Numerical simulations and exactly soluble spin-glass models

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(Received 8 November 1984)

Some general arguments based on recent numerical work are presented to explain the different behavior of short-range, random-bond and long-range, random-site spin glasses. We then analyze an exactly soluble spin-glass model, which may be solved without replicas, and show that, except for the absence of microscopic metastable states, its main features are consistent with the long-range picture.

Over the past few years considerable effort has been devoted to modeling the spin-glass transition and the spin-glass phase. Both short-range[1–5] and long-range[6,7] interactions have been studied intensely but, up to recently, only an infinite-range model, proposed by Sherrington and Kirkpatrick (SK),[8] was amenable to an "exact" solution.[9–12] However, the dispute originated by that solution still continues.

Recently one of us[13,14] has proposed a new, exactly soluble spin-glass model which contains both randomness and frustration but whose solution can be obtained *without* replicas. Like SK, it is a mean-field model. For suitable probability distributions of the coupling constants, it reproduces the well-known plateau[15] in the zero-field susceptibility for $0 \leq T \leq T_f$ and many other experimental characteristics of a field-cooled spin glass. Since exactly soluble, realistic, spin-glass models are rare, it is of prime importance to probe their microscopic phase-space structure and see whether or not this structure is consistent with the underlying physical reality one wants to model. In this paper we aim at providing such a test. We first discuss the model proposed in Ref. 13 and then comment briefly on the SK model.

We consider the following Hamiltonian $[S(i)=\pm 1]$:

$$\mathscr{H}_N = -\frac{1}{2}\sum_{\substack{i,j\\(i\neq j)}} J_{ij}S(i)S(j) - h\sum_i S(i) \ , \tag{1}$$

mostly with $h=0$. The phase space is the set of all $(\pm)$ configurations. The coupling constants J_{ij} are random variables and we first consider two typical cases.

(a) The J_{ij}'s are independent, identically distributed random variables which are nonvanishing only if $|i-j|=1$. This is a *random-bond* problem. One usually takes their distribution as Gaussian or $\pm J$ with equal weight.

(b) The spins interact via a Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, but their *positions* are random.

For these two types of interaction the following picture has emerged. The phase space of a spin system with frustrated short-range interactions consists of hills and valleys. As the temperature is lowered and passes through T_f, the system is supposed to get caught in one of the valleys. The valleys label the different low-temperature phases, which are separated by hills whose height is considerable but remains *finite* as $N\to\infty$, where N is the size of the system. For the two-dimensional $\pm J$ model[2,3] $T_f \approx 1.3J$ and the hills have a height $H\approx 15J$. So $T_f \ll H$. If one flips the spins inside a so-called zero-energy loop, one transforms the state of the system from one valley into a neighboring one.

The situation for spin systems with RKKY interactions (and anisotropy) looks rather different.[6,7] The components,[16] or valleys, are separated by (free) energy barriers which may get infinitely high as $N\to\infty$, so that the system exhibits a phase transition at a positive T_f. Inside a valley we have many small hills and valleys. Traveling from one little valley to a neighboring one by inverting the spins in a small defect region now means climbing a hill whose height H mostly does not exceed T_f; i.e., $T_f\approx H$. We show that the model under consideration corresponds to this second category.

The mean-field model we wish to study has coupling constants J_{ij} which are given by

$$J_{ij} = \frac{J}{N}(\xi_i\eta_j + \xi_j\eta_i) \ , \tag{2}$$

where the ξ_i's and η_j's are independent, identically distributed random variables with even distribution around zero and a finite variance, say, one. The J_{ij}'s ought to model the RKKY interaction in a metallic spin glass. Binder and Schröder[17] have shown that the *form* of the distribution of the RKKY coupling constants is symmetric and highly peaked at zero, because the long range of the potential samples many small J_{ij} values. This justifies taking ξ's and η's with a *continuous* probability distribution, peaked at zero, say, Gaussian. We assume this distribution throughout what follows.

As $N\to\infty$, the model has three order parameters,

$$m_N = N^{-1}\sum_{i=1}^N S(i), \quad q_{1N} = N^{-1}\sum_{i=1}^N \xi_i S(i) \ ,$$
$$q_{2N} = N^{-1}\sum_{j=1}^N \eta_j S(j) \ , \tag{3}$$

which have to be chosen in such a way that $\mathbf{m}=(m,q_1,q_2)$ minimizes a certain free-energy functional. Then q_1 and q_2 can be shown to agree.[14] Here $m=0$, so we are left with one order parameter. The number of independent random variables is $2N$ in contrast with the $\frac{1}{2}N^2$ of SK. Thus we have—in agreement with the experimental situation—a random-site problem and not a random-bond problem as in most other models.

