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Lack of Ergodicity in the Infinite-Range Ising Spin-Glass

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The size dependence of slow relaxation processes in the infinite-range Ising spin-glass is investigated by computer simulation. Below the transition temperature, relaxation of variables which do not change sign under inversion of the spins is complete by a time τ, where $\ln\tau \propto N^{1/4}$ and so diverges as N, the number of spins, tends to infinity. The "ergodic time" τ_{eg} satisfies $\ln\tau_{eg} \propto N^{1/2}$. These results are consistent with a physical picture where barriers between free-energy minima in phase space have a height proportional to the square root of the number of spins to be flipped.

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Spin-glass systems are characterized by very slow relaxation[1] below the freezing temperature. Controversy[1,2] has centered on whether this is due to a sharp phase transition or a more gradual increase in relaxation times. A simplified model which does have a transition because the range of interactions is infinite has been proposed by Sherrington and Kirkpatrick[3] (SK). Using different lines of argument various authors[4-6] have suggested that relaxation times in the SK model diverge when the number of spins, N, tends to infinity and $T<T_c$, the transition temperature. This could arise from free-energy barriers, separating minima in phase space, whose height diverges in the thermodynamic limit. It is tempting[7] to associate these minima with solutions of the mean-field equations of Thouless, Anderson, and Palmer[8] (TAP), which are known to have an enormous number of solutions.[9] An infinite system would stay close to one minimum at all times because it can never get over the infinite barrier surrounding it. By contrast statistical mechanics (ensemble average) sums over all minima with an appropriate weight. An infinite system would therefore be nonergodic because time and ensemble averages would give different results.[7]

This picture, while intuitively reasonable, rests on the assumption that relaxation times diverge for $N\to\infty$. Here we present results of Monte Carlo simulations which show directly this increase of relaxation times with system size. Furthermore we are able to quantify the relaxation processes in some detail. Our main conclusions are as follows.

(i) For excitations which do *not* involve turning over the whole system from the vicinity of one ground state to the "time-reversed" ground state, the spectrum of relaxation times extends to a rather well defined maximum value τ such that (at $T=0.4T_c$)

$$\ln\tau = 2.58N^{1/4} - 0.66 \quad (1)$$

(see Fig. 1). Lack of ergodicity then follows because $\ln\tau\to\infty$ as $N\to\infty$.

(ii) The slow relaxation of a correlation function $q^{(2)}(t)$, defined in Eq. (6) below, has been studied in detail for different sizes, mainly at $T=0.4T_c$. When plotted versus $\ln t/\ln\tau$ all our results for $q^{(2)}(t)-q^{(2)}(\infty)$ lie on a single "uni-

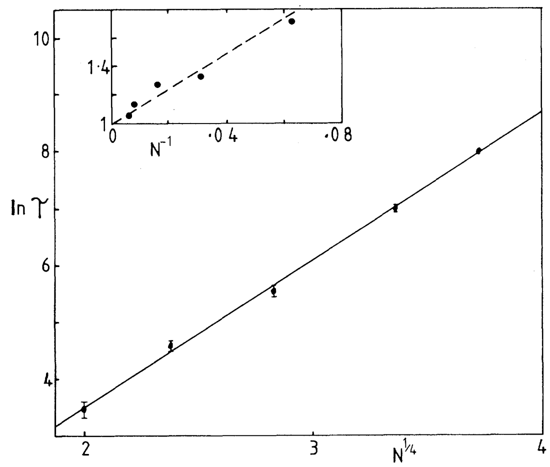

FIG. 1. A plot of $\ln\tau$ against $N^{1/4}$ for several values of N between 16 and 192 at $T=0.4$. Apart from $N=192$, for which only one run was performed, the error bars, which represent one standard deviation, are obtained from the variance of four separate runs. The straight line is a least-squares fit and is given by Eq. (1). Inset: the scale factors for the vertical axis in Fig. 2. The dashed line is a guide to the eye.

