Exact low-energy landscape and relaxation phenomena in ISING spin glasses

T. Klotz and S. Kobe *
Institut für Theoretische Physik, TU Dresden,
D-01062 Dresden, Federal Republic of Germany

Abstract
All ground states and low-lying excitations of a ± I Ising spin glass model on a cubic $4 \times 4 \times 4$ lattice with periodical boundary conditions were calculated using a method of combinatorical optimization. The structure of states in the phase space is enlightened by a representation by means of clusters in the configuration space and their connectivity. The relaxation behaviour of the system can be described by random walks in the high-dimensional phase space. Rewriting this task as an eigenvalue problem the influence of ‘entropic barriers’ in comparison with an unstructured system can be studied, leading to a better understanding of the anomalous slow dynamic behaviour.

1 Introduction
It is well established that the complicated structure of the phase space is the key to understand the unusual behaviour of spin glasses. But up to now, there is little known about the details of this structure even in the simple case of an Ising spin-glass model.

Because of the complexity of the problem and the huge number of $2^N$ configurations of the system with $N$ spins exact complete enumerations restrict the size of the system which can be considered to $N = 20 \ldots 30$. In principle, the ground state is given by the minimization task, in the zero-field case,

$$E_0 = \min_{s_i = \pm 1} \left( -\sum_{i<j} I_{ij} s_i s_j \right). \tag{1}$$

*e-mail address: KOBE@PTPRSI.PHY.TU-DRESDEN.DE
For analyzing the exact low-energy landscape the knowledge of postoptimal solutions of (1) is necessary, too. Optimization tasks of this kind are also important in other fields of physical, mathematical and biological sciences, see e.g. the Coulomb glass problem [1, 2], the Travelling Salesman problem [3] and the protein folding problem [4].

The first numerical method based on nonlinear combinatorial optimization used a branch-and-bound algorithm [5]. It was applied to find the ground state of a two-dimensional amorphous Ising system with $N = 40 \ldots 60$ antiferromagnetically interacting spins ([6] - [8]). For a $\pm I$ spin glass on a square $L \times L$ lattice the ground state can be found with polynomial in $N$ increasing computing time ([9] - [11]). The first exact analysis of the morphology of ground states of a spin system with periodical boundary conditions was given by Barahona et al. [10] for $L = 20$ using the minimal matching of frustrated plaquettes [12]. Systems with equally distributed $+ I$ and $- I$ interactions are characterized by a considerable ground-state degeneration, but there are spins, which maintain the same orientation in all ground states and thus form connected patches, the so-called ‘packets of solidary spins’ [10]. Such a ‘packet’ can be flipped as a whole without any cost in energy. An exact method to compute the complete partition function for $L$ up to 36 is described in [13].

For $\pm I$ systems with increasing concentration of antiferromagnetic bonds $p$ the ground-state threshold is determined as the critical concentration $p_c$ for the vanishing of the ferromagnetic ground state. This concentration can be calculated by heuristic algorithms (see e.g. [14, 15]) or by exact minimal matchings up to a size of $L = 300$ [16].

Two-dimensional problems with external field [17] and three-dimensional ones [18] belong to the class of NP-hard problems [19]. This makes it unlikely that an algorithm can be found which is as efficient as in the zero-field two-dimensional case. A cubic $\pm I$ system with $L = 4$ and periodical boundary conditions is considered in [20] using a recursive branch-and-bound algorithm [21]. All ground states and all low-lying excited states are characterized in respect to their connections in the configuration space. Ground-state calculations for an analogous system but using periodical boundary conditions in two dimensions and free boundaries in the third are recently given on the basis of the transfer-matrix method [22]. It should be mentioned that exact ground-state calculations are complementary to Monte Carlo (MC) calculations (cp. [23] for the three-dimensional $\pm I$ spin glass up to $L = 64$). A useful combination of MC methods and exact numerical investigations enables an analysis of the low-energy structures at least in
local regions of the phase space, see e.g. [24].

