Approach to the ground state in disordered magnetic systems: Simulated annealing study

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We present results of detailed simulated annealing studies on several models of bond-disordered Ising ferromagnets in two dimensions, both with distribution of couplings extending down to zero and with a cutoff greater than zero in the distribution. We find that in each of these cases the residual energy after cooling, $\Delta E(r)$, can be represented as a power law of the cooling rate r, i.e., $\Delta E(r)=Ar^x$. Results for the cooling-rate dependence of the magnetization, $M(r)$, are also discussed.

In spin-glasses and other disordered magnetic systems, the cooling-rate dependence of the residual energy, left after cooling to zero temperature in a finite time, is the subject of many recent studies.[1] Since the equilibrium low-temperature behavior in these systems is quite often inaccessible in experiments or in computer simulations, the nonequilibrium dynamics as a function of cooling rate invites a lot of attention.[2] Also, the concept of simulated annealing[3] and the need to find efficient numerical optimizaton schemes[4] seem to play a key role in the added interest in the problems mentioned above. Starting at high temperature T_0 and cooling slowly, significant improvement over more conventional optimization techniques was obtained for a variety of problems.[1,3,5,6]

Grest *et al.*[1] have numerically studied the residual energy after cooling, $E(r)$, of several Ising spin-glass models as a function of cooling rate r. They have found that for the one-dimensional nearest-neighbor Gaussian and two-dimensional models, the nearest-neighbor Gaussian and $\pm J$ models $E(r)=E_0+C_1r^x$, while for the three-dimensional $\pm J$ model and the infinite-range model, $E(r)\approx E_0+C_2(\ln r)^{-1}$, where C_1 and C_2 are constants and E_0 is the (unknown) energy of the true ground state. The authors interpreted that the logarithmic cooling-rate dependence seen in some of the models considered above arise from the fact that in these problems finding the ground-state energy is nonpolynomial (NP) complete.[7] On the other hand, an analytical study[2] based on the assumption that the relaxation in these systems is dominated by a distribution of classical two-level systems with low-energy excitations, predicts that the generic small-r behavior for frustrated systems is

$$\Delta E(r)\approx(\ln r)^{-\zeta}\ , \tag{1}$$

where $\Delta E(r)=E(r)-E_0$. This study is also extended to the case of bond-disordered ferromagnets with a continuous distribution of couplings (J_{ij}) with the prediction that if all the couplings are non-negative, but the distribution extends down to zero, Eq. (1) still remains valid, even though this unfrustrated system has a trivial ferromagnetic ground state. However, when the distribution of couplings is such that there is a minimum $J_{ij}>0$, $\Delta E(r)$ should vary as a power of r.

The power-law behavior seen by Grest *et al.*[1] in two-dimensional spin-glass models seems to work only over a factor of less than 3 in $\Delta E(r)$ with a small exponent and could be consistent with the logarithmic law [Eq. (1)]. Also, in these systems the ground-state energy is not known exactly and hence one needs an extra parameter for the fitting procedure which makes it more difficult to numerically extract the correct behavior. We believe that the bond-disordered Ising ferromagnets would be better systems to study, since for these systems one knows the exact ground-state energy.

In this paper we present results of detailed simulated annealing studies on several models of bond-disordered Ising ferromagnets, both with distribution of couplings extending down to zero and with a cutoff $J_{ij}>0$ in the distribution. We find that in each of these cases the residual energy $\Delta E(r)$ can be represented as a power law of r, namely,

$$\Delta E(r)=Ar^x\ , \tag{2}$$

where the exponent x is larger in the cutoff case.

