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LETTER TO THE EDITOR

Metastable states of the SK model of spin glasses

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Abstract. The remanent magnetisation and energy at zero temperature are investigated numerically for the infinite-range Ising spin glass. Three different relaxation processes are considered: sequential, random and maximum spin flip. It is shown that most of the metastable states are unstable against one spin flip only.

One of the characteristic properties of spin glasses is the existence of a huge number of metastable states (for a recent review see Binder and Young (1986)). Metastable states are spin configurations which are separated by energy barriers from other configurations; they are the origin of slow glassy dynamics. A well studied and successful model of spin glasses is the infinite-range Ising spin model with random couplings, the SK model (Sherrington and Kirkpatrick 1975). In fact, the number of metastable states has been calculated analytically (Bray and Moore 1980, De Dominicis *et al* 1980, Tanaka and Edwards 1980).

The SK model is an example of many other systems which have complex cooperative behaviour due to the existence of many stable states. Therefore, this model is discussed in the context of neural networks (Hopfield (1982), for an introduction see Kinzel (1985)), random Boolean networks (Derrida and Flyvbjerg 1986) and hard combinatorial optimisation problems (Kirkpatrick *et al* 1983).

Although much is known about the thermal equilibrium properties of the SK model (Binder and Young 1986), much less is known about the structure of the metastable states, their energy barriers and the dynamics in the multivalley structure of the energy. Recent numerical simulations have shown that the metastable states decay to thermal equilibrium at non-zero temperature (Kinzel 1986) contrary to the often used picture of valleys with infinite energy barriers, which seems to be true for the structure of equilibrium states (Bray and Moore 1980, Mackenzie and Young 1982, Parisi 1983).

In this letter we study the saturated remanent magnetisation of the SK model at zero temperature. This means that in the initial state all spins are pointing up (an infinitely strong magnetic field is applied). Then the system relaxes by decreasing its energy at zero temperature and zero magnetic field. We consider single spin-flip dynamics only. Even then different algorithms for the decay of the energy are possible and we compare the following spin flips.

(α) sequential: the spins are updated sequentially.

(β) random: the spins are visited and updated in a random sequence.

(γ) maximum: the spin with the largest internal field pointing opposite to it is flipped.

These processes are iterated until each spin points into the direction of its internal field, i.e. until each configuration has relaxed to a final metastable state.

The first two algorithms α and β correspond to the usual Monte Carlo procedures at zero temperature, while the maximum flip γ is the steepest descent of the energy.

The energy per spin of the SK model is given by

$$E = -\frac{1}{N} \sum_{i < j} J_{ij} S_i S_j \quad (1)$$

where $S_i = \pm 1$, $i = 1, \dots, N$ and the J_{ij} are independent random variables with a Gaussian distribution of zero mean and variance $J^2/(N-1)$.

The magnetisation is defined by

$$M = \frac{1}{N} \sum_i S_i. \quad (2)$$

We are interested in the mean values $\langle E \rangle$ and $\langle M \rangle$ when averaged over the distribution of bonds J_{ij} . In the ground state, i.e. the configuration S_i with the lowest energy, one finds for $N \rightarrow \infty$ (Parisi 1980)

$$\begin{aligned} \langle E_0 \rangle &= -0.7633 \pm 0.0001 J = E_0 \\ \langle M_g \rangle &= 0.0 = M_g. \end{aligned} \quad (3)$$

The last equation holds with probability one, since energy and magnetisation are self-averaging (Young *et al* 1984). This property also seems to hold for the metastable states obtained by relaxation (Kinzel 1986). Finding the ground-state energy may be considered as a problem of NP-complete combinatorial optimisation; numerically a good estimate of E_0 can be found by simulated annealing (Grest *et al* 1986).

Figure 1 shows the results for the three different relaxation processes α , β and γ described above. The bars show the standard deviations for the random flip α ; the standard deviations of the two other algorithms are basically the same. The results indicate that both $\langle (E - \langle E \rangle)^2 \rangle$ and $\langle (M - \langle M \rangle)^2 \rangle$ go to zero with $1/N$. Hence the energy and the magnetisation of the corresponding metastable states are self-averaging. Since figure 1 shows averages over 1000 samples the statistical error is $\frac{1}{30}$ times smaller than the standard deviations.

The mean energy shown in figure 1(a) seems to extrapolate with $1/\sqrt{N}$ to its value of the infinite system. The sequential flip α and the random flip β give the same metastable energy within the statistical error. The maximum flip γ leads to an energy which seems to be somewhat higher.

