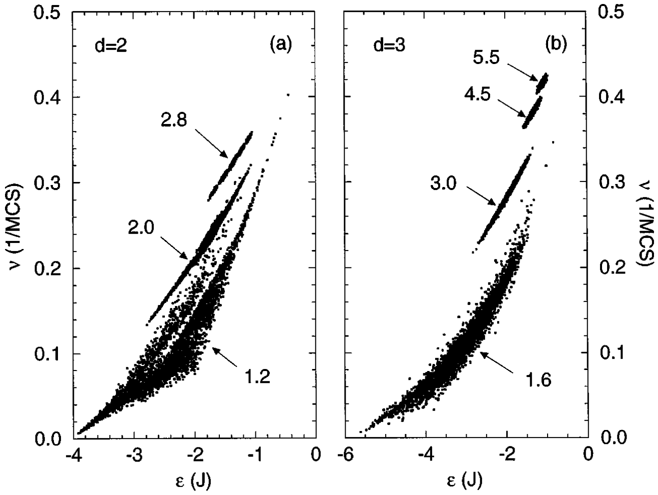

FIG. 4. Scatter plot of ν versus ϵ for all sites at various values of kT/J (a) in $d = 2$, and (b) in $d = 3$.

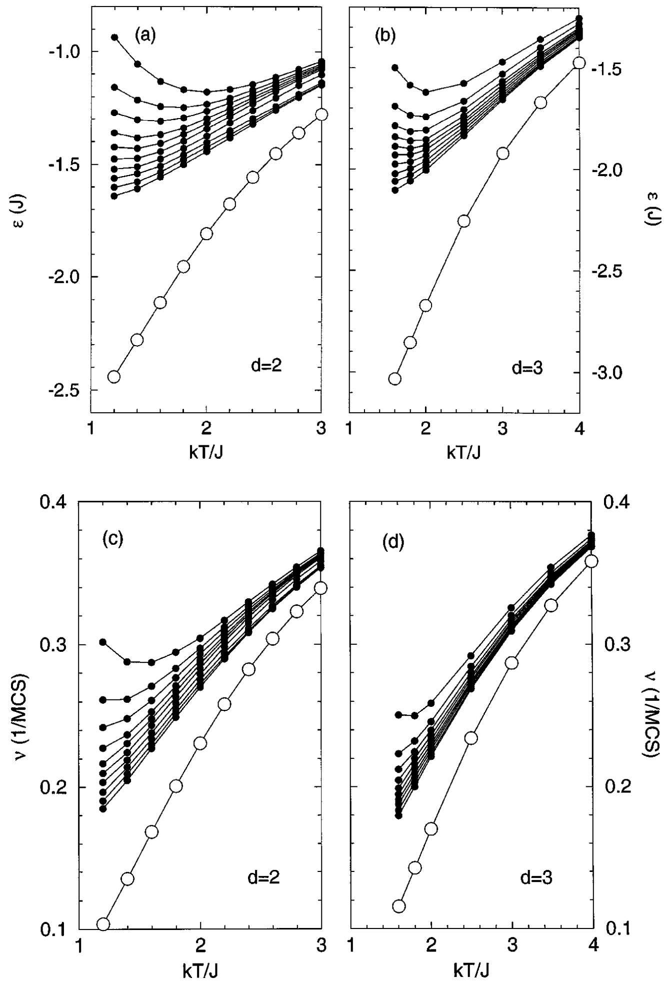

FIG. 5. As a function of T are plotted $\overline{\epsilon}_k$ (•) and $\langle\epsilon\rangle$ (∘) in (a) $d = 2$ and (b) $d = 3$; and $\overline{\nu}_k$ (•) and $\langle\nu\rangle$ (∘) in (c) $d = 2$ and (d) $d = 3$. In all plots, the curves (•) for the kth centile are shown, from bottom to top, for $k = 91, 92, \ldots, 100$. Hence the topmost curve is the average of the highest 1% of values for the indicated quantity, ϵ or ν.

the system, for various T [16]. 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 of 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}, hence ν values are influenced by interactions beyond the nn interactions quantified by ϵ.

