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Dynamical properties of a cluster model of spin-glasses

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The dynamics of small decoupled Ising clusters with Gaussian-distributed interactions is examined. The exactly solved case of 4-spin clusters shows many dynamic properties of spin-glasses. With a smoothly increasing cluster size the nonequilibrium susceptibility χ is in quantitative agreement with computer simulations of the Edwards-Anderson model of spin-glasses. A smooth change of the microscopic time constant gives a sharp peak in $\chi(T)$. Our results support the dynamical nature of the spin-glass transition.

Magnetic systems with random competing interactions very often have a transition into a spin-glass state with unusual properties.[1] After more than ten years of intensive research it is still not clear whether the freezing of spins (or groups of spins) into random directions is a nonequilibrium dynamic process which occurs on a local level or whether it is an equilibrium phase transition with an infinite correlation length below a well-defined critical temperature T_f. It turns out that a careful study of the dynamic properties of spin-glasses is necessary for a better understanding of the freezing process.

On the experimental side, T_f is remarkably well defined by a sharp cusp of the magnetic response to a small alternating field.[2] Many recent dynamical experiments have shown that a broad spectrum of relaxation times extending from 10^{-13} sec to seconds or longer exists in spin-glasses.[3] Nevertheless there may remain a transition in the infinite time limit, since (1) T_f seems to converge to a static value for low frequencies of the ac field,[4] and (2) the field-cooled susceptibility is constant with measurement times between seconds and days.[5]

On the theoretical side, the most important model for spin-glasses has been proposed by Edwards and Anderson (EA).[6] It consists of spins on a regular lattice with randomly distributed interactions. Since it has been shown[7] that anisotropic interactions are necessary for a stabilization of the spin-glass phase we restrict ourselves to the case of Ising spins. Although this model is a great simplification of the experimental situation, its properties are not trivial. Even for the mean-field version (infinite range of bonds[8]), which has an equilibrium phase transition, the introduction of a dynamics is crucial to understand the spin-glass phase.[9] It should be noted that at the transition the specific heat of this model has a cusp in clear disagreement with experimental findings.[1,10]

The properties of the *short-range* EA model have been extensively studied by Monte Carlo (MC) simulations.[11] Many qualitative observations, in particular long-time relaxation effects agree remarkably well with real experiments. However, the size dependence of exactly calculated quantities of small systems shows that there is no phase transition in thermal equilibrium.[12] So a typical length ξ_{EA} for averaged spin-spin correlations increases smoothly with decreasing temperature. At the T_f taken from computer simulations ξ_{EA} is of the order of just two lattice spacings. In fact, recent MC simulations[13] have shown that below T_f a nonzero fraction of spins freezes into *small* clusters. The rest of the spins remains close to thermal equilibrium. These results indicate that the spin-glass transition is a nonequilibrium dynamic process. However, an understanding of this transition is still missing.[14]

Since the correlation length is small at the freezing transition it might be a reasonable approximation to separate the system into independent clusters of size ξ_{EA}. This is done in the present work, which examines the following question: To what extent can the spin-glass transition be understood by a model of decoupled clusters of size ξ_{EA}?[15] We investigate the dynamics of Ising clusters with Gaussian-distributed couplings. Our main results are the following:

(1) A model of 4-spin clusters is solved exactly. For temperatures and observation times comparable to MC data we find a remanent magnetization and a nonequilibrium magnetic susceptibility χ_{ne}. For low temperatures the autocorrelation function decays nearly logarithmically over more than ten orders of magnitude in time. The dynamic structure factor has a strong "elastic" zero frequency peak.

(2) Taking a smoothly increasing cluster size ξ_{EA} into account we find good agreement (without adjustable parameter) between the calculated χ_{ne} and MC data. In two dimensions we find $T_f \sim (\ln t_{\mathrm{obs}})^{1/3}$, where t_{obs} is the observation time. Thus T_f is very insensitive to t_{obs}.

(3) A single Ising spin in our model may be considered as an effective moment of a cluster of real spins with its temperature-dependent relaxation time.[16] In this case $\chi_{\mathrm{ne}}(T, t_{\mathrm{obs}})$ is estimated and

shows a sharp cusp as a function of temperature for very large t_{obs}.

These results show that many spin-glass properties can qualitatively be understood in terms of the relaxation of a distribution of independent clusters.