We estimate

$$E = \begin{cases} -0.704 \pm 0.005 J & \text{for } \alpha \text{ and } \beta \\ -0.696 \pm 0.005 J & \text{for } \gamma. \end{cases} \quad (4)$$

Hence the final energy of the relaxation processes is about 8% and 9% higher than the ground-state energy, respectively. Therefore, the relaxation at zero temperature is a competition between the number of traps (metastable states) and the energy which drives the process. If we chose a metastable state at random we would find with probability one a state with energy $E_m = -0.506 J$ since there are $\exp(\alpha N)$ many states with $\alpha(E_m) \approx 0.2$ (Bray and Moore 1980). On the other hand, one has $\alpha(E_0) = 0.0$ and hence there are only a few ground states with $E_0 = -0.7633 J$. The relaxation leads neither to the most probable states nor to the states with lowest energy; it gives an intermediate energy. According to the analytical calculations there are $\exp(\alpha N)$ with

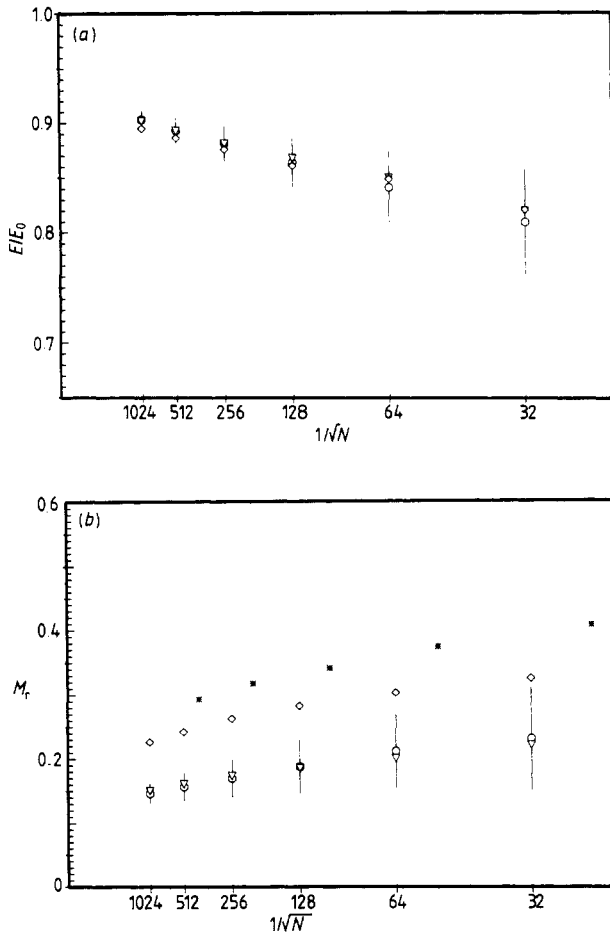


Figure 1. (a) The energy E in units of the ground-state energy $E_0 = -0.7633J$ and (b) the remanent magnetisation M_r of the metastable states obtained from relaxation plotted as functions of system size N for random flip (\circ), sequential flip (∇) and maximum flip (\diamond). The bars show the standard deviations of E and M_r for 1000 samples and random spin flip. The standard deviations for sequential and maximum flip have essentially the same magnitude. The final magnetisation obtained by parallel updating ($*$) (Gardner *et al* 1987) is included in (b).

$\alpha(-0.7) \approx 0.1$ many states with such an energy. However, we do not know whether all these states can be reached by relaxation processes.

The remanent magnetisation is shown in figure 1(b). Again random and sequential flip lead to the same result within statistical error. However, the maximum flip gives a magnetisation which is about 50% higher than the values of the two other processes.

We estimate for $N \rightarrow \infty$

$$M = \begin{cases} -0.13 \pm 0.01J & \text{for } \alpha \text{ and } \beta \\ -0.18 \pm 0.01J & \text{for } \gamma. \end{cases} \quad (5)$$

Note the magnetisation is identical to the overlap between the initial and final state. Due to the randomly distributed bonds one obtains the same result for a random initial state \bar{S}_i^0 instead of the fully aligned one $S_i^0 = +1$. Therefore, if \bar{S}_i^0 is a random initial

state and \bar{S}_i its final configuration, the average overlap

$$q = \frac{1}{N} \sum_i \langle \bar{S}_i^0 \bar{S}_i \rangle \quad (6)$$

is the same as the average magnetisation of equation (5).

