Residual Energies after Slow Cooling of Disordered Systems

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The residual energy, $\epsilon(\tau)$, left after cooling to zero temperature in a finite time τ is analyzed for various disordered systems, including spin-glasses and random-field magnets. We argue that the generic behavior for such frustrated systems is $\epsilon(\tau) \sim (\ln\tau)^{-\zeta}$ for large τ, with the exponent ζ depending on the system. This result is dominated in some cases by a distribution of classical two-level systems with low excitation energies, and in other cases by large-scale nonequilibrium effects.

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The equilibration times of frustrated systems, such as glasses, spin-glasses, or random-field systems, readily exceed the time scales of experiments at low temperatures T. For such systems we cannot directly observe the equilibrium low-temperature behavior, but must infer it from nonequilibrium behavior. Thus it is necessary to study the nonequilibrium behavior of such systems as a function of waiting time or cooling rate.

In this paper we discuss the behavior of several classes of Ising spin systems with quenched disorder and single spin-flip dynamics upon slow cooling from high temperature to $T=0$ in a finite time τ. In particular, we analyze the expected energy per spin upon reaching $T=0$ in time τ, $\langle E\rangle_\tau$. The residual energy $\epsilon(\tau)=\langle E\rangle_\tau - E_0$ is the amount by which the energy exceeds the true ground-state energy per spin, E_0. Recently, Grest, Soukoulis, and Levin[1] have speculated, on the basis of Monte Carlo simulations, that $\epsilon(\tau) \sim (\ln\tau)^{-1}$ for certain Ising–spin-glass models in which the problem of finding the ground state is not solvable in a time which grows as a power of the system size (i.e., it is *NP*-complete) and that $\epsilon(\tau)$ varies as an inverse power of τ for certain other models that are not *NP*-complete. We argue that this is not correct, but rather that the generic large-τ behavior for frustrated systems is

$$\epsilon(\tau) \sim (\ln\tau)^{-\zeta}, \qquad (1)$$

with the exponent ζ depending on the system. In certain cases, even systems whose ground state is completely trivial exhibit this behavior.

We show that the result (1) is a simple consequence of a distribution of excitations from the ground state which have small excitation energies, Δ, but are separated from it by larger activation barriers, B. We thus first consider the behavior of a single such classical two-level system as the temperature $T(t)$ is lowered during the time interval $0 \le t \le \tau$. The residual energy in the two-level system (TLS) at time τ is just $\Delta p(\tau)$ where $p(t)$ is the probability that the TLS is in its higher-energy state at time t. This probability obeys the master equation

$$\gamma^{-1} dp/dt = (1-p)\exp[-(\Delta+B)/T(t)] - p\exp[-B/T(t)], \qquad (2)$$

where γ is an attempt frequency. We will assume that the initial distribution corresponds to infinite temperature so that $p(0)=\frac{1}{2}$.

Physically, it is clear that the TLS falls out of equilibrium roughly at a temperature $\tilde{T}$ such that the rate for hopping the barrier, $\gamma e^{-B/T(t)}$, is of order $1/\tau$, i.e., the metastable state cannot decay in the remaining cooling time. At this time, $\tilde{t}$, the temperature is $\tilde{T} \approx B/\ln(\gamma\tau)$ and the probability of being in the excited state is $p(\tilde{t}) \sim e^{-\Delta/\tilde{T}} \sim (\gamma\tau)^{-\Delta/B}$. As we will see, this is roughly the correct asymptotic form in the limit of slow cooling, i.e., large τ.

For definiteness, let us reduce the temperature linearly from an initial value T_0 to 0, although it will turn out that the details of the cooling schedule are unimportant. It is convenient to define a dimensionless asymmetry of the TLS, $\mu = \Delta/B$, and a dimensionless cooling rate, $\delta \equiv T_0/B\gamma\tau$. We are then interested in the behavior of $p(\tau)$ for small δ.

Straightforward asymptotic analysis yields an expression uniformly (in μ) valid in the small-δ limit:

$$p(\tau) \approx \delta^\mu [\ln\delta/\mu]^{2\mu}\Gamma(1+\mu) - \delta^{2\mu}/(1+\delta^\mu), \qquad (3)$$

with *relative* corrections which are small. For fixed μ, we see that there are only logarithmic corrections to the naive result $p(\tau) \sim \delta^\mu$. Indeed, if the cooling schedule is chosen so as to minimize the final energy, which is achieved by $T(t) \approx B/\ln[\gamma t/(1+\mu)]$, then for large τ and fixed μ, $p(\tau) \approx (\gamma\tau)^{-\mu}(1+\mu)^{1+\mu}$, which also only differs from Eq. (3) by logarithms. Thus the simple physical argument yields roughly the correct result independent of the details of the cooling procedure.

