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Phase transitions of a nearest-neighbor Ising-model spin glass

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Monte Carlo calculations exhibit a critical point in square $S = 1/2$ Ising lattices with random nearest-neighbor interactions, which are distributed according to a Gaussian with mean zero and width ΔJ, at $\Delta J/k_B T_c \simeq 1.0$. The susceptibility χ has a cusp there, while the specific heat C has a broad peak with a maximum at somewhat higher temperatures. In nonzero external fields H the cusp of the susceptibility is rounded off, in qualitative agreement with experimental observations. Below T_c, hysteresis is found, but the remanent magnetization decays to zero very slowly. Similar nonexponential decay with time is also found for the autocorrelation function $\langle \sigma_i(0)\sigma_i(t)\rangle$. Some qualitative information on the occurrence of correlated spin clusters and their kinetics is also given.

I. INTRODUCTION

If magnetic ions (e.g., Fe) are diluted at random in a nonmagnetic metallic matrix (e.g., Au) at low concentrations ($\lesssim 1\%$), a new type of magnetic phase occurs,[1,2] which is neither ferromagnetic nor antiferromagnetic but is nevertheless characterized by some sort of ordering since a rather sharp cusp in the zero-field susceptibility is found at a freezing temperature T_c. It is believed that due to the oscillating nature of the long-range Ruderman-Kittel-Kasuya-Yosida[3] (RKKY) exchange interactions the spins interact with randomly competing forces and are frozen in below T_c (i.e., in the spin-glass state) in random directions. These systems have found enormous recent experimental[4] and theoretical[5-16] interest.

Most of the current theoretical efforts[8,10-13] concentrate upon the model of Edwards and Anderson[8] (EA) where one does not attempt to calculate the actual interaction distribution from the RKKY interaction, but rather uses random forces J_{ij} between spins at lattice sites i,j, which are distributed according to a Gaussian distribution with zero mean value:

$$P(J_{ij}) \propto \exp[-\tfrac{1}{2}(J_{ij}/\Delta J)^2] . \quad (1)$$

Mean-field approximations[8-12,17] suggest that this model exhibits a sharp phase transition where *both* the susceptibility and the specific heat have a cusp. A renormalization-group treatment[15] supports these findings, but is restricted to space dimensionalities d close to $d = 6$. The experiments, on the other hand, show a cusp in the susceptibility χ only, while the specific heat C rather exhibits[18] a broad maximum at a temperature of about 20% above T_c. In addition, the magnetic fields required to produce a rounding off of the cusp in χ similar to the experiments[1,2] are about 20 times as large as in the experiment.[11] Thus the available treatments of the EA model do not give a satisfactory account of the experiments.[1,2,4]

Two reasons for these discrepancies may be imagined: (i) the EA model does not contain the essential characteristics of real spin glasses; and (ii) the EA model is a reasonable model for a spin glass, but the mean-field approximations[8-12] are inadequate. As is well known, mean-field approximations yield only an inaccurate description of the properties of second-order phase transitions.[19] More important, mean-field approximations also predict sharp phase transitions in cases where only a gradual variation occurs in reality, such as one-dimensional spin systems (where the "transition" occurs only at zero temperature) or higher-dimensional systems of finite size (where the "transition" is rounded[20]).[21] A gradual freezing in of the spins has in fact been predicted by tunneling models.[7] On the basis of high-temperature expansions Matho[16] recently suggested that the fluctuations neglected by mean-field theory prevent the system from having a sharp transition, and that the cusp in χ is a nonequilibrium phenomenon.[22]

In order to clarify the question of whether the EA model with interactions of short range[23] has a sharp or a gradual transition, we have performed, for the first time, Monte Carlo computer simulations of a model spin glass.[24] This approach allows[25]—at least in principle—a determination of equilibrium properties with an accuracy which is much better than that of the mean-field approximation. Moreover, it allows a study of nonequilibrium relaxation phenomena, which is interesting in its own right in view of the observed irreversible behavior of the magnetization below T_c.[4,26,27] Since in the mean-field approximation there is no significant difference between Ising and Heisenberg models,[28] we treat the Ising $S = \frac{1}{2}$ case only, considering two-dimensional square

lattices with nearest-neighbor interaction only,[29] both in zero and nonzero magnetic fields. This model is much too simplified to allow a direct application to experiment,[30] but it allows a stringent test of the validity of the mean-field approximations.

In Sec. II we describe the model and our simulation technique. In Sec. III the numerical results on the time-dependent relaxation phenomena are presented, while Sec. IV contains our estimates for the "equilibrium" value of susceptibility, magnetization, energy, and specific heat. Section V summarizes our conclusions.

II. MODEL AND SIMULATION TECHNIQUE

We consider a model system of Ising spins ($\sigma_i = 2S_i^z = \pm 1$) described by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{j\neq i} J_{ij}\sigma_i\sigma_j - \mu_B H \sum_i \sigma_i , \qquad (2)$$

where the spins are situated on a $N\times N$ square lattice with periodic boundary conditions, H is the magnetic field, and the exchange constants J_{ij} between the spins are chosen at random according to the Gaussian distribution, Eq. (1). For simplicity only exchange between nearest neighbors on the lattice is taken into account (in principle, the extension to include exchange between more-distant neighbors would be straightforward, but it requires more computing time).

We emphasize the point that this model does not necessarily imply the existence of physical short-range (i.e., in the angstrom range) interactions of the type of Eq. (1). In fact, the lattice considered here is not the lattice of the host material of the spin-glass system. Imagine rather that the magnetic impurities, distributed at some concentration c in the host matrix, are labeled by some index i. We may rearrange the labels in the form of a lattice approximately preserving the topology (i.e., which spins j are nearest neighbors of spin i), to obtain Eq. (2). Since Eq. (1), which is commonly used in the mean-field theories,[8,10-12] is not at all a realistic representation of the actual distribution $P(J_{ij})$ which would follow from a more microscopic treatment based on the RKKY interaction,[3] it is legitimate to restrict the interactions to nearest neighbors: We rather are concerned with a general model of random systems with ferromagnetic and antiferromagnetic bonds equally important, rather than with a realistic theory of actual spin-glass systems. The motivation for such an idealization is, of course, that in the study of other critical phenomena[19] it turned out that many features of the phase transition do not depend on the details of the model studied, but are in common to wide classes of models ("universality"[19,31]). While we thus hope in this spirit that we nevertheless obtain results which are of qualitative use for the understanding of experimental results, we emphasize that the price paid by the above idealizations is that nothing whatsoever can be said about the concentration dependence. Apart from a trivial dependence of the number of spins per cm^3 on c, the parameter ΔJ in Eq. (1) (and hence the spin glass freezing temperature T_c) should also depend on c; and more than just a nearest-neighbor interaction should be taken into account.