The remanent magnetisation may be used for an estimate of the number of flipped spins, namely for $N = 256$ and the maximum flip γ we find that only 2.6% of the spins are flipped more than once. Therefore, the fraction p_f of flipped spins is given by

$$p_f \approx \frac{1}{2}(1 - M). \quad (7)$$

For random (sequential) updating the error of equation (7) is larger; 10.8% (10.1%) of the spins are flipped twice and 2.8% (1.5%) three times. The total duration of the relaxation process is different for the three algorithms. For $N = 256$ we obtain for the number of spin flips n divided by the number of spins N that $n/N = 0.73$ for the random flip α , $n/N = 0.65$ for the sequential flip β and $n/N = 0.42$ for the maximum flip γ . In the last case the energy decrease per spin flip is maximal, but since the total number of flipped spins is small compared to the two other algorithms the final energy is higher. It is, however, surprising that the random and sequential flips give the same energy and magnetisation although the number of spin flips is different.

The SK model may be considered as a random network of two-state elements. Recently the parallel dynamics of this model has been investigated (Gardner *et al* 1987). However, since this dynamics does not necessarily lower the energy one obtains cycles of length two in the final state with high energy. The remanent magnetisation alternates between zero and a non-zero value M_r , which we have included in figure 1(b) for comparison. Hence the overlap to a random initial state is higher for parallel updating than the one obtained by single spin-flip dynamics.

In order to understand the dynamics of spin glasses, in particular far from equilibrium, one needs knowledge about the structure of phase space with respect to energy barriers between metastable states. Not much is known about energy barriers in disordered systems in general. Recent numerical studies of the SK model indicate that metastable states are not separated from equilibrium states by infinitely high energy barriers (Kinzel 1986).

We have investigated whether the metastable states obtained from sequential spin flip are stable against one spin flip. That means that the system increases its energy by one spin flip only and then relaxes again. We have studied the following algorithm.

- (i) The spin S_i with the largest internal field is flipped and kept fixed.
- (ii) The system relaxes by sequential spin flip without considering S_i .
- (iii) After one sweep through the system the spin S_i is again included in the relaxation process.

Figure 2 shows that this process shifts the distribution of energies to lower values. Hence many of the metastable states are unstable against one spin flip and lower the energy. If S_i denotes the metastable state obtained from sequential spin flip and E its energy, this state may decay to a new state \tilde{S}_i and a new energy \tilde{E} after the stability check described above. The overlap

$$q = \frac{1}{N} \sum_i S_i \tilde{S}_i$$

is a measure of how far the state has moved in phase space. The computed energy release $\Delta E = E - \tilde{E}$ is plotted as a function of q in figure 3. Our results indicate that

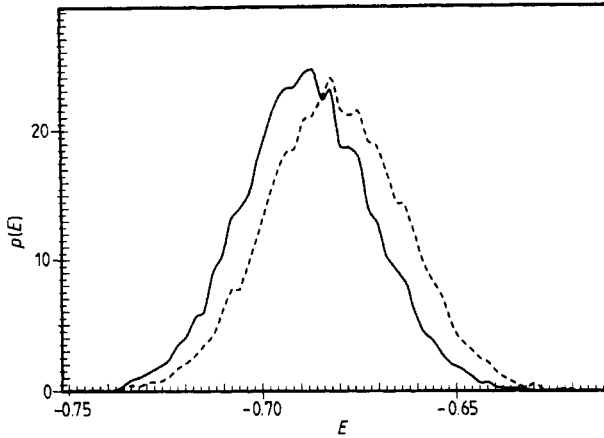


Figure 2. Distribution of energies for $N = 512$ spins and 10^4 samples. Broken curve: metastable states obtained from sequential spin flip. Full curve: metastable states after the stability check described in the text.

