Metastable states of the SK spin glass model

1988 J. Phys. A: Math. Gen. 21 L287

(http://iopscience.iop.org/0305-4470/21/5/004)

J. Phys. A: Math. Gen. **21** (1988) L287–L294. Printed in the UK

LETTER TO THE EDITOR

Metastable states of the SK spin glass model

Koji Nemoto

Research Institute for Fundamental Physics, Kyoto University, Kyoto 606, Japan

Received 24 November 1987

Abstract. The properties of metastable states at zero temperature are examined numerically for the infinite-ranged Ising spin-glass model. It is shown that the energy levels of the metastable states behave like a random energy model. Furthermore, it is found that the barrier energy between them is an increasing function of the Hamming distance. The result is consistent with the prediction that the metastable states have an ultrametric organisation in the phase space.

One of the prominent features of spin glasses is the existence of a large number of metastable states which are almost degenerate in free energy and separated from each other by huge barriers. The multi-valleyed landscape of the free energy enforces the system to the glassy dynamics or the phase transition if any. Therefore it is important to study basic characters of the landscape structure for clarifying the mechanism of anomalously slow dynamics.

A typical example having many metastable states is the infinite-ranged Ising spin-glass model (the so-called SK model [1]). It is believed that statistical mechanical averages (canonical averages) can be calculated by Parisi's replica symmetry breaking (RSB) ansatz and, in fact, many of the thermal equilibrium properties of the SK model are known (for a recent review see [2]). Furthermore the RSB is interpreted as the symmetry breaking into multi-valleyed structure in free energy. Indeed the numerical evidences for the interpretation which gives the relation between replica space and configurational space have been given by means of Monte Carlo simulation [3] and by the TAP free energy analysis [4, 5].

It seems, however, that very little is known about the detailed properties of metastable states of the SK model even at zero temperature. A few years ago Mézard *et al* pointed out, from RSB calculation, that the metastable states are organised hierarchically [6, 7]. However, it is still not so clear how this property reflects on the dynamics. In this letter we report, as the first step to reveal the problem, some basic results from numerical calculation at zero temperature. First we investigate the energetic property of metastable states and show that their energy levels are almost independent of each other like the random energy model (REM) [8, 9]. Then we take account of the statistical mechanical weight effectively and confirm the existence of ultrametric structure predicted by Mézard *et al.* Finally we evaluate the barrier energies between metastable states and find that the barrier is a non-decreasing function of the Hamming distance. The numerical analyses presented here are performed by using all the metastable states in a sample and averaging over samples.

Here we use the so-called TAP equations (equations of state) [10] to identify each metastable state. At zero temperature they are reduced to the equations for the stable state against one spin flip. Furthermore we set the external field equal to zero. Then

0305-4470/88/050287+08$02.50

the TAP equations and energy E are simply written as

$$S_i = \mathrm{sgn}\left(\sum_j J_{ij} S_j\right) \qquad (i = 1, \ldots, N) \tag{1}$$

$$E = -\sum_{ij} J_{ij} S_i S_j \tag{2}$$

where $S_i = \pm 1$ and $\{J_{ij}\}$ are independent random Gaussian variables with zero mean and the variance $(N-1)^{-1}$, N being the number of total spins. For each sample (each realisation of the set of J_{ij}) we found out all the solutions of (1) by a sequential search over half of the possible 2^N states (if a state $\{S_i\}$ is a solution, $\{-S_i\}$ is also a solution, which we call hereafter the time-reversal state of $\{S_i\}$). The numbers of samples we examined are 1000, 1000, 500 and 300 for $N = 12$, 16, 20 and 24, respectively. We found that the mean number of solutions N_s is proportional to $\exp(\alpha N)$ with $\alpha = 0.201 \pm 0.002$ and the prefactor nearly equal to one, which agrees well with the results of Tanaka and Edwards [11] and Bray and Moore [12].