As an illustration of the above remark on the inadequacy of Eq. (1) we have used the RKKY interaction[3] (k_F is the Fermi wave number of the host conduction electrons)

$$J(r_{ij}) = J_0(k_F r_{ij})^{-3}[\cos(2k_F r_{ij}) - (2k_F r_{ij})^{-1}\sin(2k_F r_{ij})] \qquad (3)$$

to calculate the actual distribution $P(J_{ij})$ by distributing 10^3 spins at random in a volume $V=(50k_F^{-1})^d$, where d is the dimensionality ($d=2$ and 3), calculating the distances r_{ij} and using Eq. (3). The results are displayed in Fig. 1 which shows that the actual $P(J_{ij})$ rather diverges for $|J_{ij}|\to 0$. On the other hand, this divergence need not be realistic either, since it comes from the distances $r_{ij}\to\infty$, where Eq. (3) need no longer be valid: these interactions may be damped out by mean-free-path effects of the electrons, finite size of mosaic blocks in the host crystal, etc. Therefore we did not attempt to use the distribution shown in Fig. 1 instead of Eq. (1) in the simulations.

The simulations are done as follows. Using pseudorandom numbers, first a set of exchange constants J_{ij} in our lattice is chosen in accordance with the probability distribution of Eq. (1). Then the initial state of the system is specified. Three types of initial states have been chosen: ferromagnetic, antiferromagnetic, or random. Then runs are made for selected values of $k_BT/\Delta J$ and $\mu_BH/\Delta J$, utilizing standard Monte Carlo techniques.[25,32] It is important to note that this technique corresponds to letting the system develop according to a Glauber equation for the probability distribution $P(\sigma_1, \ldots, \sigma_{N^d}, t)$ of the spins,

$$\frac{d}{dt}P(\sigma_1, \ldots, \sigma_{N^d}, t) = -\sum_i W(\sigma_i \to -\sigma_i)P(\ldots, \sigma_i, \ldots) + \sum_i W(-\sigma_i \to \sigma_i)P(\ldots, -\sigma_i, \ldots) , \qquad (4)$$

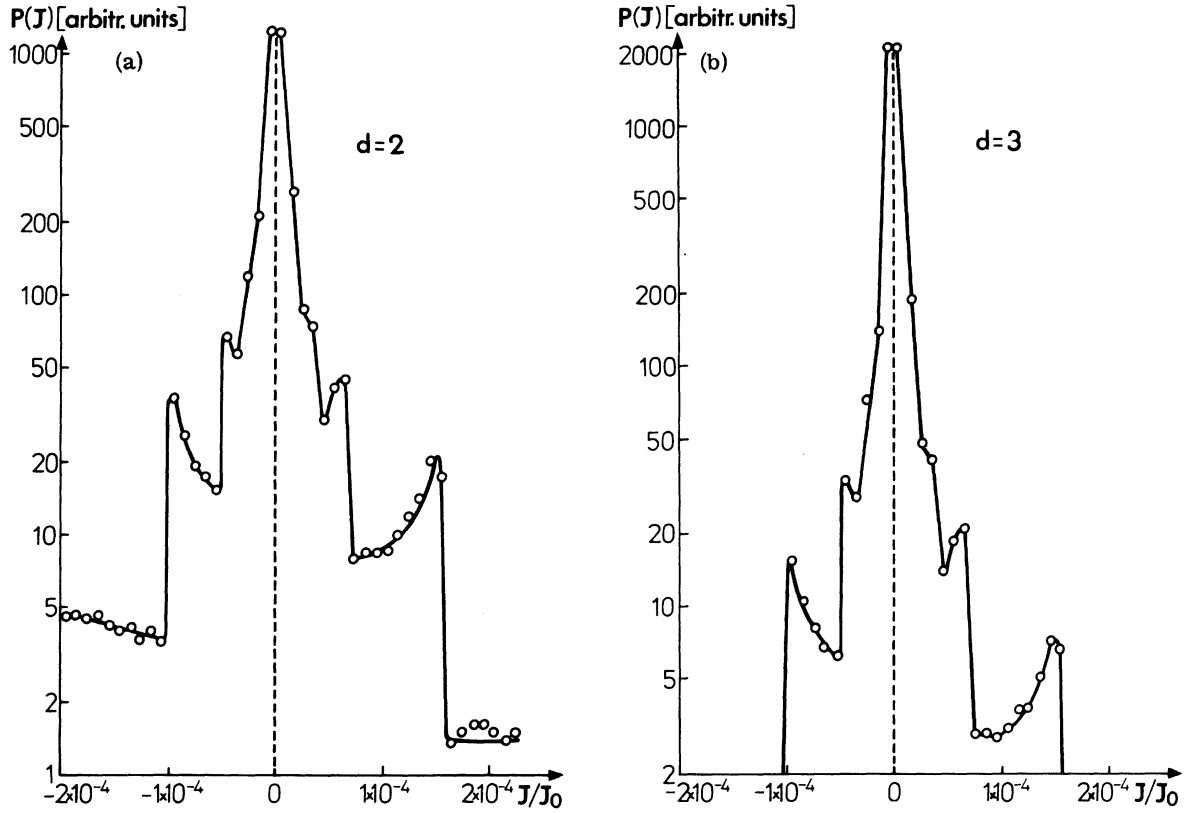

FIG. 1. Distribution of exchange constants for a system of 10^3 spins with RKKY interaction distributed at random in a volume $50k_F^{-1}$ for (a) $d=2$ and (b) $d=3$.

