"Valley structures" in the phase space of a finite 3D Ising spin glass with +or-I interactions

1994 J. Phys. A: Math. Gen. 27 L95

(http://iopscience.iop.org/0305-4470/27/4/001)

J. Phys. A: Math. Gen. 27 (1994) L95–L100. Printed in the UK

LETTER TO THE EDITOR

'Valley structures' in the phase space of a finite 3D Ising spin glass with $\pm I$ interactions

T Klotz and S Kobe

Institut für Theoretische Physik, TU Dresden, Mommsenstrasse 13, D-01062 Dresden, Federal Republic of Germany

Received 28 June 1993

Abstract. Exact results for ground states and low-lying excitations of short-range Ising spin glass systems in three dimensions are presented. Using an exact method of nonlinear discrete optimization 'valley structures' in the phase space can be analysed for finite systems. The existence of non-trivial breaking of ergodicity at zero temperature is shown by arranging the highly degenerate ground states in several valleys, which are connected only by the excited states.

The strange structure of the phase space seems to be related to the unusual behaviour of spin glasses, but up to now there has been no detailed knowledge concerning this structure. It was found that the geometry of the space of equilibrium states has a special hierarchical topology characterized by ultrametricity [1] and by bifurcation-like splitting [2]. A complex spanning phase-space structure is suggested by the method of damage spreading [3] analogous to a percolating cluster in a high-dimensional hypercube [4]. There is evidence for non-trivial breaking of ergodicity at zero temperature [5].

Because of the high dimension of phase space and the non-polynomial effort in finding ground states and excitations of spin-glass models, a detailed analysis is very difficult. For two-dimensional spin-glass systems without external field the ground states are found either by exact minimization for small lattice sizes with polynomially increasing computing time [6–8] or by heuristic algorithms (see e.g. [9–11]). However, two-dimensional problems with external field [12] and three-dimensional ones [13] belong to the class of NP-hard problems [14]. This fact suggests that it is unlikely that an algorithm that works as efficiently as in the former case can be found.

In this work the algorithm of branch-and-bound is used [15], which allows one to find exactly all ground states and all low-lying excited states for small systems in reasonable computing time. The aim is to analyse the topology of the phase space by considering distances and connections of states in the phase space.

Cubic Ising spin glass systems on a $4 \times 4 \times 4$ lattice with $\pm I$ interactions between nearest neighbours are considered. Periodic boundary conditions in all three directions are assumed. The distribution of interactions is chosen randomly with an exact distribution of 50% each of ferromagnetic and antiferromagnetic bonds. The zero-field Hamiltonian

$$H = -\sum_{(i,j)} I_{ij} s_i s_j \tag{1}$$

is considered, where the sum is over nearest neighbours.

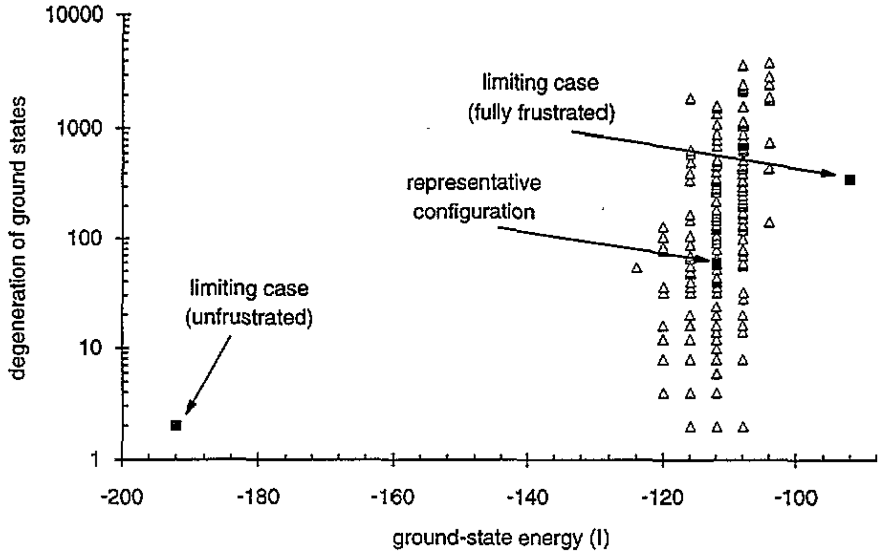

Figure 1. Energy and degeneracy of ground states for 200 random systems.