First we show the result on the density of metastable states (DOM). We evaluated DOM for one energy level $\rho(E)$ and for two energy levels $\rho(E_1, E_2)$ defined by

$$\rho(E) \equiv \left\langle \frac{1}{N_s} \sum_a \delta(E - E_a) \right\rangle_J \tag{3}$$

$$\rho(E_1, E_2) \equiv \left\langle \frac{1}{N_s^2} \sum_{ab} \delta(E_1 - E_a)\delta(E_2 - E_b) \right\rangle_J \tag{4}$$

where E_a denotes the energy of the ath solution of (1) and $\langle \ldots \rangle_J$ the average over $\{J_{ij}\}$, and the summation runs over all solutions. Figure 1 shows $\rho(E)$ for $N = 24$. In fact, $\rho(E)$ has the scaling form with N as

$$\rho(E) \simeq N^{-1/2} \tilde{\rho}\left(\frac{E - N\varepsilon_0}{N^{1/2}}\right) \tag{5}$$

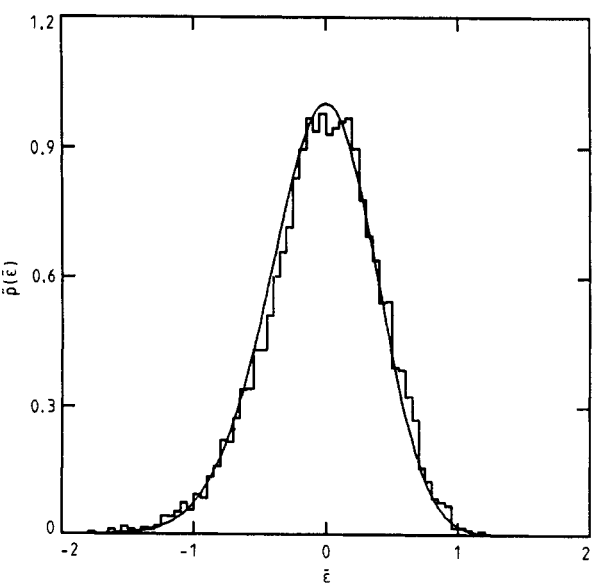

Figure 1. Scaled density of metastable states $\tilde{\rho}(\tilde{\varepsilon})$ for $N = 24$, where $\tilde{\varepsilon} \equiv (E - N\varepsilon_0)N^{-1/2}$ with $\varepsilon_0 = 0.506$. The full curve represents the analytical result of [11].

where $\varepsilon_0 \approx 0.50$ [11]. The result agrees very well with the analytic calculation [11] indicated by the full curve in the figure. In order to examine the level correlation we observed the second cumulant of DOM and found

$$\int \mathrm{d}E_1\, \mathrm{d}E_2 |\rho(E_1, E_2) - \rho(E_1)\rho(E_2)| \sim N^{-\delta} \tag{6}$$

with $\delta \approx 2$. This suggests that the energy levels of metastable states are independent of each other like the REM [8, 9].

It is well known that the distribution of statistical mechanical weight W_a for the REM:

$$W_a \equiv \frac{\exp(-\beta E_a)}{Z} \qquad Z \equiv \sum_a \exp(-\beta E_a) \tag{7}$$

has the same property as for the SK model, except that energy is to be seen as the free energy of metastable states for the latter [13, 14]. An interesting property is that the moments of $Y \equiv \Sigma_a W_a^2$ are expressed as a function of the first moment $y \equiv \langle Y \rangle_J$ alone:

$$\langle Y^2 \rangle_J = \tfrac{1}{3}(y + 2y^2) \tag{8}$$

$$\langle Y^3 \rangle_J = \tfrac{1}{15}(3y + 7y^2 + 5y^3) \tag{9}$$

and so on. We expect that these relations hold for general REM provided that DOM is well behaved. In figure 2, $\langle Y^2 \rangle_J$ and $\langle Y^3 \rangle_J$ are plotted against y for various β, where β is treated as a fictitious parameter. The full curves represent the relations (8) and (9). Rather good agreement with the analytic predictions confirms the statistical independence between energy levels of the SK model. The existence of these relations has also been observed in Kauffman's model [15], in which W_a is the normalised size of the basin of the attractor. Therefore this feature seems common to randomly connected networks.