Notably, we see from Fig. 4 the emergence at low T of high spin-flip rate, high energy sites whose ν and ϵ are larger than those observed for any other sites at higher T in the range simulated. That is, for some sites ν and ϵ are nonmonotonic functions of T [17].

To highlight this behavior, we subdivide the ordered set of ϵ values found for a particular T into 100 subgroups or "centiles": the 100th centile contains the top 1% of ϵ values, the 99th centile contains the next highest 1%, and so on down to the 1st centile which contains the lowest 1% of ϵ values. Let $\overline{\epsilon}_k$ be the average value of ϵ for the kth centile. We make an analogous definition for $\overline{\nu}_k$, the average value of ν for the kth centile of the ordered set of ν values. In Fig. 5 we plot $\overline{\epsilon}_k$ and $\overline{\nu}_k$ for $k = 91, 92, \ldots, 100$ along with the average spin-flip rate $\langle\nu\rangle$ and average energy $\langle\epsilon\rangle$ for the whole system, as a function of T for $d = 2$ and $d = 3$. We see that while $\langle\nu\rangle$ and $\langle\epsilon\rangle$ decrease monotonically with decreasing T, for the spins with the very highest ν and ϵ values, these quantities first decrease, but then increase as T decreases. In both $d = 2$ and $d = 3$ at the lowest T we simulate, the highest 5% of local ϵ values, and the highest 1%–2% of ν values, are increasing as T decreases. This nonmonotonic behavior is consistent with that found for γ shown in Figs. 2 and 3.

The trend of the curves in Fig. 5 suggests that an even greater fraction of sites will show this behavior 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. This phenomenon can be understood by considering, as an extreme case, a site i whose nn's spins j tend toward a relatively slow flipping, low energy configuration as $T \to T_{sg}$ in which the local field at site i, $h_i = \sum_j J_{ij} s_j = 0$. In this case, the spin at site i will flip quite frequently even at low T since such flips will not change the energy of the system.

In a recent experiment by Bitko *et al.* [8], 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 this, and several other recent experimental studies [2–7] we have shown here that the Ising spin glass model also exhibits a fast local relaxation that indicates the approach to the glass transition.

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[11] In heat-bath dynamics, a spin at site i is given a value $s_i = +1$ with a probability $p = \exp(Jh_i/kT)/[\exp(-Jh_i/kT) + \exp(Jh_i/kT)]$, where $h_i = \sum_j J_{ij}s_j$ is the local field at site i. See K. Binder, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1986), and B. Derrida and G. Weisbuch, Europhys. Lett. **4**, 657 (1987).

[12] We also confirm that the single spin autocorrelation function, $q_k(t) \equiv \langle s_k(0)s_k(t)\rangle$, for that site k with the *lowest* spin-flip rate decays to less than 0.01 in a time that is at least 3 orders of magnitude less than the run time.

[13] 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.

[14] For example, in $d = 2$ there are five possible combinations of frustrated and unfrustrated plaquettes than can immediately surround a given site, thus giving rise to five possible nn environments for each site. Each of these environments gives rise to a different peak in the $kT/J = 2.8$ curve in Fig. 2(a) because the correlation length at that T extends out only to nn's. As T decreases and the correlation length grows, further environments are probed, inducing new structures in the distributions. A similar situation exists in $d = 3$. Peaks in the related distribution of edge energies was first noted by A. T. Ogielski, in *Proceedings of Heidelberg Colloquium on Glassy Dynamics* (Springer-Verlag, Berlin, 1987).

[15] 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 $\gamma = (1/N)\sum_{i=1}^{N}[(x_i - \langle x\rangle)/\sigma]^3$.

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

[17] Evidence for freely flipping spins has been previously reported in D. Stauffer, J. Phys. A **26**, L525 (1993); T. S. Ray and N. Jan, J. Phys. I (France) **4**, 2125 (1993).