The relevant order parameter Q, from which other thermodynamic quantities can be obtained, such as the mean energy and specific heat, is given by

$$Q=\left\langle N^{-1}\sum_{i=1}^{N}\tfrac{1}{2}(\xi_i+\eta_i)S(i)\right\rangle_T \ . \tag{4}$$

The angular brackets denote a *thermal* average which is to be obtained by means of a Monte Carlo (MC) simulation. In Fig. 1 we show both the analytical solution of Q (full line) and the data obtained by MC simulation. Since $J=1$, the critical temperature T_f equals 1.

The simulations were carried out in the following way. We started with an arbitrary spin configuration at $T=1.3$, well above the critical temperature. Then we cooled the sample in intervals of $\Delta T=0.1$ with an average cooling time $\Delta t=200$ Monte Carlo steps per spin (MCS). We report results for different systems with size $N=200$, 400, and 800. Upon cooling, the system has some troubles around T_F but then it surprisingly follows the analytical (equilibrium) solution. As seen in Fig. 1, the numerical values approach the analytical solution in the critical region around T_f if the number of spins increases. Lowering the temperature further we reach a ground state. If we warm the system up, it follows the analytical curve again. Cooling down once again we obtain the same behavior, but in some cases the simulations give negative values of Q, indicating that inverted spin configurations are reached. This behavior is quite different from that in, say, the $\pm J$ model, where a comparable number of spins gives rise to cooling times exceeding 250 000 MCS if one wants to reach a ground state. Equilibrium values are either only reached in very long MC simulations, or never reached.[9] Thus the behavior of the present model is very surprising. It suggests that the phase space consists of some big valleys separated by high mountains (which become infinitely high as $N\rightarrow\infty$) and inside a valley the surface is relatively flat.

Further support of this picture was provided by another numerical experiment. We again started with an arbitrary spin configuration, but now at $T=0.1$. After about 200 MCS (a rather small number) we reach a ground state. In most other frustrated models this is simply impossible. Analyzing the low-temperature spin configurations, the above interpretation was confirmed. Whereas in frustrated short-range models we have quite a few microscopic, metastable states where the system may be frozen in, we now have only *two* valleys in phase space (Ising model with spin-flip symmetry). In the thermodynamic limit these two valleys are separated by infinitely high (free) energy barriers and the ergodicity is broken; we have a phase transition.[16] The expectation value in (5) is taken with respect to one component. The usual metastable states do not exist. This does not mean, of course, that the model does not have metastable *thermodynamic* states. Moreover, note that there are many low-lying excited states since the low-temperature specific heat is linear in T (Fig. 3).

Full results are presented for the internal energy (Fig. 2) with $N=800$ and the specific heat (Fig. 3) with $N=400$. The analytical solution is again indicated by a full line and

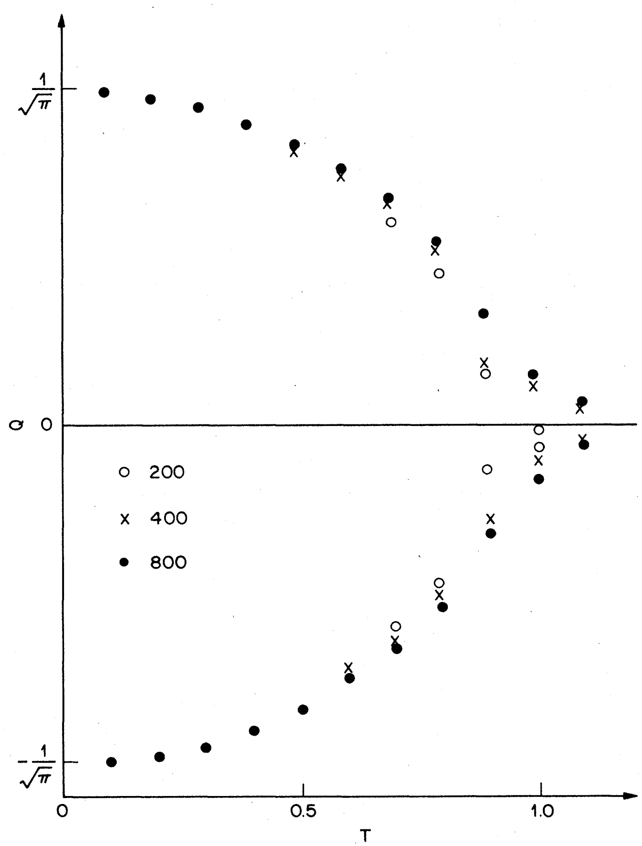

FIG. 1. Order parameter

$$Q=\left\langle N^{-1}\sum_{i}\tfrac{1}{2}(\xi_i+\eta_i)S(i)\right\rangle_T$$

vs temperature T for various system sizes.