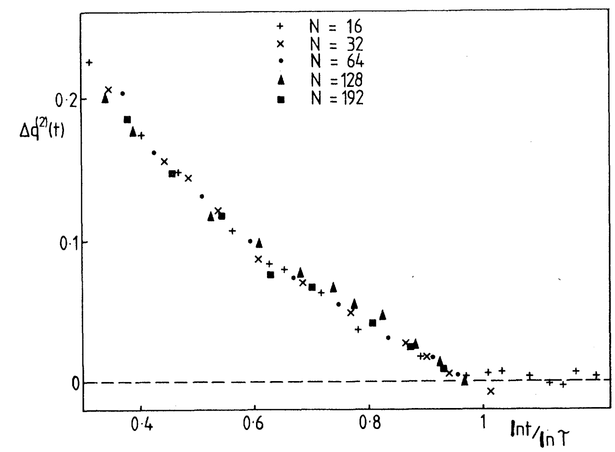

FIG. 2. A plot of $\Delta q^{(2)}(t)=q^{(2)}(t)-q^{(2)}(\infty)$ against $\ln t/\ln\tau$ where $\ln\tau$ is shown in Fig. 1 and the vertical axis has been multiplied by an amount shown in the inset in Fig. 1. The temperature is $T=0.4$. All the data appear to lie on a single universal curve with a change in slope at $\ln t=\ln\tau$.

versal curve" shown in Fig. 2, provided a small rescaling of the vertical axis (inset in Fig. 1) is made for the smaller sizes.

(iii) It was previously argued[5] that excitations from one minimum to another involve turning over a large number of spins, ΔN, where $\Delta N \propto N^{1/2}$. If we assume that $\ln\tau$ is proportional to a free-energy barrier height, Δf, then we have from Eq. (1)

$$\Delta f \propto \Delta N^{1/2}. \qquad (2)$$

In other words the barrier between two minima is proportional to the square root of the number of spins which have to be turned over to go between the minima.

(iv) There are also excitations which turn over all the spins. These control the long-time behavior of the standard correlation function $q(t)$ defined in Eq. (5) below. The time for these processes to occur, which we call the ergodic time τ_{eg}, diverges even for a ferromagnet and gives rise to spontaneous symmetry breaking. In mean-field theory $\ln\tau_{eg}\propto N$ for a ferromagnet[10] but for the SK model our calculations rule out the first power of N and are consistent with

$$\ln\tau_{eg}\propto N^{1/2}, \qquad (3)$$

as shown in Fig. 3. This result is equivalent to Eq. (2) since here $\Delta N\sim N$. Notice that $\ln\tau_{eg}\gg\ln\tau$ for large N.

We now discuss our calculations and results in more detail.

The SK model is described by the Hamiltonian

$$H=-\sum_{i<j} J_{ij}S_iS_j, \qquad (4)$$

where $S_i=\pm 1$ is an Ising spin, $i=1,\ldots,N$, and

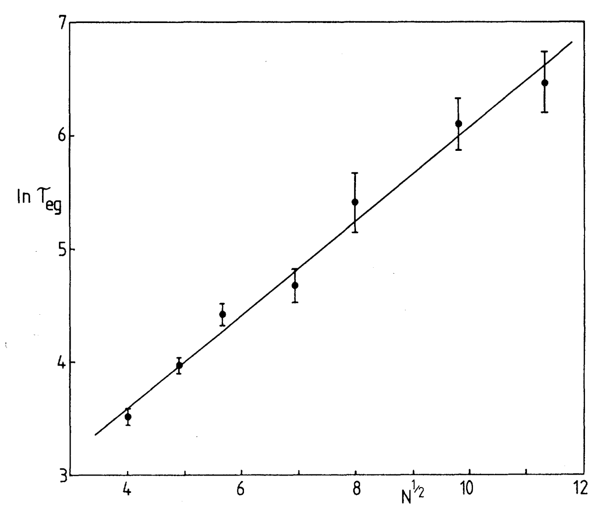

FIG. 3. $\ln\tau_{eg}$ plotted against $N^{1/2}$ for values of N between 16 and 128 at $T=0.6$. The results are consistent with $\ln\tau_{eg}\propto N^{1/2}$. The errors bars correspond to one standard deviation and are obtained from several different runs.