The Hamiltonian of the system is given by

$$H=-\sum_{\mathrm{NN}}J_{ij}\sigma_i\sigma_j \tag{3}$$

and $\sigma_i=\pm1$. The coupling constants J_{ij} are given in terms of a probability distribution function $P(J_{ij})$ which characterizes the model. In this paper we have considered three different forms for $P(J_{ij})$: (A) a Gaussian distribution with mean zero and variance unity folded about zero (the mean value of J_{ij} in this case is $\sqrt{2/\pi}$), (B) the same distribution as (A) displaced by an amount 0.5 so that the mean value of J_{ij} is $0.5+\sqrt{2/\pi}$, and (C) a uniform distribution between 0 and 1. For each of these distributions we have computed the cooling-rate dependence of energy $E(r)$ and magnetization $M(r)$ by performing a simulated annealing study. In all the cases we consider a square lattice with periodic boundary conditions and linear dimension $L=200$. In order to check that our results are not subjected to finite-size effects, we have performed in some cases test runs with $L=100$ and $L=400$ with the same results for $E(r)$. In fact, we found that the final energy is a self-averaging quantity[8] and

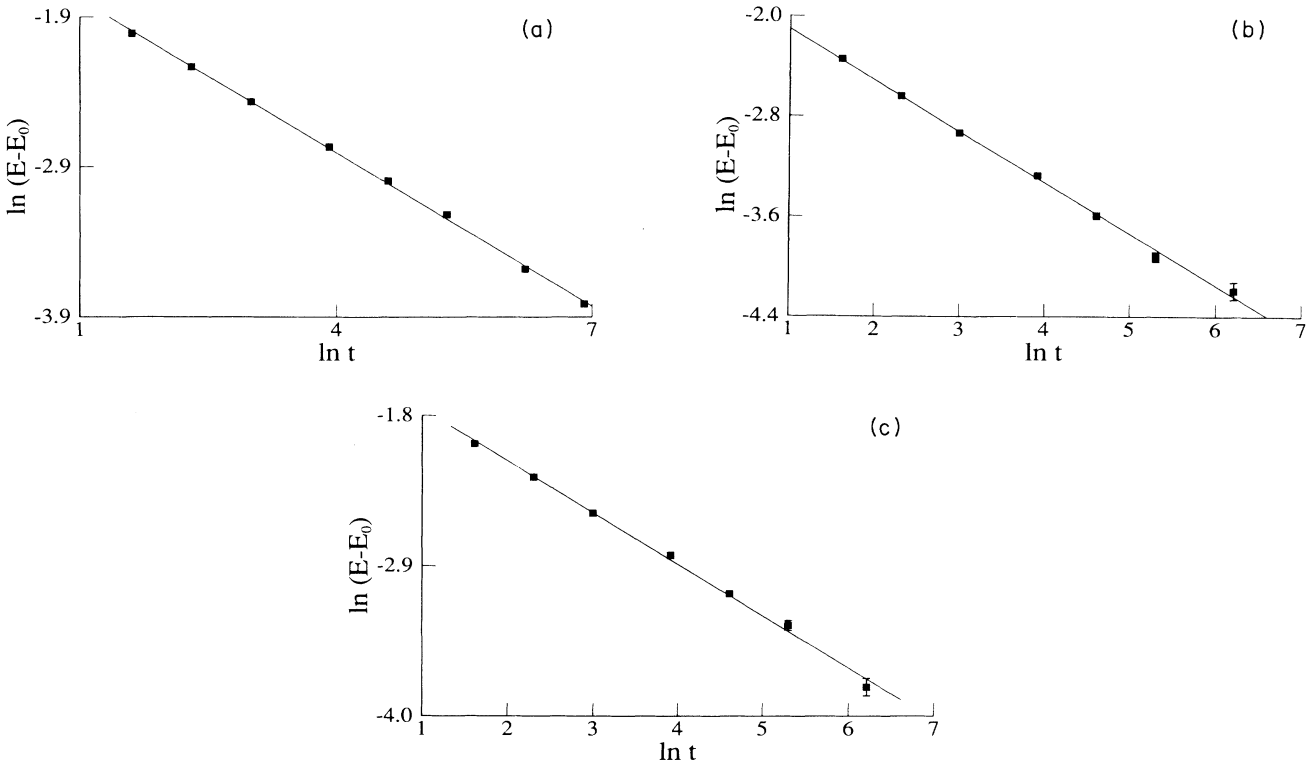

FIG. 1. (a) Log-log plot of the residual energy $E(t)-E_0$ for distribution (A) of couplings plotted against the annealing time t to verify the form (2). The solid line is the best fit to the data. The slope of this line gives a value of 0.340(5) for the exponent x. In this figure and in other figures the size of the symbol is greater than the error bars when the latter are not shown. (b) Same as (a) for distribution of couplings (B). The exponent x here is 0.41(1). (c) Same as (a) for distribution of couplings (C). The exponent x here is 0.38(1).