where the transition probability W depends on the cost in energy $\delta\mathcal{H}$ involved in the spin flip,

$$W=1/\tau, \quad \delta\mathcal{H}<0, \quad \delta\mathcal{H}=\sum_j J_{ij}\sigma_i\sigma_j+2\mu_B H\sigma_i, \tag{5a}$$

$$W=1/\tau\exp(-\delta\mathcal{H}/k_BT), \quad \delta\mathcal{H}>0, \tag{5b}$$

where $1/\tau$ is an (arbitrary) rate constant. Equations (5) are consistent with detailed balance and thus ensure that the system settles down at a thermal equilibrium state for large times, $t\to\infty$. Performing then a time averaging during these late times allows one to estimate thermal equilibrium properties. Owing to extremely slow relaxation in spin glasses, this final equilibrium is not always reached within the available computing time, and then one records only nonequilibrium phenomena. The quantities recorded are energy $\langle E(t)\rangle$ per spin, magnetization $\langle\sigma_i(t)\rangle$ per spin, staggered magnetization $\langle\sigma_i^s(t)\rangle$ per spin, and "order parameter" $q(t)$:

$$\langle E(t)\rangle=\frac{\mathcal{H}}{N^d}, \quad \langle\sigma_j(t)\rangle=\sum_j\frac{\sigma_j(t)}{N^d}, \quad \langle\sigma_j^s(t)\rangle=\sum_j\frac{e^{i\vec{r}_j\cdot\vec{Q}}\sigma_j(t)}{N^d}, \tag{6a}$$

$$\langle E\rangle=\int_{t_i}^{t_f}\frac{\langle E(t')\rangle\,dt'}{t_f-t_i}, \quad m=\int_{t_i}^{t_f}\frac{\langle\sigma_j(t')\rangle\,dt'}{t_f-t_i}, \quad m_s=\int_{t_i}^{t_f}\frac{\langle\sigma_j^s(t')\rangle dt'}{t_f-t_i}, \tag{6b}$$

$$q(t)=\sum_{j=1}^{N^d}\left(\int_{t_i}^{t}\frac{\sigma_j(t')\,dt'}{t-t_i}\right)^2\Big/N^d. \tag{6c}$$

[The order parameter q originally is defined as $q=\langle\langle\sigma_j\rangle^2\rangle=\langle m^2\rangle$, where the inner brackets denote thermal averaging in equilibrium. The resulting square of the magnetization $\langle\sigma_j\rangle^2=m^2$ is then averaged ($\langle m^2\rangle$) over all possible configurations of exchange interactions according to their given probability distribution, Eq. (1). Our computer program simulates the thermal averaging by a time averaging, $\langle\ \rangle\to\int dt'/t$, and the configurational averaging by spatial integration, $\langle\ \rangle\to N^{-d}\sum_j$. Thus Eq. (6c) is a reasonable definition for ergodic systems in the thermodynamic limit.]

The time t_i after which the system is considered to be "in equilibrium" is determined from an inspection of the fluctuations of energy and magneti-

zation. The time t_f up to which the simulation is extended is typically about 2000 Monte Carlo steps per spin (i.e., $2000 \times N^d$ attempted spin flips). $\vec{Q}$ in Eq. (6a) is the reciprocal-lattice vector of antiferromagnetic ordering. From the fluctuations we compute the specific heat C, susceptibility χ, and staggered susceptibility $\chi_s [n_l = (t_f - t_i)/\Delta t$, Δt being typically 10 Monte Carlo steps per spin]:

$$C = N^d \sum_{l=1}^{n_l} \frac{[\langle E(t_l)\rangle - \langle E\rangle]^2}{n_l (k_B T)^2}, \tag{7a}$$

$$\chi = N^d \sum_{l=1}^{n_l} \frac{[\langle \sigma_i(t_l)\rangle - m]^2}{n_l k_B T}, \tag{7b}$$

$$\chi_s = N^d \sum_{l=1}^{n_l} \frac{[\langle \sigma_i^s(t_l)\rangle - m_s]^2}{n_l k_B T}. \tag{7c}$$

Also the autocorrelation function of the spins is recorded:

$$\langle \sigma_j(0)\sigma_j(t)\rangle = N^{-d}\left(\sum_j \int_{t_i}^{t_f - t} \sigma_j(t')\sigma_j(t'+t)\,dt'\right)\Big/(t_f - t - t_i). \tag{8}$$

For large times t, this quantity should reduce to the "order parameter" q defined in Eq. (6c).

Since the linear dimension N of the lattice chosen was not very large ($N = 24$ to 160 for $d = 2$), we have made several runs with different sets of J_{ij} [for the same $P(J_{ij})$] in order to reduce the effect of fluctuations.

While Eqs. (1)–(5) represent a well-defined dynamical model, one has to worry about the question to what extent it corresponds to the actual kinetics of a physical spin-glass system. Such a correspondence exists only if the kinetics of the lattice is due to a coupling of the spins to the other degrees of freedom of the host lattice (like lattice vibrations), and not due to the exchange interaction. However, in the latter case one can have at least a qualitative similarity of the time evolution.