the J_{ij} are independent random variables with a Gaussian probability distribution of width[3,5] $(N-1)^{-1}$, the same for all pairs of spins. In the thermodynamic limit there is a transition at $T_c=1$, in these units. We shall not include a magnetic field. The spins are flipped by the "heat bath" Monte Carlo procedure,[11] and time is given in units of Monte Carlo steps per spin.

Starting from an initial spin arrangement the simulation proceeds for a time t_0 in order to equilibrate the system. One needs $t_0 \geq \tau$ for the energy to relax and we check *a posteriori* that this condition is satisfied. The simulation then continues and we calculate the correlation functions

$$q(t)=N^{-1}\sum_i \langle S_i(t_0)S_i(t+t_0)\rangle_J \quad (5)$$

and

$$q^{(2)}(t)=\frac{2}{N(N-1)}\sum_{i<j}\langle S_i(t_0)S_j(t_0) \times S_i(t+t_0)S_j(t+t_0)\rangle_J. \quad (6)$$

Here $\langle\cdots\rangle_J$ denotes an average over samples. For the calculations of $q^{(2)}(t)$ presented here the number of samples, N_s, satisfies $NN_s \simeq 100\,000$, which is necessary in order to get good statistics.

The Hamiltonian in Eq. (1) is invariant under the "time-reversal" operation $S_i \to -S_i$ for all i. $q(t)$ changes sign if all the spins flip over between t_0 and t_0+t. It will only reach its equilibrium value, which is zero because no symmetry-breaking field is applied,[12] for times longer than the ergodic time τ_{eg}. On the other hand $q^{(2)}(t)$ follows the fluctuations of a pair of spins S_iS_j ($i\neq j$), which does not change sign under inversion of all the spins. Hence it is insensitive to fluctuations which turn over the whole system and will reach its (nonzero) equilibrium value $q^{(2)}$ for times greater than some value, τ, which will be much less than τ_{eg}. Hence

$$q^{(2)}(t)\to q^{(2)}=\langle\langle S_iS_j\rangle_T{}^2\rangle_J \quad (7)$$

for $\ln t>\ln\tau$, where $\langle\cdots\rangle_T$ denotes a statistical mechanics average. In fact $q^{(2)}$ is related to the energy per spin, $U(T)$, by[5,13] $q^{(2)}=1-2T|U(T)|$. This is useful because $U(T)$ is obtained at time t_0, the end of the equilibration process, and so we know to what value $q^{(2)}(t)$ is relaxing as $t\to\infty$.

In order to study the size dependence of $q^{(2)}(t)$ carefully we have mainly considered the single temperature $T=0.4$. Plotting $\Delta q^{(2)}(t)=q^{(2)}(t)-q^{(2)}$ against $\ln t$ we obtain zero for $\ln t$ greater than a certain value $\ln\tau$, which is rather well defined since a change in slope is observed at this point. Furthermore $\ln\tau$ is found to increase with system size, as shown in Fig. 1, and is accurately given by Eq. (1) for $16\leq N\leq 192$. If one assumes the form $\ln\tau=aN^x+b$ and allows the exponent x to vary we find $x=0.27\pm0.10$. We strongly suspect that the exact value is $x=\frac{1}{4}$.