Using the method of branch-and-bound all ground states of one system are found in a CPU time of about one minute on an IBM3090-200J VF computer.

The results for an ensemble of 200 systems with different distributions of interactions are shown in figure 1. The values of energies found are very similar to those found in [5]. The limiting cases of an unfrustrated and a fully frustrated system are especially marked. The ground-state energy and entropy per spin are calculated as

$$E/N = 1.733(\pm 0.013)I$$
$$S/N = 0.073(\pm 0.007)\,k_B \qquad (2)$$

where I is the strength of interaction, k_B is the Boltzmann constant and N is the number of spins. The given errors are statistical ones.

The ground-state energy per spin is in good agreement with results in [16–18], however the entropy values found in [16, 17] are significantly too small.

In [16] the entropy value $(0.04 \pm 0.01)\,k_B$ was estimated from systems with periodic boundary conditions in only two directions. Obviously, the significantly different results are caused by the different boundary conditions. This can be confirmed by comparing calculations for systems as considered in [16], which have led to a good agreement.

A ground-state entropy per spin of $0.062k_B$ was found by the Monte-Carlo method [17] for systems with $20 \times 20 \times 20$ spins. The deviation from (2) is presumably caused by the fact that not all ground states are found by this method. Otherwise, because of the non-polynomially increasing effort in finding ground states, the influence of finite-size effects could not proved by our method for larger systems.

In the following, one representative system taken from the ensemble of 200 systems in figure 1 is studied in more detail. For this system the values for energy and degeneracy up to the third excitation are given in table 1.

Table 1. Energy and degeneracy of the ground state and the low-lying excitations for the representative system.

Excitation	Energy / I	Degeneracy
0	−112	60
1	−108	3.910
2	−104	94.740
3	−100	1.537.086

To classify the states found, first the neighbouring relations in the phase space are investigated. Doing this, the 60 ground states can be arranged into four groups, which we call *clusters in the phase space*.

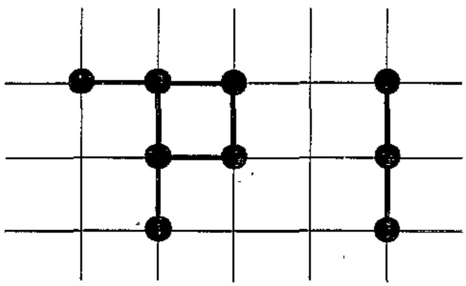

Figure 2. Schematic representation of clusters in the phase space.

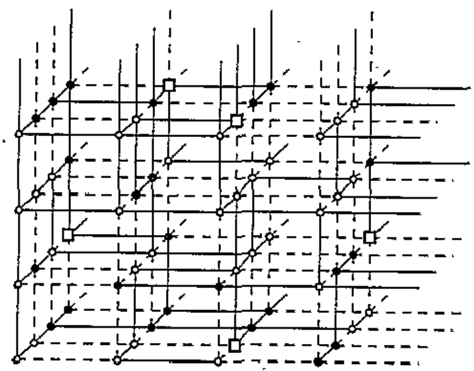

Figure 3. Ground-state cluster 1 (● denotes spin up, ○ denotes spin down, □ denotes spin not fixed, —— denotes ferromagnetic interaction and - - - denotes antiferromagnetic interaction).

To illustrate the term *cluster* we assume that the lattice in figure 2 represents the phase space of the spin system. One node of this lattice belongs to one spin configuration. The spin configurations of two *neighbouring* nodes differ in the orientation of only one spin, this means they have the Hamming distance (HD) one. Assuming that nodes marked by full circles in figure 2 represent a certain subset of all configurations, a classification into two clusters is possible. In general, two-spin configurations belong to the same *cluster* if there exists a chain connecting them, which is built up by neighbouring members of this cluster, i.e. there exists no way between different clusters. In contrast to earlier investigations the knowledge of all ground states and energetically low-lying states makes it possible to find exactly all these clusters. As a result of an analysis of the ground states of the representative system, four clusters can be found (table 2). Due to the symmetry of the Hamiltonian, for every ground-state cluster a mirror image exists. In addition to this trivial breaking of ergodicity at zero temperature there is a non-trivial one, caused by the two remaining different clusters.