there is no advantage in computer time when using either smaller systems (which could lead, on the other hand, to finite-size effects) or larger systems (since a minimum number of measurements is required in order to be able to apply statistical methods). The initial starting temperature T_0 has been chosen for each distribution such that the relaxation time is small at that temperature and the final energy after cooling does not depend on it. For distributions (A) and (C) we use $T_0=2.0$ and for distribution (B), $T_0=3.0$. We used a temperature decrement $\Delta T=0.1$ and we have checked that smaller values of this quantity (with a constant cooling rate) do not affect the final energy. Since the cooling rate is defined as $r=\Delta T/t$ where t is the annealing time (number of Monte Carlo steps spent at every temperature) and ΔT is a constant throughout our calculation, the results can be expressed either as a function of the cooling rate r or the annealing time t, with $t=\Delta T/r$. Our results for $E(t)$ and $M(t)$ are summarized in Table I. In this table and in the following figures the energies for all the distributions have been normalized in such a way that the energy of the ground state is -2. This makes it easier to compare energy values for the different distributions.

The cooling-rate dependence of the ground-state energy for distributions (A), (B), and (C) are presented in Figs. 1 and 2. For each of these distributions we show a log-

TABLE I. Values for the energy and magnetization for a 200×200 system after annealing through t Monte Carlo steps and $\Delta T=0.1$ for distributions (A), (B), and (C) of couplings. The statistical errors shown in parentheses are obtained after averaging over N configurations of J_{ij}.

	Distr. (A)			Distr. (B)			Distr. (C)		
t	N	$-E$	$\lvert M\rvert$	N	$-E$	$\lvert M\rvert$	N	$-E$	$\lvert M\rvert$
5	250	1.865 79(26)	0.0426(21)	150	1.903 51(40)	0.0815(47)	50	1.865 50(70)	0.0569(63)
10	100	1.892 53(41)	0.0590(46)	100	1.928 13(51)	0.1137(85)	30	1.894 54(79)	0.0546(79)
20	100	1.914 97(43)	0.0698(47)	100	1.946 58(52)	0.147(11)	30	1.918 88(70)	0.071(12)
50	50	1.937 06(44)	0.0891(93)	50	1.962 03(69)	0.170(20)	20	1.940 5(11)	0.108(19)
100	50	1.949 91(59)	0.107(11)	50	1.972 53(72)	0.269(29)	20	1.955 2(10)	0.141(29)
200	50	1.959 99(48)	0.143(16)	50	1.980 20(73)	0.388(37)	20	1.964 5(13)	0.166(39)
500	25	1.972 16(57)	0.206(28)	25	1.984 9(10)	0.456(70)	15	1.977 4(14)	0.326(63)
1000	25	1.977 91(67)	0.237(31)						