III. KINETICS OF THE RELAXATION TOWARDS EQUILIBRIUM

In Figs. 2(a) and 2(b), typical examples of "raw data" are shown. Figure 2(a) gives the relaxation of the magnetization at low temperatures in zero field. Although the model does not favor ferromagnetism, the system settles down at a nonzero remanent magnetization m_r, if one starts out with a ferromagnetic initial spin configuration, while the staggered magnetization stays at zero. If instead we start with a random initial state, both the magnetization and the staggered magnetization remain zero. The energy, on the other hand, approaches rather quickly nearly the same value in both cases. Our simulations support the conclusion[7] that in a spin glass there should be a large number of states with (at least nearly) the same energy, and that hence the relaxation via tunneling should be important. No tunneling is included in our simulation, however, which amounts to purely classical statistical mechanics. Nevertheless such simulations may be used as valuable input data for a calculation of tunneling rates in a spin glass, too.[33]

Since the state with a remanent magnetization m_r of Fig. 2(a) is clearly not a true equilibrium state but (at best) a metastable state, we have carefully checked if there is any dependence of m_r on the linear dimension N, performing runs for $N = 40$, 80, and 160. Curves for $n = 80$ and 160 were indistinguishable, while the curve for $N = 40$ gave again the same average value for m_r, but showed statistical fluctuations more distinctly,

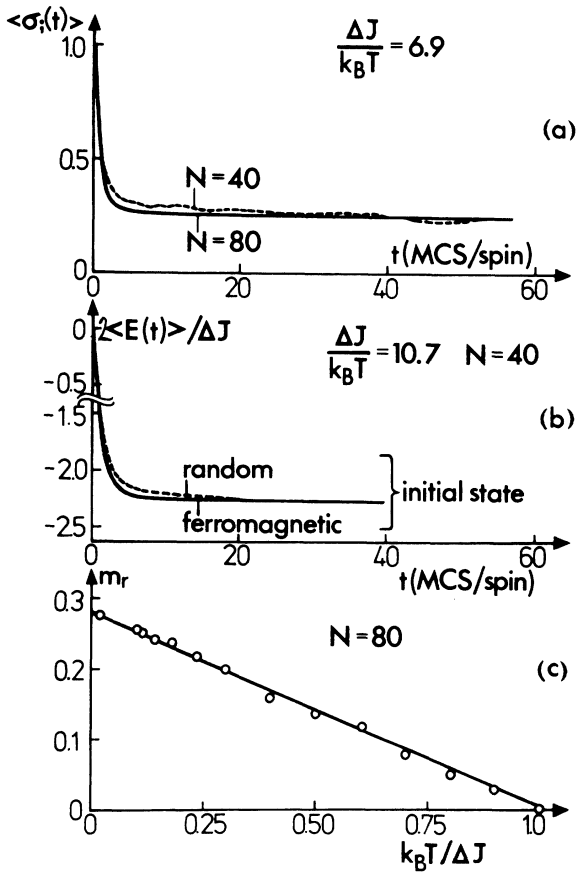

FIG. 2. (a) Relative magnetization per spin as a function of time [in units of Monte Carlo steps per spin]; (b) energy per spin plotted versus time; (c) remanent magnetization plotted versus temperature.

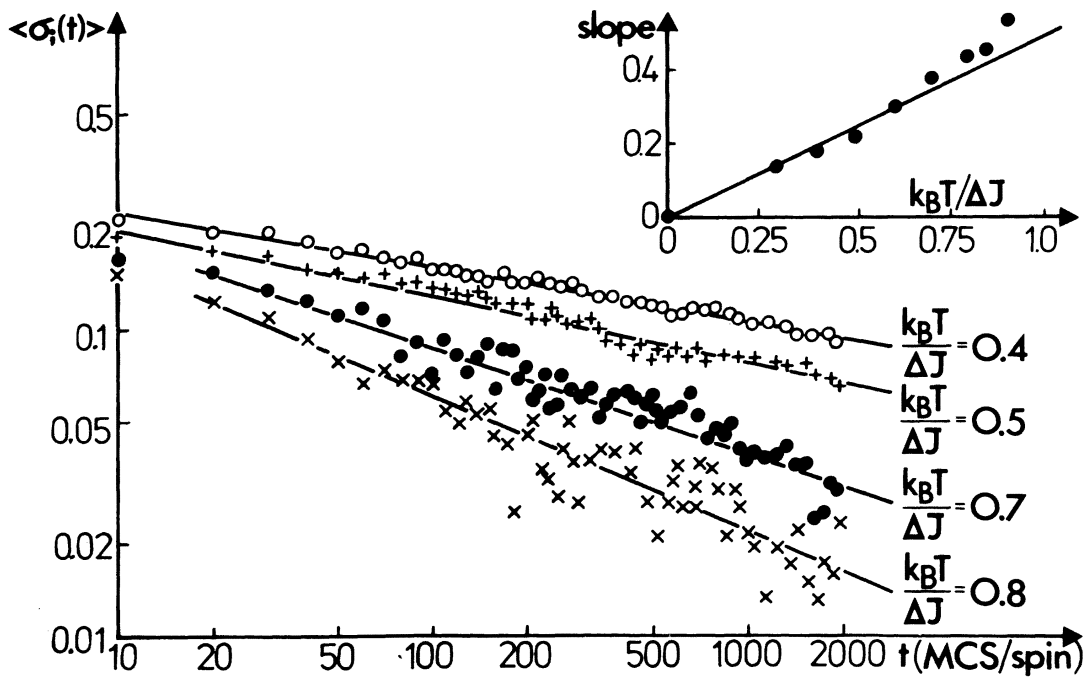

FIG. 3. Log-log plot of magnetization versus time for several temperatures in a 80×80 system. Inset shows temperature variation of the exponent a, Eq. (10).

as expected [see, e.g., Fig. 2(a)]. In order to define the remanent magnetization precisely, we used

$$m_r = \int_{50}^{250} \tfrac{1}{200} \langle \sigma_i(t') \rangle \, dt' \,. \tag{9}$$

The temperature dependence of this quality is linear, as seen in Fig. 2(c). A similar linear variation of m_r vs T has been found in recent experiments.[26,27]

In Eq. (9) we have used a rather small value for t_f since it turned out that $\langle \sigma_i(t) \rangle$ did *not* stay in the vicinity of m_r for larger times, but rather decays to zero. Hence the remanent magnetization cannot uniquely be defined; it depends on the observation time. This result is again qualitatively similar to experimental results where it was found that the remanent magnetization decreases with time t according to a log t behavior and vanishes typically after a few days or hours. The time dependence of $\langle \sigma_i(t) \rangle$ as observed in the simulation is also consistent with a logarithmic behavior over the same range of times. It would be best consistent (Fig. 3) with a power-law behavior:

$$\langle \sigma_i(t) \rangle \propto t^{-a}, \quad a \simeq \tfrac{1}{2} k_B T/\Delta J \quad (T \to 0) \,. \tag{10}$$

We failed to detect any influence of the magnitude of the linear dimension N on this behavior.