Our model consists of an ensemble of decoupled Ising clusters. The dynamics is a Glauber master equation[17] for the probability of a spin configuration as used in MC simulations.[11] Thus we model pure relaxation processes with a one-spin-flip dynamics.[18] To obtain an analytic solution we first consider a ring of four spins with energy

$$\mathcal{H} = -J \sum_{ij} S_i S_j - h \sum_i S_i \ ,$$

where J is a nearest-neighbor coupling constant. The transition probability for a spin $S_i \epsilon \{-1, +1\}$ is taken as[17] (for $h=0$)

$$W(S_i) = \frac{1}{2\tau}[1 - S_i \tanh(KS_{i-1} + KS_{i+1})] = \frac{1}{2\tau}\left[1 - \frac{\tanh 2K}{2} S_i (S_{i-1} + S_{i+1})\right] \ , \quad (1)$$

with $K = J/k_B T$, and τ is the microscopic relaxation time of a single spin. With Eq. (1) one easily obtains equations for all correlation functions $\langle S_i(t_0) \times S_j(t_0 + t)\rangle$ in the cluster where t is the time in units of τ and $\langle \dots \rangle$ is an ensemble average over the probability of spin configurations. For $t_0 \rightarrow \infty$ one obtains the thermal expectation value.

Now we introduce an ensemble of clusters by an Gaussian distribution of couplings J:

$$P(J) = \frac{1}{(2\pi)^{1/2}} \exp(-J^2/2(\Delta J)^2) \ . \quad (2)$$

We are interested in ensemble averaged quantities $[\langle \dots \rangle]_{av}$, where the average is taken with the distribution equation (2). Adding a small oscillating magnetic field $h(t) = h_0 e^{i\omega t}$ a straightforward calculation gives the averaged dynamic susceptibility

$$\chi(\omega) = \left. \frac{d[\langle S_i \rangle]_{av}}{dh_0} \right|_{h_0 = 0} = \frac{1}{T}[(\sinh^4 K + \cosh^4 K)^{-1}(1 - \tanh 2K + i\omega\tau)^{-1}]_{av} \ . \quad (3)$$

The autocorrelation function in thermal equilibrium is given by

$$[\langle S_i(0) S_i(t)\rangle]_{av} = (\alpha_1 e^{-\lambda_1 t} + \alpha_+ e^{-\lambda_+ t} + \alpha_- e^{-\lambda_- t})_{av} \quad (4)$$

with

$$\alpha_1 = (1 - \langle S_i S_{i+2}\rangle)/2 \ ,$$
$$\alpha_\pm = (1 + \langle S_i S_{i+2}\rangle \mp 2\langle S_i S_{i+1}\rangle)/4 \ ,$$
$$\lambda_1 = 1/\tau, \quad \lambda_\pm = (1 \pm \tanh 2K)/\tau \ ,$$
$$\langle S_i S_{i+2}\rangle = (\tanh K + \tanh^3 K)/(1 + \tanh^4 K) \ ,$$
$$\langle S_i S_{i+1}\rangle = 2\tanh^2 K/(1 + \tanh^4 K) \ .$$

Also nonequilibrium properties can be calculated, e.g., for the thermoremanent magnetization (TRM) one obtains, after switching off the field h at $t=0$

$$(\langle S_i \rangle)_{av}(t) = \{\langle S_i \rangle_{eq} \exp - [(1 - \tanh 2K)t/\tau]\}_{av} \quad (5)$$

with

$$\langle S_i \rangle_{eq} = (e^{4K} \sinh 4H + 2\sinh 2H)/(e^{4K}\cosh 4H + 4\cosh 2H + e^{-4K} + 2); \quad H = \frac{h}{k_B T} \ .$$

We are interested in the question whether relaxational effects are present for temperature and time scales comparable to computer simulations. There $k_B T$ is of the order of ΔJ and the observation time t_{obs} is of the order 10^3 to $10^4 \tau$. Indeed, for $k_B T \lesssim \Delta J$ and $t_{obs} = 10^3 \tau$, Eq. (5) gives a nonzero TRM with temperature, field, and time dependence which are similar to MC results. Also, even for very low frequencies, the susceptibility $\chi'(\omega = \mathrm{Re}\chi(\omega)$ is very different from the equilibrium one $\chi_{eq} = \chi(\omega = 0)$. For instance, for $\omega\tau = 10^{-4}$, Eq. (3) gives, for the deviations from equilibrium $\Delta\chi = (\chi_{eg} - \chi')/\chi_{eq}$, the values $\Delta\chi = 0.0004$, 0.006, 0.06, 0.35, and 1, for $k_B T/\Delta J = 2$, 1.5, 1.0, 0.5, and 0, respectively. The presence of very long relaxation times is even more evident from Fig. 1. There for $k_B T < \Delta J$ the averaged autocorrelation decays over many orders of magnitude in time inaccessible to any numerical calculations.