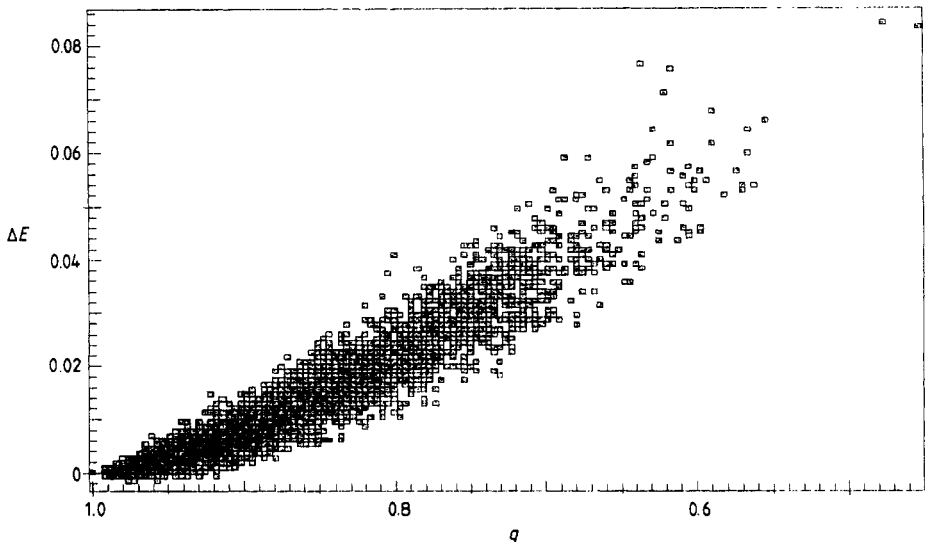


Figure 3. Energy decrease ΔE as a function of overlap q for the stability check ($N = 512$ and 10^4 samples). The intensities of the dots scale logarithmically with the number of samples.

for $N \rightarrow \infty$ one obtains a well defined function $\Delta E(q)$. For larger distances one finds a larger energy decay. However, in the thermodynamic limit the state does not move macroscopically far away; the average energy decay ΔE and the average distance $1 - q$ go to zero for $N \rightarrow \infty$. Figure 4 shows that the total distance $(1 - q)N$ and the total energy decay ΔEN increase with \sqrt{N} . On average, the energy increase made by one spin flip leads to a new state which has \sqrt{N} spins changed. Figure 4 shows that only 15% of the metastable states do not move at all by our stability check.

In summary, the relaxation process at zero temperature from a totally magnetised state to a state with remanent magnetisation is a complicated competition between the number of metastable states and the decrease of energy. The system neither falls into

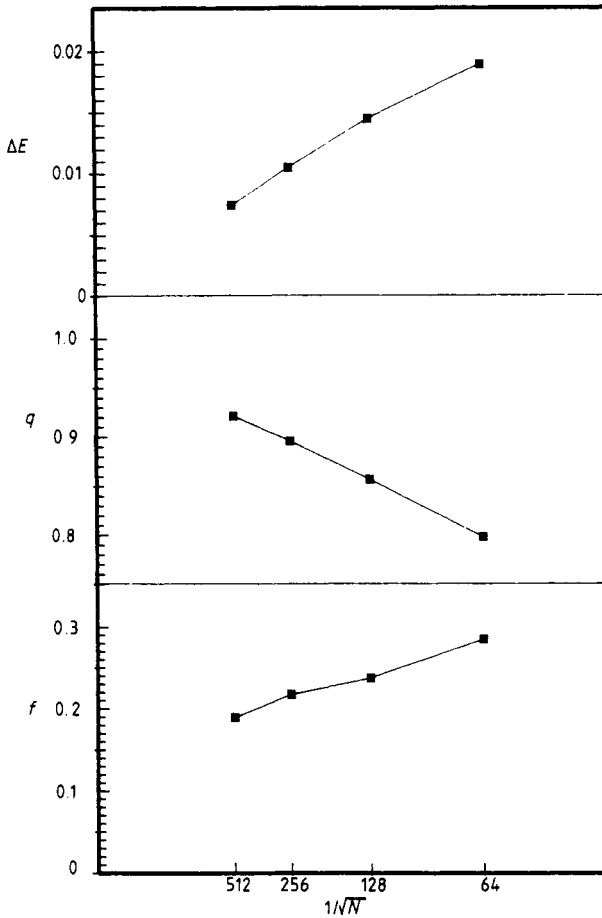


Figure 4. Energy decrease ΔE , overlap q and fraction f of states which do not move by the stability check as a function of system size N .

one of the most probable states nor into the state of lowest energy. Random and sequential updating of the spins gives the same energy and magnetisation in the final metastable states; both values are lower than the ones obtained from steepest descent. Most of the metastable states are unstable against increasing the energy by one spin flip. Hence these states are not the bottoms of deep smooth valleys in energy space; there are many metastable states with low-energy barriers very close to each other.

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