From Eq. (3), we see that the residual energy in the TLS, $\Delta p(\tau)$, is largest for fixed γ, B, and τ when $\Delta \approx B/\ln\gamma\tau$. Thus, in a system with a distribution of TLS, those with small asymmetry μ dominate the residual energy for slow cooling.

In disordered Ising systems with frustration, there are generally TLS which consist of small clusters of spins flipped from the ground state. If the distribution of the randomness controlling the frustration is continuous, then there are no exact degeneracies, but there are small-scale excitations with excitation energies Δ arbitrarily close to zero. Indeed, generically the density of states goes to a positive constant as $\Delta \to 0$. Examples of such systems, which we will discuss in more detail later, are short-range spin-glasses with a continuous distribution of exchanges for which the TLS have ben discussed in some detail,[2] disordered ferromagnets with a small number of antiferromagnetic bonds with variable magnitude, and random-field magnets with a continuous distribution of bond or random-field strengths in which the TLS consist of (possibly rare) regions where the cumulative random field is approximately the critical strength needed to flip the spins in that region in the ground state.[3] In all these cases the barriers B for the creation of excitations are typically of the order of some fraction of the number of spins in the excitation and thus, for small scale excitations, of the order of the characteristic exchange-energy scale J.

We are thus led to consider, as an approximation, a collection of *independent* TLS with excitation energies Δ and barriers B with density per spin $\Phi(\Delta,B)\,d\Delta\,dB$. The residual energy per spin is then simply

$$\epsilon(\tau)=\int dB \int d\Delta\, \Phi(\Delta,B)\Delta p_{\Delta,B}(\tau). \tag{4}$$

As argued above, we expect a positive density of TLS with arbitrarily small excitation energies for fixed B, i.e., $\Phi(0,B)>0$. Then, for large τ, the integral over Δ in Eq. (4) is dominated by $\Delta \sim B/\ln\gamma\tau$, which yields

$$\epsilon(\tau)\approx C\int dB\, \Phi(0,B)B^2/\ln^2\gamma\tau. \tag{5}$$

The coefficient C depends on the cooling schedule; for constant cooling rate $C=\pi^2/12$. We have assumed that γ is independent of Δ for $\Delta \to 0$ as expected physically.

In the disordered systems of interest, the small-scale low-energy excitations are not independent but interact, at least at positive temperature. However, the TLS in which most of the energy is trapped on cooling have energies of order $B/\ln\gamma\tau$, which is smaller than typical so that these TLS are dilute for large τ and thus independent to a good approximation, especially at the low temperature $\tilde{T}\sim B/\ln\gamma\tau$ at which they fall out of equilibrium. We thus expect the result $\epsilon(\tau)\sim 1/(\ln\gamma\tau)^2$ from the small-B part of the integral in Eq. (5) to generally be at least a lower bound for systems with a continuous distribution of frustration; this yields $\zeta\leq 2$ in (1). However, for some systems, excitations with large barriers B may dominate $\epsilon(\tau)$ at large τ; when this occurs the true decay is slower than that given by Eq. (5). In these cases, the temperatures $\tilde{T}$ at which the TLS with large B fall out of equilibrium are large and we must consider the effects of entropy and thermal disorder at these high temperatures. It is convenient to absorb the effects of varying attempt frequencies γ into temperature-dependent barrier heights B, so that we henceforth measure all times in units of the microscopic time. We now analyze various kinds of systems in detail, relying considerably on recent developments in the understanding of their dynamics. We focus on Ising systems, but very similar results should obtain for systems with frustration and continuous degrees of freedom.[2]

Spin-glasses with $T_c>0$.—In three (or more) dimensions d, there is now reasonably compelling evidence that for short-range Ising spin-glasses in zero magnetic field there is a positive transition temperature, T_c, below which the spin-flip symmetry is broken.[4] We have recently presented arguments[2] that the static and dynamic properties of the ordered phase for any $T<T_c$ are dominated at long distances and/or long times by droplet excitations (droplets of coherently flipped spins) which occur on all length scales with a distribution of excitation free energies, $F=\Delta$, with nonvanishing density at $\Delta\to 0$ and characteristic scale $F\sim L^\theta$ for large length scale L. The exponent θ, which lies in the range $0<\theta\leq(d-1)/2$, is minus the renormalization-group eigenvalue of temperature at the nontrivial zero-temperature fixed point governing the spin-glass phase. In our picture, these droplet excitations are two-level systems with barriers which scale as L^ψ for large L, where $\theta\leq\psi\leq(d-1)$. Therefore the temperature at which the droplets at length scale L fall out of equilibrium is $\tilde{T}(L)\sim L^\psi/\ln\tau$.