We also observed the geometrical distribution of metastable states in the phase space by evaluating the overlap function $P_0(q)$:

$$P_0(q) = \left\langle \frac{1}{N_s^2} \sum_{ab} \delta(q - q_{ab}) \right\rangle_J \tag{10}$$

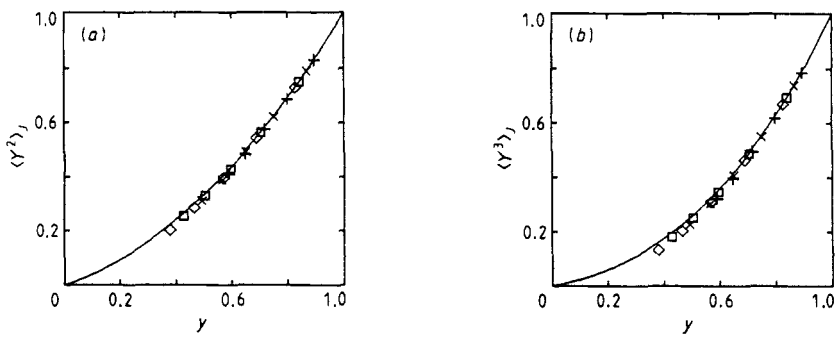

Figure 2. (*a*) $\langle Y^2 \rangle_J$ plotted against $y = \langle Y \rangle_J$ for various β ($2 \leq \beta \leq 10$) and for $N = 12$ (+), 16 (×), 20 (□) and 24 (◇). (*b*) $\langle Y^3 \rangle_J$ plotted against y. The full curves in (*a*) and (*b*) represent the relations (8) and (9), respectively.

where q_{ab} is the overlap between two states, a and b. If the metastable states are distributed randomly $P_0(q)$ can be calculated from the binary distribution and in the large-N limit it is written as

$$P_0(q) \simeq \left(\frac{\gamma N}{2\pi}\right)^{1/2} \exp\left(-\frac{\gamma N q^2}{2}\right) \tag{11}$$

with $\gamma = 1$. In figure 3 we show $P_0(q)$ of the present data scaled by $N^{1/2}$. It fits well to the scaling form described by (11) with $\gamma \sim 0.37$. We can see from the result that the metastable states of the model are distributed almost randomly in the phase space with reduced degree of freedom, γN, due to the interactions.

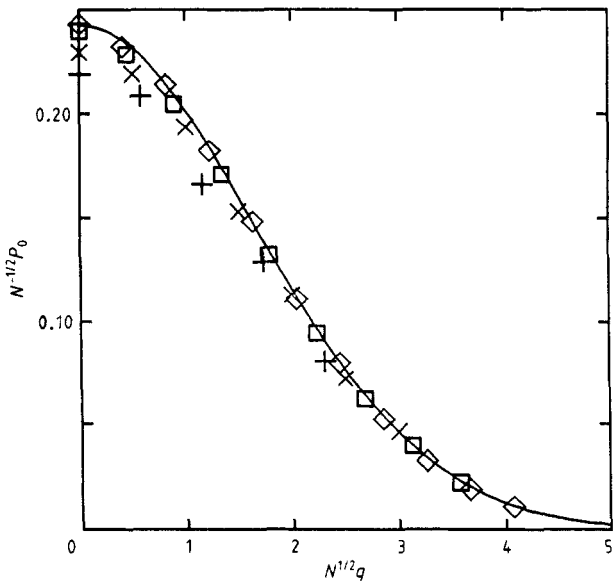

Figure 3. Scaled overlap function $N^{-1/2}P_0(q)$ plotted against $N^{1/2}q$ for $N = 12$ (+), 16 (×), 20 (□) and 24 (◇). The full curve represents the scaling function (11) with $\gamma = 0.37$.