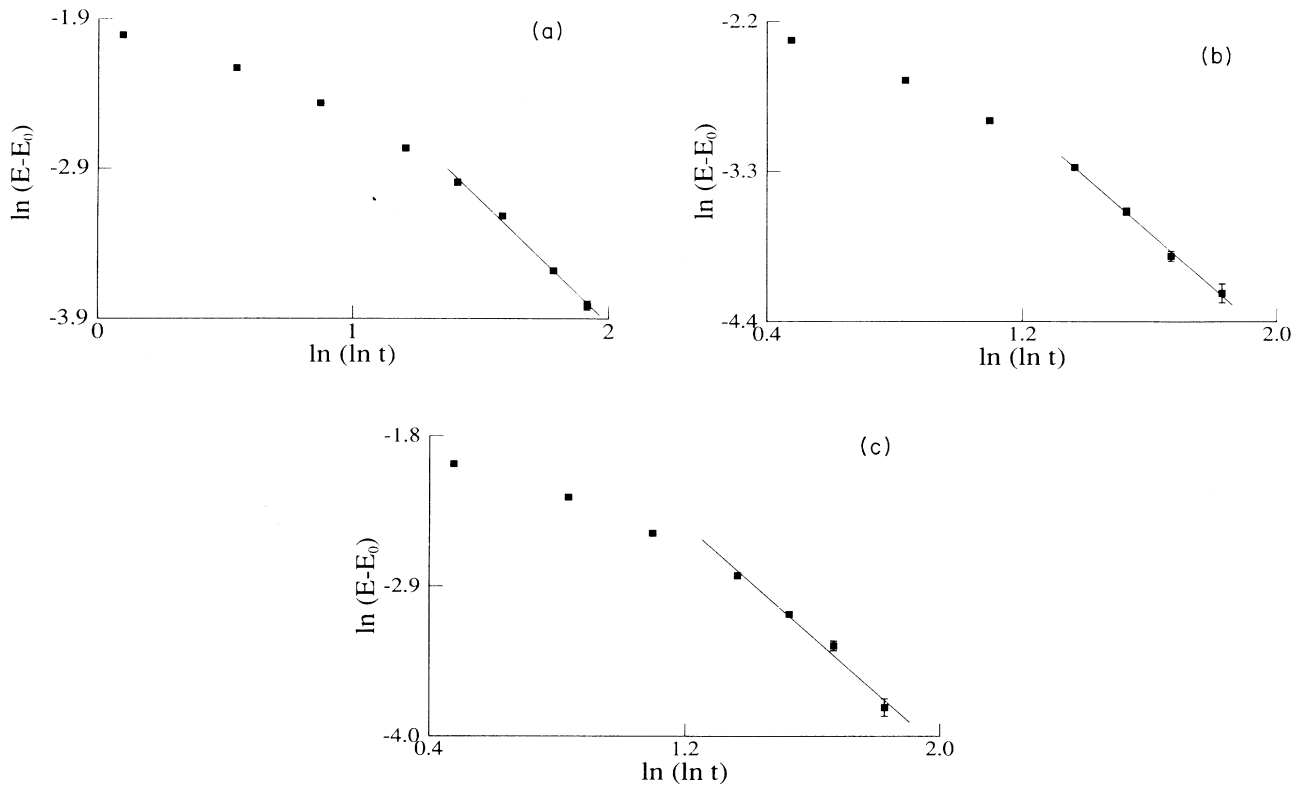

FIG. 2. (a) Plot of the logarithm of the residual energy $E(t)-E_0$ vs the double logarithm of annealing time t for distribution (A) of couplings. The form (1) predicts that this plot should be a straight line with slope $-\zeta$. The attempted fit of the last four points yields $\zeta \approx 2$. (b) Same as (a) for distribution of couplings (B). In this case also the attempted fit of the last few points to form (1) yields $\zeta \approx 2$ although there is no theoretical basis for form (1) to hold in this case. (c) Same as (a) for distribution of couplings (C). The exponent ζ here again is ≈ 2.

log plot of $\Delta E(t)$ versus t in Figs. 1(a), 1(b), and 1(c), respectively, to compare with functional form (2). It seems clear from these figures that a power law is a good description of the data in every case over the whole range of t values considered here. The exponent x of Eq. (2) has been calculated by a least squares fit to the data and is given by $x=0.340(5)$ for distribution (A), $x=0.41(1)$ for distribution (B), and $x=0.38(1)$ for distribution (C). It is interesting to note that the exponent x is larger in distribution (B) when compared to the exponent in distribution (A) and that they are both larger than the exponent found for the spin-glass model in two dimensions with a full Gaussian distribution of couplings.[1] Although these results support functional form (2), we plot $\ln\Delta E(t)$ versus