In considering the effects of large droplets there are several subtleties which must be taken into account. The most important is the temperature dependence of the droplets' free energies. The droplet free energy is, by $F=E-TS$, a difference of energy and entropy terms which individually can be much larger than the free energy. For a given droplet of size L, at sufficiently low temperatures the energy term dominates and the lower *free*-energy level of the TLS corresponds to the true $T=0$ ground state. However, at low temperatures the entropy difference between the two levels is a sum, over sections of the domain wall surrounding the droplet, of roughly independent random terms, and hence scales as $S\sim T^{n-1}L^{d_s/2}$ for small T and L. This entropy is important for large enough L, since the fractal dimensionality of the domain wall, d_s, lies in the range $d-1\leq d_s\leq d$ and thus $d_s/2\geq\theta$.[2] For spin-glasses with a continuous distribution of exchanges the entropy of the domain wall arises from a distribution of small-scale two-level systems on the domain wall so that the exponent $n=2$, while for discrete distributions (e.g., $\pm J$) there is a nonzero entropy at $T=0$ so that $n=1$. The temperature $T_S(L)$ at which the entropy term starts to play an important role in the determination of the free energy is therefore given by $L^\theta \sim T_S^n L^{d_s/2}$. For higher temperatures $T > T_S(L)$ the lower *free*-energy level of the TLS has a probability of order $\frac{1}{2}$ is *not* being the ground state. Therefore, a droplet of length scale L such that the temperature at which it falls out of equilibrium $\tilde{T}(L) \gtrsim T_S(L)$ is just as likely to end up in its excited state after cooling to $T=0$ as in its ground state. The amount of residual energy per spin in such droplets is $\epsilon(\tau) \sim L^{\theta-d}$, and so is dominated by the smallest such L, for which $\tilde{T}(L) \sim T_S(L)$. These frozen-in droplets, which are large for slow cooling rates, contribute to the residual energy an amount of order $(\ln\tau)^{-\zeta}$, where $\zeta = n(d-\theta)/(d_s/2+n\psi-\theta)$. For a continuous distribution of exchanges these large-scale effects may or may not dominate over the small TLS with $\zeta=2$ and so we have Eq. (1), with

$$\zeta = \min[2, 2(d-\theta)/(d_s/2+2\psi-\theta)],$$

while for a discrete distribution there is no $(\ln\tau)^{-2}$ contribution from the small TLS and $\zeta=(d-\theta)/(d_s/2+\psi-\theta)$.

Spin-glasses with $T_c=0$.—It is now relatively well established that in two dimensions there is no spin-glass phase at nonzero temperature.[5] There does, however, exist a critical point at $T_c=0$ with a diverging correlation length $\xi \sim 1/T^\nu$, at least when there is a continuous distribution of exchanges. In this case, droplet excitations should be well defined for scales $L < \xi$, and their free energies scale as L^θ, with $\theta = -1/\nu < 0$. These have arbitrarily low energies and may have surfaces with fractal dimension $d_s = d$. However, it is possible, although by no means clear, that the barrier exponent ψ is still positive (this occurs even in one dimension if there is a power-law tail of the distribution of exchanges J at large J), in which case the equilibration time diverges as $\exp(T^{-1-\nu\psi})$. If $\psi > 0$, then the large droplets again fall out of equilibrium at a temperature $\tilde{T} \sim L^\psi/\ln\tau$. The same arguments as used above for $T_c > 0$ apply here, which yields

$$\zeta = \min[2, 2(d-\theta)/(d_s/2+2\psi-\theta)].$$

If $\psi=0$, we have $\zeta=2$ from the small TLS. It is not clear at this point what happens in the discrete case, $\pm J$, when $T_c=0$.

Random-field magnets.—In random-field Ising magnets (realized experimentally, for example, by diluted antiferromagnets in a field[6]) there is frustration induced by the competition between the exchange and the random field.[7] For continuous distributions of the disorder, this leads to small TLS with arbitrarily low excitation energies consisting of clusters for which the random field almost exactly balances the exchange energy of flipping the cluster. Thus we again have the bound $\zeta \leq 2$.