Spin glasses appear as suitable model systems to discuss relaxation and aging processes in glassy systems. On a purely phenomenological level the anomalously slow dynamical behaviour is described in terms of empirical laws. Mostly the Kohlrausch law [25] is used to characterize the time dependence of physical quantities by stretched exponentials. Various attempts have been made to give a physical understanding of this picture. The heuristic basis is attributed to the morphology of the phase space, assuming that it is partitioned in ‘components’ by bifurcation-like splitting [26], which at first was mentioned as an idea by Krey [27]. A complex spanning phase-space structure is suggested by the method of damage spreading [28] analogous to a percolating cluster in a high-dimensional hypercube [24]. Theoretical concepts on the basis of the infinite-range Sherrington-Kirkpatrick (SK) model [30] support a special hierarchical topology of the phase space characterized by an ultrametric organization of metastable states which are separated by energy barriers [31]. This picture seems to be consistent with exact results for systems with up to \( N = 24 \) spins [32], heuristic estimations (up to \( N = 96 \)) [33] and experiments [34, 35]. However, there are also arguments against hierarchically constrained dynamics at least for certain time scales [36].

In mesoscopic models special plausible assumptions on the phase-space structure are made. Random walks on tree structures [37] belong to this class of theoretical concepts. Another picture is the droplet model ([38 - 40]), which seems to be related with the above mentioned ‘packet of solidary spins’ in the \( \pm I \) spin glass [10]. Starting with the assumption of only one ground state (apart from the mirror symmetry of the problem) a droplet of the length scale \( l \) is that multi-spin cluster of coherently flipped spins which contains a certain spin and belongs to the lowest excitation energy due to flipping [39]. Such droplets were also found earlier in two-dimensional amorphous Ising systems with antiferromagnetic interactions (\( N = 40 \ldots 60 \)) [4, 5, 11]. Experiments on relaxation of the magnetization of spin glasses qualitatively agree with the results found on the basis of the droplet concept of low-lying excitations which dominate the long-distance and long-time correlations [42]. Further theoretical investigations e.g. on aging in spin glasses [43] support the droplet scenario, too. The question, whether or not the droplet model for short-range spin glasses is in contradiction with hierarchical concepts for the infinite-range SK model, is actively discussed [35, 44]. Especially, the validity of the droplet theory in more than two dimensions is not yet clear [45, 46].
It is expected that a number of still open questions can be handled by means of microscopic concepts. First investigations which make use of the exact knowledge of the low-energy landscape in the phase space of complex systems let this approach appear to be promising. In [3] all configurations connected to a certain suboptimal solution of a Travelling Salesman problem \((N = 32)\) are considered. They form a ‘phase space pocket’ around this minimum. This method has been extended to two-dimensional \((L = 8)\) and three-dimensional \((L = 4)\) short-range Gaussian Ising spin glass systems [47].

The purpose of the present work is to extend the idea of microscopic considerations using for the first time the exact knowledge of the global low-energy phase-space structure of a three-dimensional \(\pm I\) spin glass (section 2). The long-time behaviour of random walks on this structure represented by the largest nontrivial eigenvalue of the transition matrix in the case of infinite temperature is calculated and compared with that of an unstructured system (section 3).

2 Model

A cubic Ising spin glass system on a \(4 \times 4 \times 4\) lattice with \(\pm I\) interactions between nearest neighbours and periodical boundary conditions in all three directions is considered. The distribution of interactions is randomly chosen with an exact portion of 50% of ferromagnetic and of antiferromagnetic bonds. For this system (1) was solved by the method of recursive branch-and-bound [21]. Additional, all energetically low-lying states were calculated with this method.

In [21] the mean ground-state energy per spin \(E(T \to 0)/N = 1.733 (\pm 0.013) I\) and the mean ground-state entropy per spin \(S(T \to 0)/N = 0.073 (\pm 0.007) k_B\) \((k_B -\) Boltzmann constant) were found by calculating the ground-state properties of 200 systems with different distributions of the interactions (Fig. 1).