The results presented above do not conflict with the prediction that the metastable states are organised hierarchically (ultrametrically) in the free energy space [6, 7], because the proper weights (7) considerably reduce the effective number of metastable states. To confirm this, we examined the weighted three-state overlap function defined by

$$P(q_1, q_2, q_3) \equiv \left\langle \sum_{abc} W_a W_b W_c \delta(q_1 - q_{bc}) \delta(q_2 - q_{ca}) \delta(q_3 - q_{ab}) \right\rangle_J . \tag{12}$$

According to the RSB calculation, two of the three overlaps are always equal and another one is equal to or greater than these. This statement naturally leads to the hierarchy indexed by the overlaps (ultrametricity) of metastable states (for a review of ultrametricity see [16]). We evaluated the following function using our solutions:

$$P_2(q_1, q_2) \equiv \int_\Omega \mathrm{d}q_3 \, P(q_1, q_2, q_3) \tag{13}$$

where Ω denotes the integral region of q_3, $q_3 \geqslant \max(q_1, q_2)$ (in which time-reversal symmetry is taken into account). If the ultrametricity holds (13) should be zero except on the line $q_1 = q_2$ [17]. In figure 4 we show the contour map of $P_2(q_1, q_2)$. In the case of a white average ($\beta = 0$) it is essentially the same as that of random distribution as expected from the result presented above. With proper weights ($\beta = 5$), on the other hand, non-trivial structure along the line $q_1 = q_2$ is seen, which suggests the existence of non-trivial ultrametricity (here 'trivial ultrametricity' means ultrametricity where all the states are equidistant from each other and no structure exists).

In order to understand the structure of the phase space in more detail, we investigated the relation between the Hamming distance d_{ab} (in the present case $d_{ab} = N(1-q_{ab})/2$) and energy barrier E_{ab} separating two states a and b defined by

$$E_{ab} \equiv \min_{\substack{\text{paths} \\ a \to b}} \{ \max_{\substack{\text{along} \\ \text{the path}}} E \} \tag{14}$$

where 'paths $a \to b$' means that minimisation is taken over all paths from a to b connected by one-spin-flip passages. It was claimed that the distance $\{E_{ab}\}$ defines an ultrametric space [18]. Although, strictly speaking, $\{E_{ab}\}$ is not a distance (note that $E_{aa} \neq 0$), it is easily seen by the definition (14) that

$$E_{ab} \leqslant \max(E_{ac}, E_{bc}). \tag{15}$$

Thus one can construct a hierarchical tree indexed by $\{E_{ab}\}$ [16].

Here we used a method of simulated annealing to evaluate all of E_{ab} (the exact evaluation is desperately hard!). Let us explain the basic idea of the method. We introduce the one-spin-flip operator $\mathcal{P}_i$ which has the function $\mathcal{P}_i S_i = -S_i$. Then any paths from the ath state $\{S_i^a\}$ to the bth state $\{S_i^b\}$ can be described by the product of $\mathcal{P}_i$ which satisfies the relation

$$\{S_i^b\} = \mathcal{P}_{i_1} \mathcal{P}_{i_2} \ldots \mathcal{P}_{i_n} \{S_i^a\} \tag{16}$$

where n is the length of a specified path. This product is the target of our simulation. As a trial we adopted the commutation of two adjoining operators. The cost is easily evaluated because the commutation changes only one transient state along the path. We used the heat bath method for the acceptance rule of such trials. Among the highest energies on each path realised during annealing, the lowest one was evaluated as E_{ab}. Of course n can be varied by considering creation and annihilation of $\mathcal{P}_i \mathcal{P}_i (=1)$. However it turned out, from preliminary observations, that the length of the path having the lowest barrier is almost always equal to d_{ab} or there exist other metastable states on the path. Therefore we performed the annealing with n fixed to d_{ab} for all