These clusters are not closely packed, but the large values of the minimal Hamming distances between different clusters (table 2) leads to the conclusion that they seem to spread out over the whole phase space.

To visualize which spin configurations form a single cluster, the spins, which are fixed in all configurations of this cluster, are marked by filled ($s = +1$, spin up) or empty ($s = -1$,

Table 2. Size of the four ground-state clusters for the representative system and the minimal Hamming distances between them.

		Minimum HD			
Cluster	Size	1	2	3	4
1	18	—	21	59	34
2	12	21	—	34	59
3	18	59	34	—	21
4	12	34	59	21	—

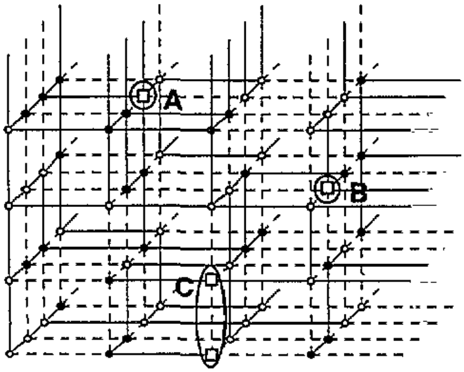

Figure 4. Ground-state cluster 2 (● denotes spin up, ○ denotes spin down, □ denotes spin not fixed, —— denotes ferromagnetic interaction and - - - denotes antiferromagnetic interaction).

spin down) circles in the cubic $4 \times 4 \times 4$ lattice (figures 3 and 4). The variable spins are marked by squares. In cluster 2 (figure 4) there are two isolated spins at A and B. The minimal energy of the two spins at C is realized by three of the four possible states. So this cluster is formed by $2 \times 2 \times 3 = 12$ spin configurations. Analogously there are $2 \times 3 \times 3 = 18$ possible configurations in the first cluster (figure 3).

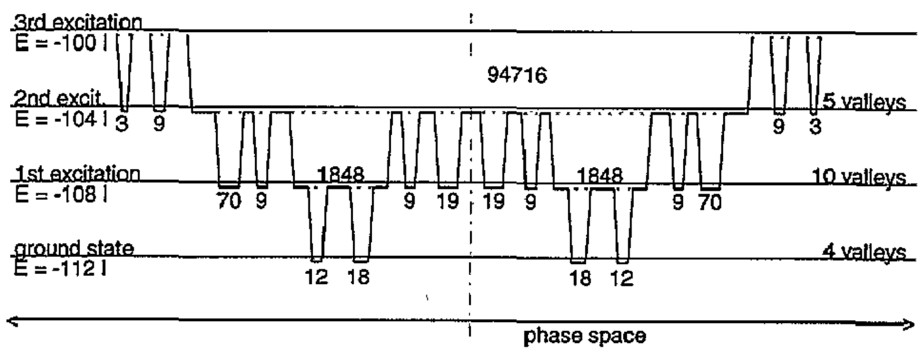

Figure 5. Schematic picture of the 'valley structure' of the representative system.

If, additionally, the spin configurations of energetically low-lying excitations are taken into consideration, an analogous analysis of existing clusters in the phase space leads to a schematic picture of the phase space (figure 5).

With increasing excitation there exist the following effects:

- the appearance of new clusters;
- the fusion of low-lying clusters;
- the fusion of low-lying clusters with their 'mirror images' in the phase space to form a large cluster in the second excitation.

The last effect is of special interest. The cluster, which is built by most of the configurations up to the second excitation, already connects each spin configuration with its 'mirror image' in phase space, which have the maximal Hamming distance of $N = 64$. Otherwise, this cluster is very small in comparison with the whole number of states ($\approx 10^{-11}\%$).

A first attempt to analyse the inner structure of this cluster is made by a calculation of the frequency of relative Hamming distances (figure 6). The symmetry in figure 6 for the Hamming distance 32 is caused by the mirror symmetry of the phase space. However the maxima and minima seem to result from the four ground-state valleys.