A classification of the found states of the representative system in Fig. 1 by means of their neighbouring relations in the configuration space leads to an exact first schematic picture of the ‘valley structure’ in the configuration space [20]. This was done by arranging all the states with an energy lower than a chosen energy in clusters. By definition, two spin configurations belong to the same cluster whenever a chain connecting them exists building on neighbouring members of this cluster. Neighbours in the configuration space may differ only in the orientation of a single spin. There are no paths
between different clusters.

At first glance the schematic picture in [20] could be explained by a hierarchical organization of the clusters [37, 48] as shown in Fig. 2a. But another more detailed investigation of the structure with respect to ‘microcanonical’ clusters (i.e. all members of a cluster have the same energy) leads to a more complex picture (Fig. 2b). The found closed circle paths cannot be described by a hierarchy. Moreover, there are connections between different clusters which do not go across energy barriers but underrun such barriers by going first to intermediate states with lower energy.

It should be mentioned here that the connections drawn in Fig. 2b only show that at least one path between the concerned clusters exists, but there is no information about the total number of paths and how difficult it is to find them.

3 Random Walk

One method to quantify the connectivity of the phase space is the concept of the random walk. A random walk on the subset of $M$ low-lying states can be written in matrix notation and solved as an eigenvalue problem [49, 50]. This will be outlined briefly below.

Let $p(t)$ be the vector of probabilities, whose elements $p_i(t)$ give the probability, that at time $t$ the system is in the state $i$. One time step in the random walk will then be described by

$$ p(t + 1) = Ap(t) $$

(2)

where $A$ is the transition matrix with

$$ A_{ij} = \begin{cases} 
  w_{ij} & \text{for } i \neq j \\
  1 - \sum_{k=1,k\neq i}^{M} w_{ki} & \text{for } i = j
\end{cases} $$

(3)

The element $w_{ij}$ denotes the transition probability per unit time from state $j$ to state $i$ and is given by

$$ w_{ij} = \begin{cases} 
  0 & \text{if states } i \text{ and } j \text{ are not nearest neighbours (i.e. Hamming distance > 1)} \\
  \frac{1}{N} & \text{if states } i \text{ and } j \text{ are nearest neighbours and } E_i \leq E_j \\
  \frac{1}{N} \exp(-\beta(E_i - E_j)) & \text{if states } i \text{ and } j \text{ are nearest neighbours and } E_i > E_j
\end{cases} $$

(4)
where $\beta = 1/k_B T$, $E_i$ denotes the energy of state $i$ and $N$ is the maximal number of nearest neighbours, i.e. the number of spins. Because of the definition of $A$ the total probability in the system is constant.

Only for $\beta = 0$ is the matrix $A$ symmetric. For $\beta > 0$ the problem can be transformed into a symmetric one taking into consideration the detailed balancing in the equilibrium distribution [49]. So in the following we restrict ourself to the case $\beta = 0$.

For calculating the time evolution of the system it is useful to split any starting state at time $t = 0$ by the system of eigenvectors of $A$:

\[ p(0) = \sum_{i=0}^{M-1} \alpha_i b_i, \quad Ab_i = \lambda_i b_i \quad (i = 0 \ldots M - 1). \tag{5} \]

Because the matrix $A$ is real and symmetric, all $\lambda_i$ must be real and can be ordered by $\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_{M-1}$. Furthermore all eigenvalues are restricted to $|\lambda_i| \leq 1$. The largest eigenvalue $\lambda_0 = 1$ is the trivial one and describes the equilibrium state $b_0 = p(\infty)$ with $p_i(\infty) \propto \exp(-\beta E_i)$.