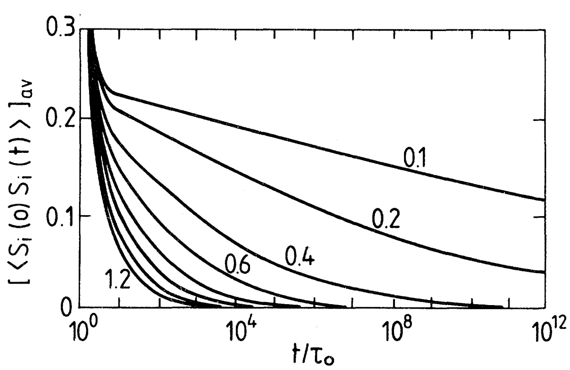

FIG. 1. Configuration-averaged spin-spin autocorrelation as a function of time for different temperatures. $k_B T/\Delta J$ 0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.1, and 1.2.

Another interesting quantity of spin-glasses is the dynamical structure factor which has been measured by quasielastic neutron scattering.[3] For low frequencies (compared to k_BT) it is proportional to $S(\omega) = \mathrm{Im}\,T\chi(\omega)/\omega\tau$. This quantity is shown in Fig. 2. For low temperatures we see a large increase of the zero frequency maximum, as shown in the inset. In experiments $S(\omega)$ is analyzed by fitting a Lorentzian through the wings and taking the difference contribution around $\omega=0$ as elastic scattering intensity.[3] From Fig. 2 it is obvious that by such a fitting procedure one would obtain a large "elastic" scattering intensity for $k_BT \lesssim J$.

Up to now we have studied a simple exactly solvable cluster model with a distribution of 4-spin clusters. Although this model shows many long-time relaxation properties similar to the EA model, it does not reproduce the maximum of the susceptibility for $t_{\mathrm{obs}} \simeq 10^3\tau$. However, if in fact our cluster size is determined by the correlation length $\xi_{\mathrm{EA}}(T)$, as mentioned above, we should consider a cluster model with smoothly varying cluster size. For this case we still can give a simple estimate for the nonequilibrium susceptibility. We expect that the longest relaxation time λ^{-1} for the cluster moment should be given by the Arrhenius law

$$\lambda^{-1} \approx \tau \exp(J\xi_{\mathrm{EA}}^2/k_BT) \quad , \tag{6}$$

where the parenthetical expression is proportional to the number ξ_{EA}^2 of spins in the cluster (for a two-dimensional system). Exact calculations for small systems of the EA model[12] have shown that $\xi_{\mathrm{EA}}(T)$ follows roughly the first term of a high-temperature expansion of the correlation $[\langle S_iS_j\rangle^2]_{\mathrm{av}}$. This gives (for the square lattice)

$$\xi_{\mathrm{EA}}(T) \approx 2\Delta J/T \quad . \tag{7}$$

Taking again the distribution equation (2) for the couplings J of different clusters, one obtains an estimate for the fraction P of cluster which are slower than a given observation time t_{obs}

$$P(T,t_{\mathrm{obs}}) = \int_{J_0}^{\infty} \frac{dJ}{(2\pi)^{1/2}} \exp\left[-\frac{J^2}{2(\Delta J)^2}\right] \tag{8}$$

with

$$J_0 = \frac{(k_BT)^3}{4} \ln\frac{t_{\mathrm{obs}}}{\tau} \quad .$$

Only the clusters which are faster than λ^{-1} can contribute to the equilibrium susceptibility (which for finite EA systems is just a Curie law), therefore

$$\chi(T,t_{\mathrm{obs}}) \simeq (1-P)/T \quad . \tag{9}$$

In fact, recent computer simulations of the two-dimensional EA model[13] have shown that Eq. (9) is a reasonable approximation. In Fig. 3 we show again our results: the dots and crosses are the data of the right and left side of Eq. (9), respectively. Figure 4 also shows our estimate of χ when P is taken from Eq. (8). For $t_{\mathrm{obs}} = 10^3\tau$ which was also used in the MC simulation we see a remarkable agreement between the analytic form of Eqs. (8) and (9) and the MC data. It should be noted that although we have used a rough estimate only there is no adjustable parameter. Therefore we think that this agreement justifies our approach. From Eq. (8) we see that T_f defined by the maximum of χ is very insensi-