In order to clarify what goes on in the system during this process on the microscopic scale, we have recorded the microstates, examples of which are given in Fig. 4. Reversed spins are shown as black dots; up spins are not shown. It is seen that the spins form an irregular percolating network of rather ramified clusters. As time goes on, these clusters become slightly more compact while the general structure of the pattern stays the same.

It is interesting to note that this slow nonexponential variation with time is suppressed in the presence of an external magnetic field H, where the magnetization settles down much more quickly to a nonzero equilibrium value $m = \langle \sigma_i(\infty) \rangle$; see Fig. 5.

According to the conjectures of Refs. 8–12 one would expect that the autocorrelation function $\langle \sigma_i(0) \sigma_i(t) \rangle$ relaxes to a nonzero value of the "order parameter" q below T_c as t goes to infinity. Figure 6 shows that our data are consistent with that conjecture. The same data are replotted versus log t in Fig. 7, however, which shows that the data are well accounted for by a decay similar to the remanent magnetization (apart from $k_B T/\Delta J = 0.5$ where definite approach to equilibrium seems to occur, as indicated by the broken line).

A more conclusive answer to the question if a spin glass has a nonzero "order parameter" is

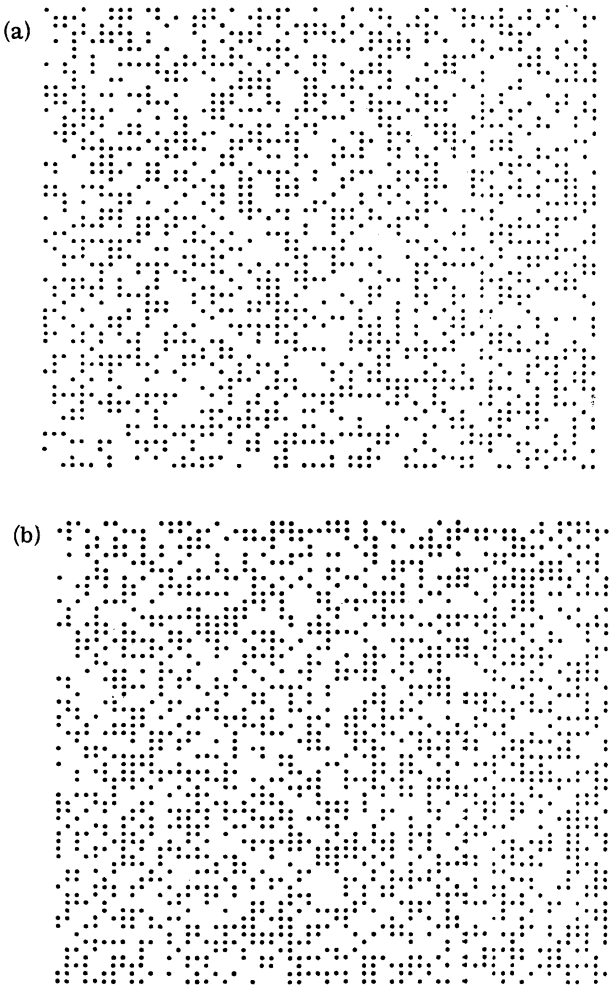

FIG. 4. Snap-shot picture of the state of a 60×60 system at temperature $k_B T/\Delta J = 0.7$ at a time of 30 Monte Carlo steps per spin after the start from (a) a ferromagnetic initial configuration and (b) at a time of 900 Monte Carlo steps per spin. Reversed spins are shown as black dots; up-spins are not shown.

obtained from the time dependence of $q(t)$ [Eq. (6c)], cf. Fig. 8(b). For $k_B T/\Delta J \gtrsim 1.0$, $q(t)$ relaxes monotonically towards zero very slowly (Figs. 8 and 9). At lower temperatures it first decreases [note $q(0) \equiv 1$], but then increases again and approaches a nonzero equilibrium value after very slow damped oscillations [Fig. 8(b) shows only parts of the recorded variation with time]. Owing to this nonmonotonic variation we could not make a reliable extrapolation to $t \to \infty$, which would be necessary to estimate the temperature dependence of the order-parameter reliably. We expect that it behaves qualitatively like the broken curve in Fig. 8(a).

At this point it is in order to comment why the

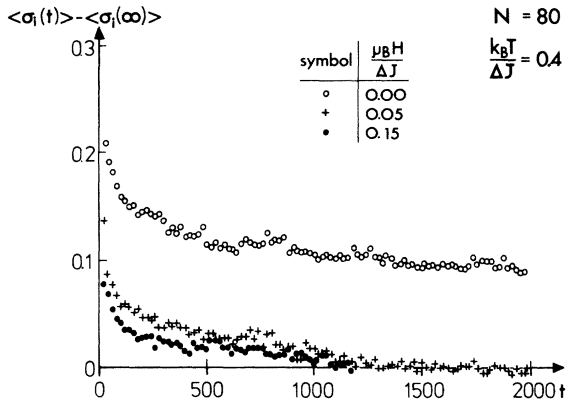

FIG. 5. Magnetization plotted versus time (in units of Monte Carlo steps per spin) at $k_B T/\Delta J = 0.4$ and at various fields.