Rewriting (2) with respect to (5) the probability distribution at time $t$ is given by

\[ p(t) = AAp(t-1) = AA \ldots Ap(0) = A^t p(0) = A^t \sum_{i=0}^{M-1} \alpha_i b_i \]

\[ = \sum_{i=0}^{M-1} \lambda_i^t \alpha_i b_i. \tag{6} \]

A simple measure of the spreading in the configuration space is the mean distance $r_k(t)$ from the starting configuration $k$ of a random walk. If $h_k$ denotes the vector of Hamming distances to the configuration $k$, $r_k(t)$ can be written as $r_k(t) = h_k^T p(t)$. The deviation $q_k(t)$ to the equilibrium distance is then

\[ q_k(t) = r_k(\infty) - r_k(t) = h_k^T \left( b_0 - \sum_{i=0}^{M-1} \alpha_i b_i \lambda_i^t \right) \]

\[ = - \sum_{i=1}^{M-1} \alpha_i h_k^T b_i \lambda_i^t = \sum_{i=1}^{M-1} \gamma_{ki} \exp(t \ln \lambda_i) \quad \gamma_{ki} = \alpha_i h_k^T h_i \tag{7} \]

using $\alpha_0 = 1$. In the limit of large times one gets

\[ q_k(t \to \infty) \propto \exp(t \ln \lambda_1). \tag{8} \]
Fig. 3 shows $q_k(t)$ for random walks in the representative system with different starting configurations $k$ and $\beta = 0$. The considered subset consists of all states with an energy lower or equal to the second excitation. As expected for long times all curves show an exponential decay with the same exponent $\ln \lambda_1 = -2.98 \cdot 10^{-6}$, which does not depend on the starting position. The time belonging to this value $\tau_1 = 3.36 \cdot 10^5$ is considerable larger than that of an unstructured system, which was calculated in a comparing calculation as $\tau_1^* = 74$, see Appendix A.

4 Conclusions

Based on the exact knowledge of the global low-energy phase-space structure for a $4 \times 4 \times 4 \pm I$ Ising spin glass it is possible to obtain a schematic detailed picture, which shows clusters in the phase space and their connections. The appearence of closed circle paths and the possible underrunning of energy barriers are difficult to describe solely by a simple hierarchical concept.

By the reason of this complicated structure, in general, the relaxation behaviour should be determined not only by the existing energy barriers but also by ’entropic barriers’ [26]. In the case of increasing temperature the influence of the energetic barriers should decrease. Thus, if there is any entropic effect it should be found first in the limes of infinite temperature. However, it should be noted that there is an influence of the cut-off energy, which is necessary in our calculations.

In first approximation the long-time behaviour of a random walk in the low-energy landscape of the system can be characterized by the largest non-trivial eigenvalue of the transition matrix. It could be shown that in comparison with an unstructured system there is a slowing down by a factor of about $10^3$ in the relaxation.

The additional temperature-dependent influence of energy barriers on the dynamics is the subject of further investigations.

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Appendix A - Unstructured Systems

An unstructured system in our sense is a system with minimal structural information. For the reason of comparing it with our system it should have the same number of states $M$. For every state of the unstructured system the number of nearest neighbours $d$ has to be equal to the mean number of nearest neighbours in our system. The number of spins $N$ and thus the dimension of the hypercube describing the whole configuration space is equal for both systems.

The construction of a fictive approximated unstructured system was done by dilution of a $D$-dimensional hypercube where $D \leq N$. This hypercube is embedded in the large hypercube with dimension $N$. Every state of the subcube has to be occupied with a probability of $d/D$ to get $d$ nearest neighbours instead of $D$ for the fully occupied subcube. Since for $d \geq 1$ this probability is larger than the percolation threshold of such a hypercube [24] the remaining subset should form at least one large connected cluster.

Starting the random walk from state $i$ because of the symmetry of the system the occupation probability of state $j$ should only depend on the distance between these two states. Therefore the states of the diluted subcube can divided into $D + 1$ layers where the occupation probability of a state in the $k$-th layer with Hamming distance $k$ to the starting configuration at time $t$ is denoted by $p_k(t)$.