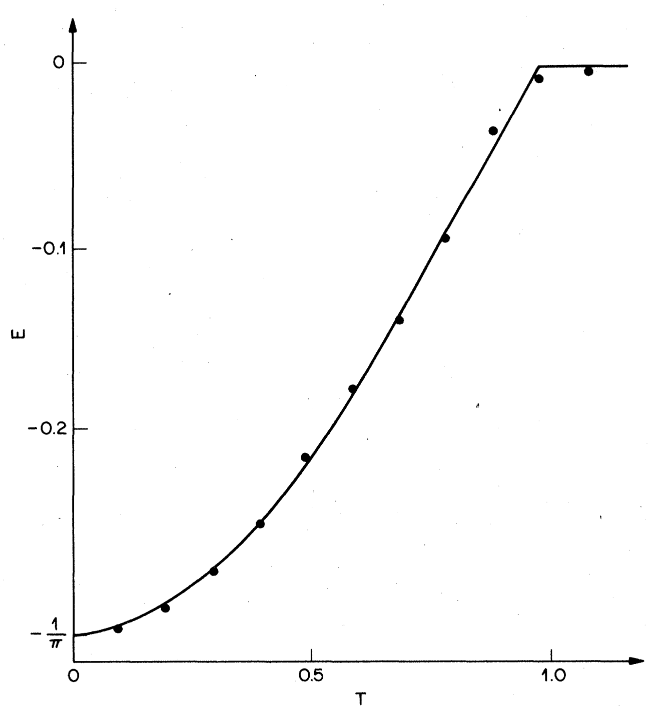

FIG. 2. Internal energy E vs temperature T for an $N=800$ system. The full line corresponds to the analytic solution.

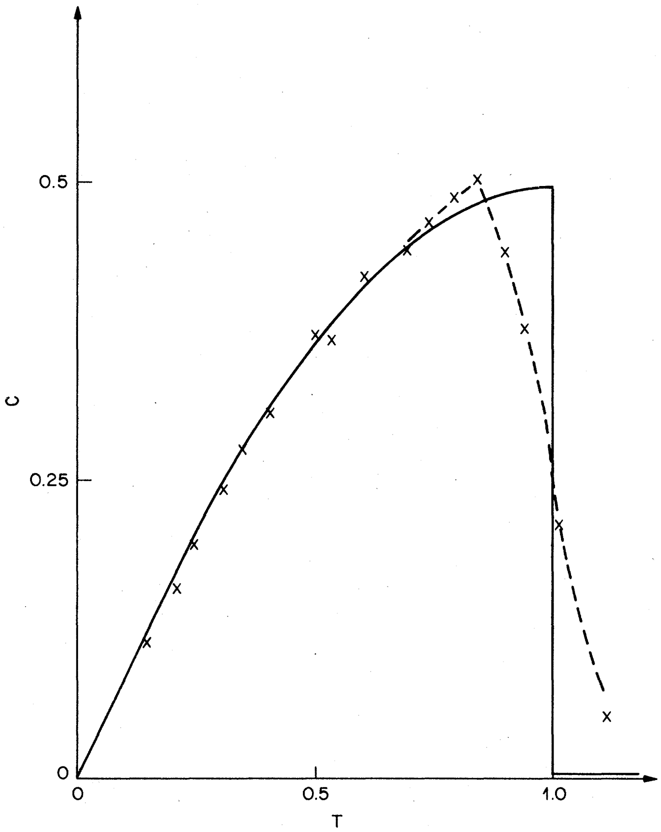

FIG. 3. Specific heat C (broken line) vs temperature T for an $N=400$ system. The full line is the analytic solution. The low-temperature specific heat is *linear* in T, indicating the existence of many low-lying excited states.

we note that the agreement is rather good except for the specific heat near T_f where the MC procedure breaks down. Increasing the time Δt to 1000 MCS we nevertheless found a fair overall agreement. But it is clear that the present simulations fully confirm the analytical solution of the model as given in Refs. 13 and 14. As to Figs. 1 and 2, similar results were obtained for the case where ξ and η are taken as ± 1 with equal probability.