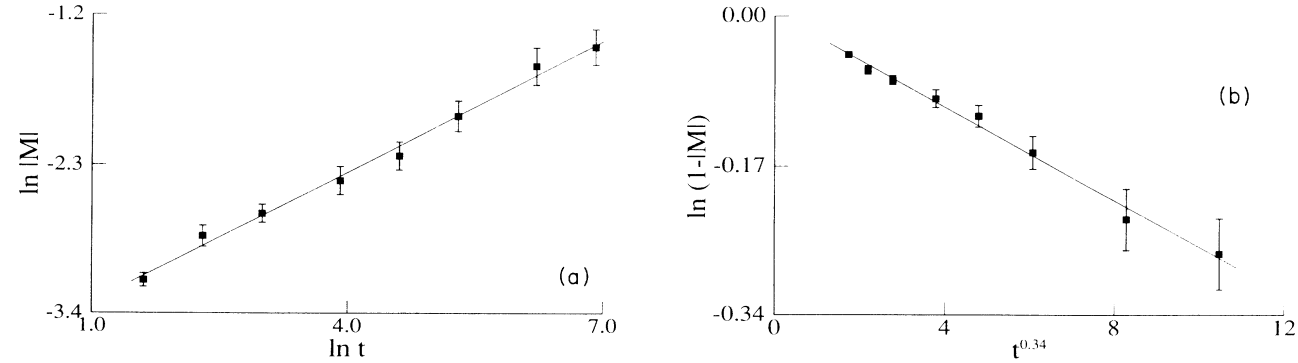

FIG. 3. Logarithm of the magnetization, $|M(t)|$ for distribution (A) of couplings and a 200×200 system plotted against the logarithm of annealing time t. The solid line is the best fit to the data. The slope of this line gives a value of 0.32(3) for the exponent x. This exponent is equal within error to the one obtained in Fig. 1(a) for the residual energy. (b) Logarithm of the residual magnetization, $1-|M(t)|$ for distribution (A) of couplings and a 200×200 system plotted against the power of annealing time $t^{0.340}$, which is the same power obtained in Fig. 1(a) for the residual energy. The solid line is the best fit to the data.

$\ln(\ln t)$ for each of the distributions in Figs. 2(a), 2(b), and 2(c) to explicitly check functional form (1). We note that the last few points of Figs. 2(a) and 2(c) are somewhat consistent with functional form (1) with an exponent $\zeta \approx 2$ which is close to the upper bound on ζ found in Ref. (2) for several frustrated systems. However, this seems to be also true for Fig. 2(b) where functional form (1) is not supposed to hold. Although this could be an indication that we are not yet in the asymptotic regime where Eq. (1) should hold, our data for $\Delta E(t)$ covers almost a factor of 7 and extrapolates smoothly to zero in the infinite-annealing-time limit when fitted to form (2).

We now present the results for the cooling-rate dependence of the residual magnetization. We have found that the magnetization per spin $M(r)$ is system size dependent and actually goes as $1/L$, where L is the linear dimension of the system. One can understand that by a simple domain argument;[9] if domains of linear size $R(r)$ are left when T goes to zero, the total magnetization per domain is approximately R^2, and the number of domains is of the order $(L/R)^2$. Then the final magnetization per spin is of the order of R/L. One also finds from a similar argument that $\Delta E(r) \approx 1/R$ in that case. Then one expects that $|M| \approx 1/\Delta E$ and consequently exhibits a power-law behavior as shown in Fig. 3(a). However, this relation should break down when ΔE goes to zero since $|M|$ is bounded from above by unity. We have found that an empirical fit such as a stretched exponential $|M(r)| = 1 - e^{-\alpha r^{-x}}$ fits the data for $|M|$ over the whole range of annealing time as shown in Fig. 3(b). This empirical fit reduces to the power-law behavior when $|M|$ is small and has also the correct limit when $t \to \infty$. Similar behavior is seen for distributions (B) and (C).

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