Monte Carlo method yields here rather poor results, while it has yielded very accurate results in ordinary Ising and Heisenberg model simulations, especially for the respective order parameters.[25] The reason for this failure is twofold: (i) in ordinary (kinetic) Ising models, the relaxation is exponential and hence the systems reach their equilibrium rather quickly, apart from the immediate vicinity of critical points where critical slowing down occurs; and (ii) in equilibrium one may obtain the order parameter not only from time or ensemble averages but also from a spatial average of a single configuration (since fluctuations are of the order $N^{-d/2}$ and hence negligible for large N). In contrast, the "order parameter" $q(t)$ in Eq. (6) is meaningless for a single observation, of course $q(0) \equiv 1$ at any temperature. One could circumvent this difficulty if one introduces phase functions $\phi_i^{(l)}$ for the ground state of the system such that in the ground state (which has the degeneracy n_g)

$$\Psi \equiv \sum_i \frac{\phi_i^{(l)} \sigma_i}{N^d} = 1, \quad l = 1, 2, \ldots, n_g . \tag{11}$$

In an ordinary ferro- and antiferromagnet, $n_g = 2$ and $\phi_i^{(1)} = 1$, $\phi_i^{(2)} = -1$ (for the ferromagnet), or $\phi_i^{(1)} = e^{i\vec{r}_i \cdot \vec{Q}}$, $\phi_i^{(2)} = -e^{i\vec{r}_i \cdot \vec{Q}}$ (for the antiferromagnet). The quantity Ψ on the left-hand side of Eq. (11) is the order parameter of the system (ferro- or antiferromagnet) at arbitrary temperatures, the susceptibility and correlation length associated with its fluctuations diverge at the critical point. We speculate that the behavior of the spin glass is analogous, only the determination of the phase functions ϕ is highly nontrivial. We have not yet attempted to find Ψ for the spin-glass problem[34] but note that from the above remarks it is clear that the energy and magnetization are obtained

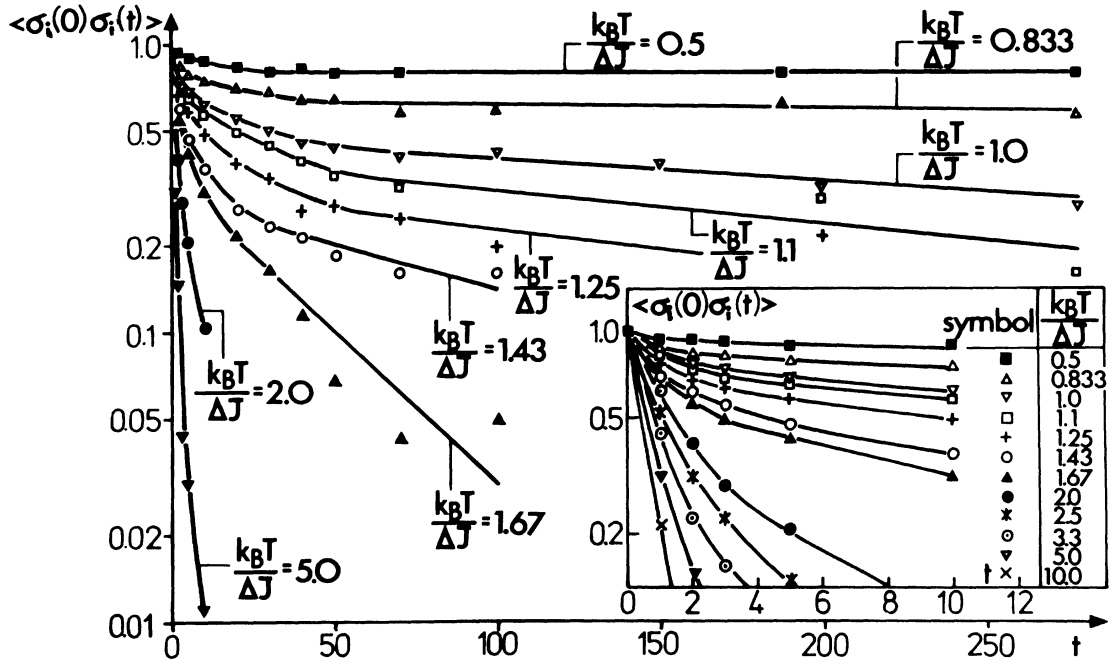

FIG. 6. Autocorrelation function plotted versus time (in units of Monte Carlo steps per spin) for various temperatures. The inset shows the behavior at short times. All data refer to a 24×24 system.

with much better precision than the "order parameter" q; and hence in the following we concentrate on the former quantities.

IV. EQUILIBRIUM PROPERTIES OF THE SPIN GLASS

In Fig. 10 the temperature variation of the energy is plotted for some of the calculated values of the field. These data are typically based on the last 1000 Monte Carlo steps per spin of runs with 2000 Monte Carlo steps per spin. It is seen that in the vicinity of the freezing temperature ($k_BT_c/\Delta J \simeq 1.0$) the energy is still rather close to its ground state value. In Fig. 11 we present selected data on the magnetization process of the spin glass (ferromagnetic starting configuration; i.e., Fig. 11 corresponds to the physical situation where the system is cooled to the considered temperature in a very high field and the field then is put to the considered value). The values of the remanent magnetization in Fig. 11 differ from that of Fig. 2(c) since in Fig. 11 we used $t_f = 2000$ throughout instead of $t_f = 250$.

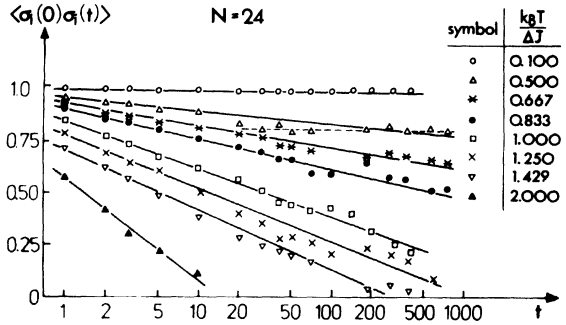

FIG. 7. Semilog plot of autocorrelation function versus time (in units of Monte Carlo steps per spin). Solid straight lines indicate a $\langle\sigma_i(0)\sigma_i(t)\rangle \propto$ const-log t behavior.

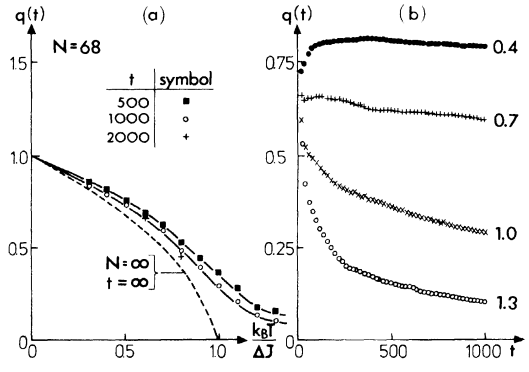

FIG. 8. (a) "Order parameter" $q(t)$ plotted versus temperature for various values of time (in units of Monte Carlo steps per spin). (b) "Order parameter" $q(t)$ plotted versus time. The parameter of the curves is $k_BT/\Delta J$.