As for the spin-glass case, we must also consider the effects of large-scale nonequilibrium effects. These are especially important in dimensions $d > 2$, where for weak disorder it has recently been proven that there exists long-range ferromagnetic order.[8] We will restrict our discussion to $d > 2$ and the regime of random-field strengths for which the ferromagnetic phase exists.

In contrast to spin-glasses, large low-free-energy droplet excitations are very rare in the ordered phase of random-field magnets[3] and they would not play an important role if the system were initially in equilibrium with $T(0) < T_c$. However, as has become apparent over the past few years, the random fields make the time scales for the establishment of the long-range order extremely long when the system is cooled from the paramagnetic phase.[9] For temperatures below T_c, Villain, Grinstein, and Fernandez[9] have argued that because of the barriers to motion of domain walls, the characteristic domain size, L, grows with time as $L \sim \ln t$. Villain and Fisher[10] have analyzed the behavior near the critical point and found that the characteristic scale on which equilibrium is attained also grows logarithmically at T_c as $L \sim (\ln t)^{1/\theta}$, where the exponent θ describes the violation of hyperscaling via $(d-\theta)\nu = 2-\alpha$.[10]

We are interested in the effects of cooling through T_c to $T=0$ in a time τ. From the above discussion it can be seen that there are domain walls frozen in with a characteristic separation, L, which is $(\ln\tau)^{\max(1,1/\theta)}$. It is likely that θ is greater than 1 in all dimensions[10,11] $(d > 2)$ and hence we find that the energy density frozen in the domain walls, which is proportional to $1/L$, yields $\epsilon(\tau) \sim 1/(\ln\tau)$; i.e., $\zeta=1$.

Bond-disordered ferromagnets.—Ferromagnets with a continuous distribution of exchanges J have small TLS with a positive density of states at $\Delta=0$ if the couplings can be negative, which causes frustration and logarithmic decay of $\epsilon(\tau)$ with $\zeta=2$. If all the couplings are nonnegative, but with the distribution extending down to zero, there is still a logarithmic decay of the residual energy, even though this unfrustrated case has a trivial ferromagnetic ground state. However, ζ depends on the distribution of couplings. If there is a minimum $J > 0$, on the other hand, $\epsilon(\tau)$ varies as a power of τ.

Huse and Henley[12] have argued that even weak bond disorder causes domains to grow logarithmically with time following a *quench* to below T_c. However, in contrast to the random-field case, the equilibration times near T_c grow as a power of the length scale so that rapid growth of the domains near T_c as the system is slowly cooled yields a domain size proportional to a power of τ. Thus, in bond-disordered ferromagnets there is no logarithmic contribution to $\epsilon(\tau)$ arising from large-scale nonequilibrium effects.

Conclusions.—We have shown that logarithmic dependence of the residual energy on the cooling rate is a generic property of disordered systems with frustration. In some systems, the behavior is dominated by small low-energy excitations, while in others, large-scale nonequilibrium effects are more important. We expect the results to apply also to frustrated Heisenberg magnets and other systems with continuous symmetry, since these systems have defect excitations which play a similar role to the droplets in Ising systems.[2,13]

Contrary to speculation,[1] there should not be a direct correlation between the dynamics upon slow cooling and whether or not the corresponding ground-state problem is *NP*-complete. In particular, one- and two-layer $d=2$ Ising spin-glasses should behave similarly, although the former corresponds to a polynomially solvable ground-state problem while the latter is *NP*-complete.[14] (Grest, Soukoulis, and Levin[1] have found that Monte Carlo data for one-layer spin-glasses fit better to a power law than to $(\ln\tau)^{-1}$; however, the power-law fits work only over a factor of less than 3 in $\epsilon(\tau)$ and the exponent is small, so that the results are consistent with the logarithmic law we propose.) In addition, random-field systems, whose ground states can be found in polynomial time,[15] also show logarithmic behavior of the residual energy. Thus logarithmic dynamics does not imply *NP*-completeness. The reason for the absence of a connection should be clear: For the nontrivial polynomial problems, the algorithms that can find the ground state in polynomial time bear no resemblance to Monte Carlo or physical dynamics. However, there is a connection in the opposite direction: *NP*-complete problems must have slower than power-law relaxation with *any* dynamics.[1]

We note that the analysis we have presented here yields new predictions about nonequilibrium behavior of the energy in various frustrated systems. Nonequilibrium scaling arguments of the sort used here may well be useful for analysis of nonequilibrium experiments in spin-glasses and other frustrated systems.

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