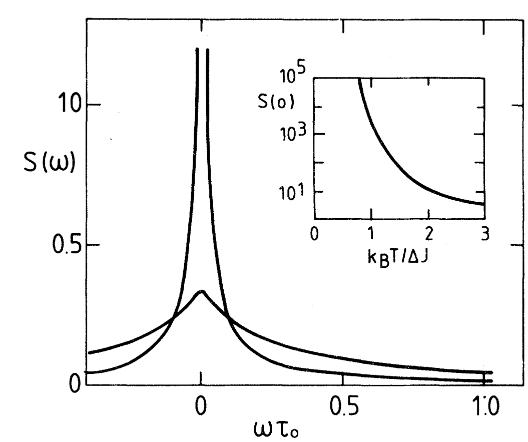

FIG. 2. Dynamic structure factor $S(\omega) = \mathrm{Im}\,T\chi(\omega)/\omega\tau$ as a function of frequency ω for $k_BT/\Delta J = 3$ (low max) and 0.5. The inset shows the zero frequency maximum as a function of temperature.

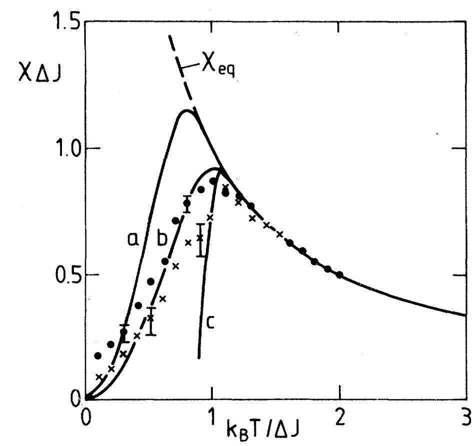

FIG. 3. Nonequilibrium susceptibility for different estimates as discussed in the text. a: $t_{\mathrm{obs}} = 10^6\tau$, b: $t_{\mathrm{obs}} = 10^3\tau$. Curve c is for a slightly different model with $t_{\mathrm{obs}} = 10^3\tau(T) = 10^3 e^{30/k_BT}\tau_0$. The points and crosses show MC data for the EA model taken from Ref. 13.

tive to t_{obs}; one has $T_f \sim (\ln t_{obs}/\tau)^{1/3}$. So even if one could increase the time in MC simulations by a factor 100, T_f would decrease by just 15%.

Although our cluster model reproduces the magnetic susceptibility of the EA model, $\chi(T)$ has still a rather broad maximum, in contrast to the experimentally observed ac susceptibility.[1,2] Of course the maximum becomes sharper in higher dimensions and, if cluster size increases stronger with decreasing temperature. However, there may be another possibility of understanding the cusp in χ from a cluster picture. In order to get a quantitative agreement between MC and experimental temperature and time scales it has been suggested[16] that each Ising spin represents an effective moment of a group of real spins. In this case the microscopic time scale τ has its own exponential temperature dependence $\tau \simeq \tau_0 e^{E/k_B T}$, where E is again of the order of the number of spins in the cluster and $\tau_0 \simeq 10^{-12}$ sec.[3] In remanence experiments one usually has $t_{obs} \simeq 10^{15}\tau_0$, while in computer simulations $t_{obs} \simeq 10^3 \tau$. This would give $E \simeq 30\Delta J$ for $k_B T \lesssim \Delta J$ $(\simeq k_B T_f)$. With these times t_{obs} and $\tau(t)$, Eqs. (6), (7), and (8) give the susceptibility c in Fig. 3. This demonstrates that a smooth variation of cluster size and time constant with physically reasonable parameters can produce a sharp cusp in the dynamic susceptibility.

Our model helps to understand the qualitative behavior and temperature and time scales of a cluster approach to spin-glass dynamics. For a more quantitative description one has to go to more microscopic models and use the computer to study the cluster dynamics. This has still to be done.

Note added in proof. Recent numerical calculations[19,20] have shown that the exponent in Eq. (6) seems to increase in proportion to ξ_{EA} instead of ξ_{EA}^2. However, since $\xi_{EA}(T)$ seems to diverge more strongly, than in Eq. (7),[2] we expect $\chi(t)$ to behave in a similar fashion to Fig. 3. Only the exponent x in $T_f \sim (\ln t_{obs}/\tau)^x$ changes from $\frac{1}{3}$ to a larger value.

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