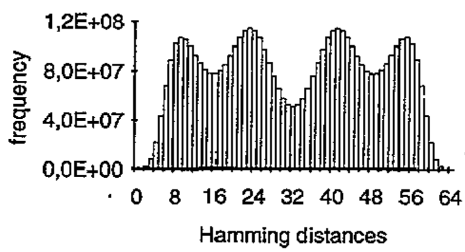

Figure 6. Frequency of Hamming distances for all spin configurations with maximum second excitation.

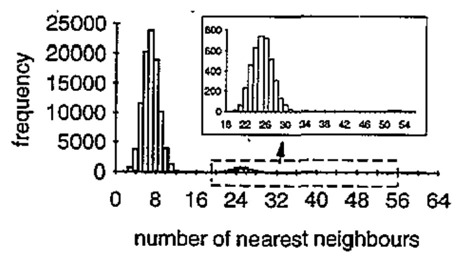

Figure 7. Frequency of the number of nearest neighbours for all spin configurations with maximum second excitation (there is a third, very small peak at 52 nearest neighbours).

The number of nearest neighbours in the phase space that belong to the same cluster, is a measure for a kind of 'local dimension'. In figure 7 the frequency of the number of nearest neighbours for the cluster of second excitation is shown. There are three separate peaks in this curve. By a detailed test these peaks could be identified as being caused by the spin configurations of the second excitation, the first excitation and the ground state, respectively. Although there are large quantitative sample-to-sample fluctuations, the qualitative picture of the phase-space structure is the same, except for samples with a very small degeneracy of the ground state (see figure 1) showing only a trivial ergodicity breaking.

In this letter we have shown that even in simple, very small spin-glass model systems, non-trivial breaking of ergodicity at zero temperature definitely exists as suggested in [5]. Different ground-state valleys are separated by energy barriers with respect to single-spin flips. There are no zero-energy paths between them. It is suggested that this effect is more pronounced with increasing size of the sample, cf also [5]. By including the energetically low-lying excitations one can find complex phase-space structures, which are characterized by the existence of clusters in phase space, which appear, expand and join with increasing excitation. In particular, the internal structure of the ground states is very compact ('high-dimensional'). The ground states are surrounded by the spin configurations of the first and second excitation with a more net-like organization. This picture is in good agreement with the structure suggested in [3].

References

[1] Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M 1984 *Phys. Rev. Lett.* **52** 1156
[2] Palmer R G 1982 *Adv. Phys.* **31** 669
[3] Campbell I A and de Arcangelis L 1990 *Europhys. Lett.* **13** 587
[4] Campbell I A, Flesselles J M, Jullien R and Botet R 1988 *Phys. Rev.* B **37** 3825
[5] Sourlas N 1988 *Europhys. Lett.* **6** 561
[6] Bieche I, Maynard R, Rammal R and Uhry J P 1980 *J. Phys. A: Math. Gen.* **13** 2553
[7] Barahona F, Maynard R, Rammal R and Uhry J P 1982 *J. Phys. A: Math. Gen.* **15** 673
[8] Bendisch J 1992 *J. Stat. Phys.* **67** 1209
[9] Freund H and Grassberger P 1989 *J. Phys. A: Math. Gen.* **22** 4045
[10] Bendisch J 1991 *J. Stat. Phys.* **62** 435
[11] Kawashima N and Suzuki M 1992 *J. Phys. A: Math. Gen.* **25** 1055
[12] Grötschel M, Jünger M and Reinelt G 1987 *Heidelberg Colloquium on Glassy Dynamics* ed J L van Hemmen and I Morgenstern (Berlin: Springer) p 325
[13] Barahona F and Maccioni E 1982 *J. Phys. A: Math. Gen.* **15** L611
[14] Barahona F 1982 *J. Phys. A: Math. Gen.* **15** 3241
[15] Hartwig A, Daske F and Kobe S 1984 *Comp. Phys. Commun.* **32** 133
[16] Morgenstern I and Binder K 1980 *Z. Phys.* B **39** 227
[17] Kirkpatrick S 1977 *Phys. Rev.* B **16** 4630
[18] Berg B A, Celik T and Hansmann U 1993 *Europhys. Lett.* **22** 63