If $\Delta q^{(2)}(t)$ is plotted against $\ln t/\ln\tau$ all the data for different sizes at $T=0.4$ appear to lie on a single universal curve, as shown in Fig. 2. A small rescaling of the vertical axis is also necessary but this scale factor tends to unity for large N as shown in the inset in Fig. 1. The universal curve is almost a straight line, with negative slope, up to $\ln t/\ln\tau=1$. At this point there is apparently an abrupt change of slope and $\Delta q^{(2)}(t)=0$ for $\ln t/\ln\tau>1$. In terms of barriers these results can be interpreted as an almost constant density of barrier heights up to some critical value Δf_c where $\beta\Delta f_c\simeq\ln\tau$, beyond which there are no more barriers. A $\ln t$ dependence is also seen in many remanance magnetization experiments[14] and in simulations of $q(t)$ on short-range models.[15] Earlier simulations[16] on the SK model report a $t^{-1/2}$ variation of $q(t)$ but this is for shorter times and larger samples, and so represents fluctuations in the vicinity of one minimum. Our results provide evidence for Sompolinsky's[4] idea that there is a spectrum of relaxation times which all diverge in the thermodynamic limit.

We have also studied the times at which the system turns over from the vicinity of a ground state to the "time-reversed" one. If the time between the successive flips of the whole system is Δt, then we define $\ln\tau_{eg}=\langle\langle\ln\Delta t\rangle_S\rangle_J$, where $\langle\cdots\rangle_S$ denotes an average over all flips for a given sample. Results for $\ln\tau_{eg}$ at $T=0.6$ are shown in Fig. 3 and are consistent with an $N^{1/2}$ behavior. Since these large flips involve of order N spins the data in Fig. 3 agree with the free-energy barrier formula, Eq. (2). One of us (A.P.Y.) and, independently, Morgenstein[17] have also obtained Eq. (2) for a nearest-neighbor spin-glass model in two dimensions but with ΔN, and hence Δf, finite in the thermodynamic limit, implying the absence of a transition in that model.

Since $\ln\tau\ll\ln\tau_{eg}$ for large N the earlier stages of relaxation of $q(t)$ are not affected by reversals of the whole system and for $\ln t\ll\ln\tau_{eg}$ we find $[q(t)]^2=q^{(2)}(t)$ apart from expected differences of order $N^{-1/2}$. Consequently a single "order parameter" $q(t)$ is adequate up to times where reversal of the whole system starts to occur.

To conclude, we feel that the SK model is qualitatively understood and that the central feature is the many minima in phase space, corresponding to TAP solutions, which become infinitely long lived in the thermodynamic limit. They are therefore strictly speaking stable rather than metastable states. If a uniform field, H, is included the SK solution is correct above the Almeida-Thouless[18] instability line in the H-T plane and there is only one TAP solution[9] in this region. We therefore expect that $\ln\tau \propto N^{1/4}$ everywhere below this line, but with a coefficient which vanishes as the line is approached, and we anticipate that above the instability line $\ln\tau$ will saturate at a finite value as $N\to\infty$. This conjecture will be verified in future calculations.

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Reduction of the Fokker-Planck Equation with an Absorbing or Reflecting Boundary to the Diffusion Equation and the Radiation Boundary Condition

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It is shown, from microscopic considerations based on the Fokker-Planck equation, that the boundary condition (used in conjunction with the diffusion equation) in which the particle density is set to zero on a perfectly absorbing surface is untenable, and, for the first time, the boundary condition for any plane (partially or perfectly) absorbing surface is derived.

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By treating Brownian motion as a simply Markoff process in phase space, Klein,[1] Kramers,[2] and Chandrasekhar[3] demonstrated (independently) that $f(x,v,t)$, the distribution function of a free Brownian particle of mass m, satisfies the so-called field-free Fokker-Planck equation

$$\left(\frac{\partial}{\partial t}+v\frac{\partial}{\partial x}\right)f=\beta\frac{\partial}{\partial v}\left(v+\frac{q}{\beta}\frac{\partial}{\partial v}\right)f, \tag{1}$$

in which β is the friction coefficient, $q/\beta=kT/m$,