The number of states in the $k$-th layer can be calculated as

$$n_k = \frac{d}{D} \binom{D}{k}.$$  \hfill (9)

If $c_k^+$ and $c_k^-$ are the numbers of nearest neighbours for a state of the $k$-th layer in the $(k+1)$-th layer and the $(k-1)$-th one, respectively, it follows that

$$c_k^+ + c_k^- = d. \hfill (10)$$

The number of all connections between layer $k$ and $k + 1$ must be the same as between layer $k + 1$ and $k$ and therefore

$$n_k c_k^+ = n_{k+1} c_{k+1}^- = n_{k+1} \left( d - c_{k+1}^+ \right) \Rightarrow c_{k+1}^+ = d - \frac{k+1}{D-k} c_k^+$$ \hfill (11)

and

$$c_0^+ = d \Rightarrow c_1^+ = d \frac{D-1}{D} \Rightarrow \ldots \Rightarrow c_k^+ = d \frac{D-k}{D} \Rightarrow c_k^- = d \frac{d}{D}. \hfill (12)$$
Now the occupation probability of a state in the $k$-th layer at time $t+1$ can be written as

\begin{align*}
    p_k(t+1) &= p_k(t) \left(1 - \frac{d}{N}\right) + p_{k+1}(t) \frac{c^+_k}{N} + p_{k-1}(t) \frac{c^-_k}{N} \\
    &= p_k(t) \left(1 - \frac{d}{N}\right) + p_{k-1}(t) \frac{dk}{DN} + p_{k+1}(t) \frac{d(D-k)}{DN}.
\end{align*} 

(13)

Eq. (13) is equivalent to a matrix multiplication $p(t+1) = Bp(t)$ where the matrix $B$ is given by

\begin{equation}
    B_{kj} = \begin{cases} 
        \frac{d(D-k)}{DN} & \text{if } j = k-1 \\
        1 - \frac{d}{N} & \text{if } j = k \\
        \frac{dk}{DN} & \text{if } j = k+1 \\
        0 & \text{otherwise}
    \end{cases}.
\end{equation} 

(14)

The long-time behaviour of the unstructured system is given by the largest nontrivial eigenvalue of $B$. For a given set of $N$, $D$ and $d$ this can easily be done using numerical standard methods.

The values of $N$ and $d$ are defined by the number of spins and the mean number of nearest neighbours in the configuration space of our representative system ($N = 64$, $d \approx 7.7$). $D$ has to be chosen in such a way that the total number of states is correct (i.e. $\approx 10^5$ in our case). The total number of states in the unstructured system is

\begin{equation}
    M = \frac{d}{D} \sum_{k=0}^{D} \left( \frac{d}{D} \right)^k = \frac{d}{D} 2^D \Rightarrow D \approx 18.
\end{equation} 

(15)

Using this combination of $N$, $D$ and $d$ the eigenvalue can be calculated as $\lambda_1 = 0.987$ and $\ln \lambda_1 = -1.4 \cdot 10^{-2}$. The time belonging to this values is $\tau_1^* = 74$.

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Figures

1. Energy and degeneration of ground states for 200 random systems.

2. Detailed structure of the configuration space up to and including the second excitation for the representative system. The drawn circles denote microcannoncial clusters. For each excitation the size of a circle is proportional to the number of states in the cluster, where the scaling factor differs for different excitations.
   a) Explanation by a schematic picture of a hierarchical structure
   b) Result of an exact detailed analysis (the full lines mark an example of a closed circle path).

3. $q_k(t)$ for random walks in the representative system with different starting configurations $k$ for $\beta = 0$. 
Ground-state energy $I$

Degeneration of ground states

- Limiting case (unfrustrated)
- Limiting case (fully frustrated)

Representative configuration

Ground-state energy $I$
configuration space

a) b)