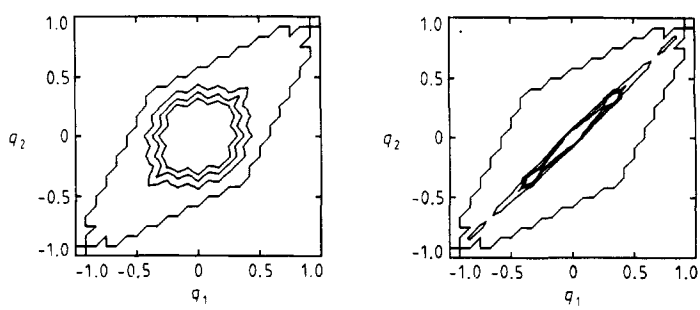

Figure 4. Contour map of $P_2(q_1, q_2)$ for $N = 24$ in the case for $\beta = 0$ (left) and $\beta = 5$ (right).

pairs of metastable states and from the result we constructed the minimal spanning tree [16] to obtain $\{E_{ab}\}$.

Figure 5 shows an example of the tree for a sample of $N = 20$. As shown in the figure the greater part of metastable states, which is dominated in the REM property, is over the lowest time-reversal barrier (indicated by an arrow). Here the time-reversal barrier means the one between a state and its time-reversal state.

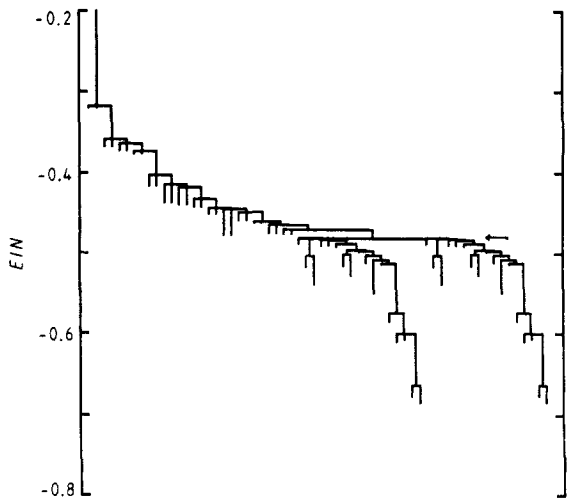

Figure 5. Hierarchical tree indexed by energy barrier for a sample of $N = 20$, $N_s = 62$. The arrow indicates the lowest energy barrier. Metastable states are represented by positions where vertical lines terminate. Horizontal lines are drawn at the value of the barrier energy between two sheafs suspended under the lines. Two identical sheafs are suspended under the lowest time-reversal barrier.

It is a plausible statement that the further two states are separated, the higher the barrier between them is. In order to see this feature we define a function as

$$B(d) \equiv \left\langle \left(\sum_{ab} \Delta E_{ab} W_a W_b \delta(d - d_{ab}) \right) \left(\sum_{ab} W_a W_b \delta(d - d_{ab}) \right)^{-1} \right\rangle_J \tag{17}$$

where

$$\Delta E_{ab} \equiv E_{ab} - E_{GS} \qquad E_{GS} \equiv \min_a E_a. \tag{18}$$

Again we treat β in (7) as a fictitious parameter (remember that we discuss the case where $T = 0$ so β should be taken to be large). The result from our data with $\beta = 5$ is plotted in figure 6. As expected $B(d)$ is a non-decreasing function of d and the plausible statement above is really correct. Therefore the metastable states have, on average, an ultrametric structure with respect to the Hamming distance, which is described by the same hierarchical tree as that of the energy barriers.

In the figure plateau-like behaviour is seen for $d \geq 0.5N$ because the lowest time-reversal barrier is dominated there. We could not estimate the scaling form of $B(d)$ since the system sizes we studied are rather small. Nevertheless an interesting observation is that, in the small-d limit, a finite barrier of the order of unity seems to exist, namely