In conclusion, frustrated short-range systems with bond disorder have many ergodic components which are separated by free-energy barriers whose height H remains finite as $N \rightarrow \infty$. Nevertheless, H is relatively large ($H \approx T_F$) so that at *low* temperatures these systems are in quasiequilibrium. One goes from one component to a neighboring one by flipping spins inside a certain contour.[3] Below T_f, long-range RKKY systems have a few ergodic components separated by infinitely high free-energy barriers and, hence, allow an equilibrium phase transition. Inside a component we have many small valleys separated by barriers whose height H is about T_f, thus accounting for metastability. Here, too, one may go from one valley to a neighboring one by flipping some spins in a defect region.[6] Plainly, mean-field models are not expected to reproduce this soft, local structure. Their first and foremost task is to reproduce thermodynamic behavior and this is what the model under consideration does—and it does so pretty well.[14] The MC data are in surprisingly good agreement with the analytical results, even for very short observation times. Cooling and warming experiments indicate that there are *no* microscopic metastable states. We have finitely many valleys, with quite a few low-lying excited states, separated by infinitely high free-energy barriers. In a sense, the phase space of the model agrees rather well with the above picture for RKKY interactions with *site* disorder. The appropriate analytical description of this type of disorder in spin glasses is still an open problem, however.

The SK model[18] exhibits qualitatively the same behavior as the previous model. As $N \rightarrow \infty$, the valleys which are relevant to thermodynamics do not contain finite-energy barriers and are relatively flat. The freezing which is suggested by Sompolinsky's theory[12] exists only in the case of *finite N*.

We gratefully acknowledge many stimulating discussions with several participants of the Heidelberg Colloquium on Spin-Glasses. We also thank J. Canisius and A. C. D. van Enter for their help and advice. J.L.H. acknowledges the support of the Deutches Forschungsgemeinschaft under Sonderforschungsbereich 123, Universität Heidelberg, 6900 Heidelberg, Federal Republic of Germany.

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[1]S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

[2]I. Morgenstern and K. Binder, Phys. Rev. Lett. **43**, 1615 (1979); Phys. Rev. B **22**, 288 (1980); Z. Phys. B **39**, 277 (1980).

[3]I. Morgenstern and H. Horner, Phys. Rev. B **25**, 504 (1982).

[4]I. Morgenstern, J. Appl. Phys. **53**, 7682 (1982); Phys. Rev. B **27**, 4522 (1983).

[5]A. P. Young, Phys. Rev. Lett. **50**, 917 (1983).

[6]R. E. Walstedt and L. R. Walker, Phys. Rev. Lett. **47**, 1624 (1981).

[7]R. E. Walstedt, in *Heidelberg Colloquium on Spin-Glasses*, edited by J. L. van Hemmen and I. Morgenstern (Springer-Verlag, Berlin, 1983).

[8]D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1792 (1975); S. Kirkpatrick and D. Sherrington, Phys. Rev. B **12**, 4384 (1978).

[9]N. D. Mackenzie and A. P. Young, Phys. Rev. Lett. **49**, 301 (1982).

[10]A. P. Young, in Ref. 7.

[11]G. Parisi, J. Phys. A **13**, L115 (1980); Philos. Mag. B **41**, 677 (1980).

[12]H. Sompolinsky, Phys. Rev. Lett. **47**, 935 (1981); H. Sompolinsky and A. Zippelius, Phys. Rev. B **25**, 6860 (1982).

[13]J. L. van Hemmen, Phys. Rev. Lett. **49**, 409 (1982).

[14]J. L. van Hemmen, A. C. D. van Enter, and J. Canisius, Z. Phys. B **50**, 311 (1983).

[15]S. Nagata, P. H. Keesom, and H. R. Harrison, Phys. Rev. B **19**, 1633 (1979).

[16]R. G. Palmer, Adv. Phys. **31**, 669 (1982); A. C. D. van Enter and J. L. van Hemmen, Phys. Rev. A **29**, 355 (1984).

[17]K. Binder and K. Schröder, Phys. Rev. B **14**, 2142 (1976).

[18]A. P. Young (private communication).