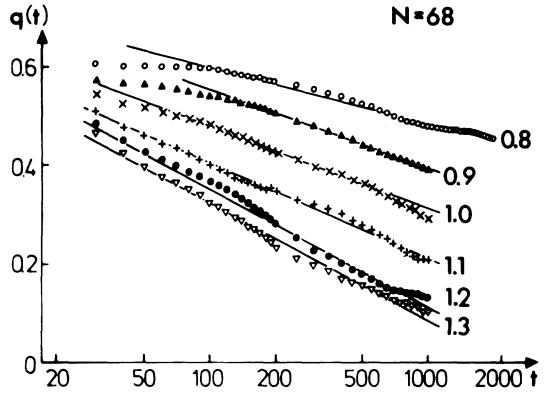

FIG. 9. Semilog plot of the "order parameter" $q(t)$ versus time (in units of Monte Carlo steps per spin), showing that $q(t) \propto$ const-log t over more than one decade of times. The parameter of the curves is $k_BT/\Delta J$.

By graphical differentiation of the curves shown in Figs. 10 and 11 (and of similar data at other fields and temperatures) we obtain the results for specific heat and susceptibility shown in Fig. 12. The specific heat has (at zero field) a broad peak at about $k_BT/\Delta J \simeq 1.25$; in nonzero field this peak is slightly reduced in height and shifted to higher temperatures.

In zero field, data on the energy and specific heat for linear dimension $N = 40$ have been obtained as well. We did not observe any finite-size effect which exceeds the statistical error (which has the size of the data points in the case of C, and is about twice as large in the case of χ). This absence of appreciable finite-size rounding effects is not surprising, of course: Previous studies[20,25] of finite-size effects in ordinary Ising and Heisenberg models revealed that large rounding effects occur for quantities only which have a critical divergence, and they are restricted to temperatures where the correlation length is compatible

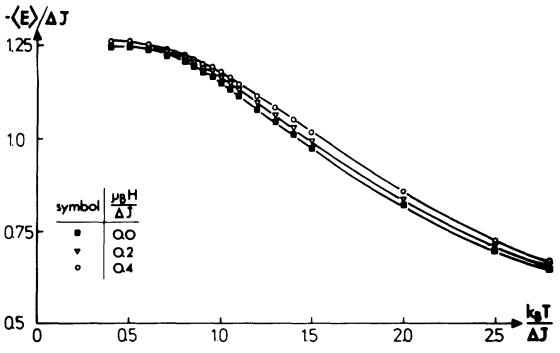

FIG. 10. Normalized energy per spin plotted versus temperature for various values of the magnetic field.

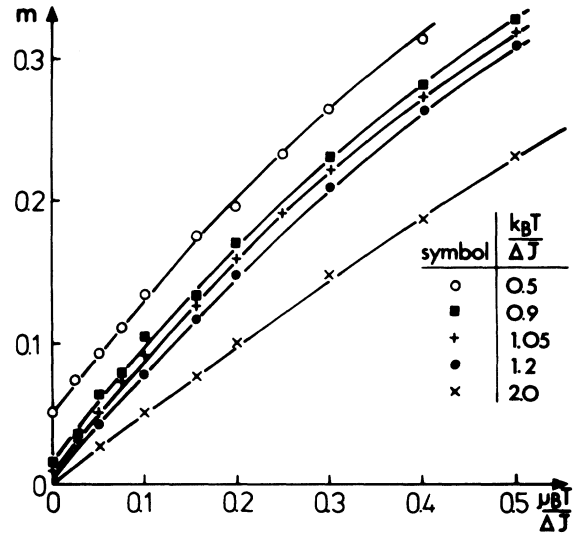

FIG. 11. Magnetization plotted versus magnetic field at various temperatures.

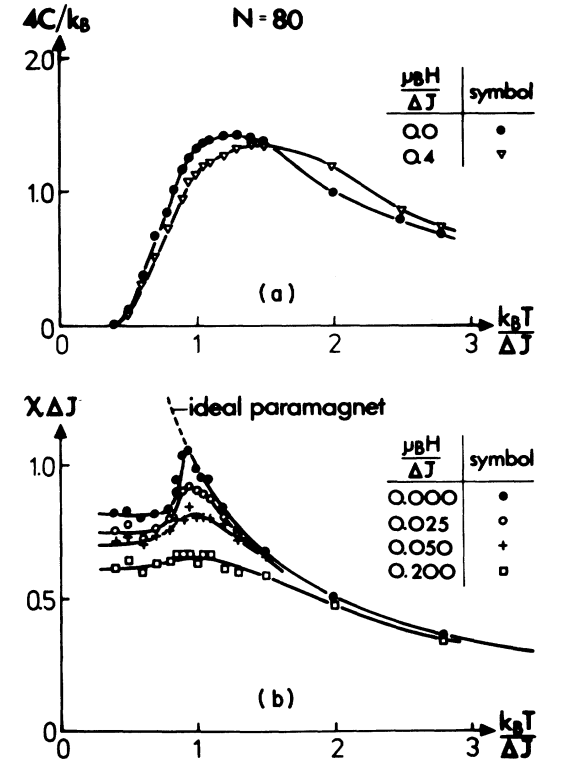

FIG. 12. (a) Specific heat plotted versus temperature for two values of the magnetic field. These data are obtained via $C = \partial E/\partial T$ from the data on which Fig. 10 is based. (b) Susceptibility plotted versus temperature for four values of the field. These data are obtained via $\chi = \partial m/\partial H$ from the data on which Fig. 11 is based.

to the linear dimensions of the system (for $n = 80$ in an ordinary Ising system, rounding is thus restricted to $|1 - T/T_c| < 2\%$, which would be of no interest for the scale of Fig. 12!). Hence we believe that the round maximum of C in Fig. 12 is a real effect, which is strikingly similar to experimental findings.[18]

The susceptibility in zero field is identical to that of a noninteracting paramagnet for temperatures larger than T_c, and has a rather sharp cusp at T_c. It goes to a constant value at lower temperatures. In nonzero fields the cusp is rounded off. Again the results are in striking qualitative agreement with experimental observation.[1,2] There is a large disagreement concerning the numerical values of the fields necessary to produce appreciable rounding, however: For $T = 15$ K in Au-Fe alloys the cusp is reduced in height by 20% in Fig. 12 by a field of about 6000 Oe while experimentally one needs only about 600 Oe. A similar discrepancy occurs in the mean-field treatment[11] as well, which indicates that the EA model as a whole is not sufficient for a quantitative description of real spin glasses.