$$B_0 \equiv \lim_{d/N \to 0} B(d) \sim 0.13. \tag{19}$$

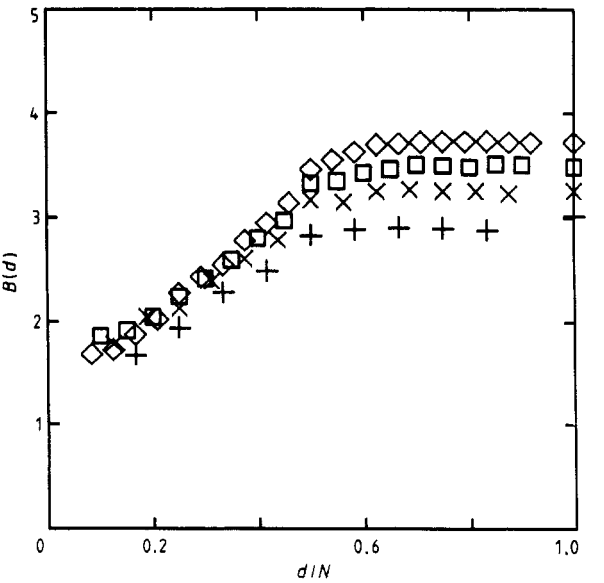

Figure 6. $B(d)$ defined by (17) plotted against normalised distance d/N for $N = 12$ (+), 16 (×), 20 (□) and 24 (◇), for $\beta = 5$.

If B_0 is assumed to be a correction term to the asymptotic form of the N dependence of the plateau value, we can estimate the form as

$$\lim_{d/N \to 1} B(d) \sim N^{\eta} + B_0 \tag{20}$$

with $\eta \sim 0.51$. This can be compared with the estimation of Mackenzie and Young [19], $\eta = \frac{1}{2}$, although our estimation need not be considered so seriously.

In summary, we have found that the metastable states of the SK model behave energetically like the REM and the distribution in phase space also seems random with reduced degree of freedom. When the metastable states are weighted properly, the energy barrier is, in the mean, an increasing function of the Hamming distance, which suggests the existence of the ultrametric structure in phase space.

In the very low temperature region where entropy effect is negligible, the behaviour of the system can be described by the structure of metastable states in phase space. Therefore it is of great interest to consider the relaxation process on the hierarchical tree, such as that shown in figure 5, of which analysis is now in progress.

The author is grateful to Professor H Takayama for invaluable discussions and for a critical reading of the manuscript. This work was financially supported by a Grant-in-Aid for Scientific Research for the Ministry of Education, Science and Culture of Japan.

References

[1] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792
[2] Binder K and Young A P 1986 *Rev. Mod. Phys.* **58** 801
[3] Young A P 1983 *Phys. Rev. Lett.* **51** 1206
[4] Nemoto K and Takayama H 1986 *J. Magn. Magnet. Mater.* **54–57** 135

[5] Nemoto K 1987 *J. Phys. C: Solid State Phys.* **20** 1325
[6] Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M A 1984 *Phys. Rev. Lett.* **52** 1156
[7] Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M A 1984 *J. Physique* **45** 843
[8] Derrida B 1980 *Phys. Rev. Lett.* **45** 79
[9] Derrida B 1981 *Phys. Rev.* B **24** 3613
[10] Thouless D J, Anderson P W and Palmer R G 1977 *Phil. Mag.* **35** 593
[11] Tanaka F and Edwards S F 1980 *J. Phys. F: Met. Phys.* **10** 2769
[12] Bray A J and Moore M A 1980 *J. Phys. C: Solid State Phys.* **58** 801
[13] Mézard M, Parisi G and Virasoro M A 1985 *J. Physique Lett.* **46** L217
[14] Derrida B and Toulouse G 1985 *J. Physique Lett.* **46** L223
[15] Derrida B and Flyvbjerg H 1986 *J. Phys. A: Math. Gen.* **19** L1003
[16] Rammal R, Toulouse G and Virasoro M A 1986 *Rev. Mod. Phys.* **58** 765
[17] Kirkpatrick S and Toulouse G 1985 *J. Physique* **46** 1277
[18] Mézard M, Sourlas N and Toulouse G 1987 *Proc. Heidelberg Coll. on Glassy Dynamics* ed J L van Hemmen and I Morgenstern (Berlin: Springer) p 238
[19] Mackenzie N D and Young A P 1983 *J. Phys. C: Solid State Phys.* **16** 5321