In Fig. 13 we finally present results on specific heat and susceptibility in zero field, as estimated from the fluctuations of energy and magnetization, Eq. (7). We also computed the staggered susceptibility, Eq. (7c), and found that it agreed with the susceptibility within the statistical error. Figure 13 confirms the qualitative features of Fig. 11. For $k_B T/\Delta J \gtrsim 1.4$, Figs. 12 and 13 even give identical answers. For temperatures closer to the freezing temperature ($1.0 \lesssim k_B T/\Delta J \lesssim 1.4$) the results based on the fluctuations are systematically somewhat smaller. We believe that this is a systematic error due to too short observation time. Figures 7 and 9 show that in this regime the relaxation time is comparable to the observation time, and therefore Eq. (7) is not expected to yield equilibrium phenomena. A similar slowing down occurs at very low temperatures with respect to the difference between the magnetization and its frozen-in part: there the "susceptibility" based on observation of fluctuations over a finite time interval probably goes to zero.

V. CONCLUSIONS

On the basis of the analysis of our above Monte Carlo simulation data we suggest the following behavior:

(i) The Edwards-Anderson model of a spin glass with nearest-neighbor random (Gaussian) interactions on the square lattice has a critical point $k_B T_c/\Delta J \simeq 1.0$ where freezing-in of the spins sets in (Figs. 2, 6, 8, 12, and 13).

(ii) Above the transition, the susceptibility is that of an ideal noninteracting paramagnet while below T_c it drops off to lower values. This cusp is smeared out by an applied magnetic field. The field strengths needed to produce a smearing out comparable to the experiment are about 10 times larger than in the experiment, however (Fig. 12).

(iii) The specific heat does not show any detectable anomaly at T_c, but rather exhibits a broad peak at temperatures which are about 25% higher (Figs. 12 and 13). This result agrees surprisingly well with experimental observation, but disagrees with mean-field treatments of the EA model. We believe that this discrepancy is due to the incorrect treatment of fluctuations in the mean field approximation.

(iv) In a magnetic field the peak in the specific heat is both slightly suppressed and shifted to higher temperatures (Fig. 12).

(v) The "order parameter" $q \equiv \langle\langle\sigma\rangle^2\rangle$ of the spin glass decreases linearly with T at low tempera-

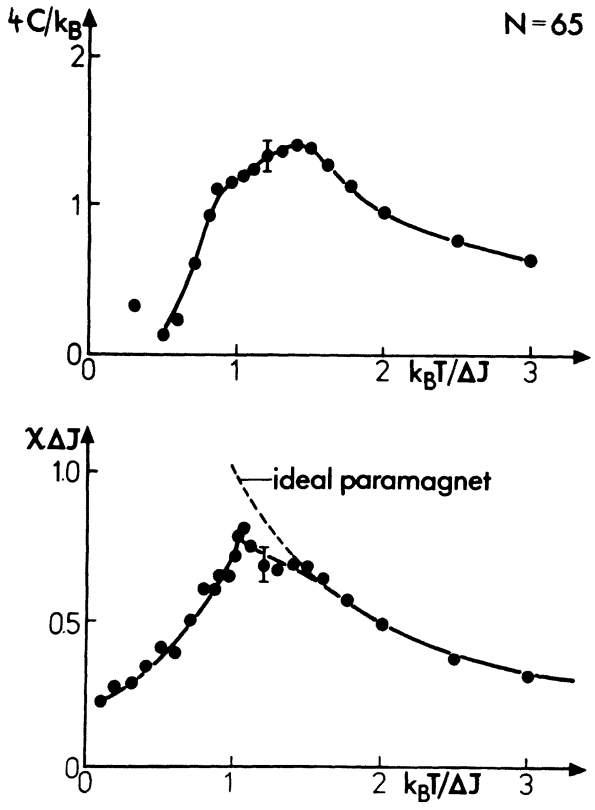

FIG. 13. Specific heat (upper part) and susceptibility (lower part) plotted versus temperature. These data are obtained from the fluctuations of energy and magnetization, respectively. Typical error bar, not including systematic effects due to short observation time, is shown at one temperature.

tures and vanishes at T_c (Fig. 8). This quantity is particularly cumbersome to obtain from Monte Carlo techniques since it is meaningless for a single observation (equal to the microstate), and hence we are not able to estimate its critical exponent. We argue, however, that q may be not the best possible choice for an order parameter (the susceptibility of this *local* quantity, which describes its fluctuations, is finite at T_c), and we discuss in which way a *global* quantity Ψ playing the role of an order parameter can be introduced.

(vi) The kinetic behavior of our stochastic Ising spin glass is characterized by very slow nonexponential relaxation (close to log t or t^{-a} behavior, with $a \ll 1$). This slow relaxation distinctly shows up above T_c in the autocorrelation function (Fig. 7) and in the approach to equilibrium of the "order parameter" $q(t)$ (Fig. 9); below T_c it also appears in the decay of the remanent magnetization (Figs. 3 and 5). Qualitatively this behavior could be related to the behavior of ramified clusters of reversed spins, which become slightly more compact during the course of the time evolution (Fig. 4).

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[23]Probably one can construct limiting cases of infinite-range interactions where the approximations of Refs. 8 and 10–12 become correct. It is unclear to what extent these cases are experimentally relevant.

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