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The state space of short-range Ising spin glasses: the density of states

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Abstract. The state space of finite square and cubic Ising spin glass models is analysed in terms of the global and the local density of states. Systems with uniform and Gaussian probability distribution of interactions are compared. Different measures for the local state density are presented and discussed. In particular, the question whether the local density of states grows exponentially or not is considered. The direct comparison of global and local densities leads to consequences for the structure of the state space.

PACS. 02.70.-c Computational techniques – 05.50.+q Lattice theory and statistics; Ising problems – 75.10.Nr Spin-glass and other random models

1 Introduction

The often very unusual dynamic behaviour of complex systems like spin glasses [1,2] is significantly determined by the properties of their state space. One key to understand the relaxation and aging effects in this class of systems, in particular for the low-temperature region, is given by the structure of local minima and barriers in the low-lying energy landscape. In order to construct models of this landscape, which are useful for simulating the non-equilibrium dynamics, it is necessary to extract and to quantify the important structural properties of this landscape. Unfortunately, in experiments the state-space structure is only indirectly accessable. For systems with long-range interactions analytical mean-field-like methods have been applied to investigate the state-space properties. The situation for short-range systems is more complicated. Due to the computational effort needed the exact calculation of the energetically low-lying excitations of a system is restricted to small system sizes. Nevertheless the analysis of small sytems can give a first understanding of effects in principle and help to check model assumptions.

One of the simplest models for complex systems is the Ising-spin glass. There has been a great amount of research concerning the long-range SK-model [3]. A few numerical and experimental works tried to analyse the state-space structure more or less directly [4,5]. This was mostly done in order to check the interesting theoretical predictions for the hierarchical structure of the phase space of the SK model [6]. For short-range systems the situation is more unsatisfying. For small $\pm J$ model systems a detailed analysis of the state-space has be made in [7]. It is unclear how strongly the state-space structure found is influenced by the discretness of the interactions. As a counterpart to the $\pm J$ systems, usually systems with Gaussian distributed interactions between nearest neighbours are treated. An extensive analysis of the morphology of the state space was undertaken in [8] by use of the so called lid method.

An interesting outcome of these investigations was, that the local density of states inside a state-space pocket seem to grow exponentially. Such an exponential increase of the local density of states with increasing energy would have drastic thermodynamic consequences. For temperatures below a critical temperature the occupation probability would reach its maximum at the ground-state energy. Thus the system is trapped in a certain state-space valley for a long time or even forever, provided that the barriers surrounding this pocket are high enough. For increasing temperatures the maximum of the occupation probability jumps at a critical temperature T_c from the minimal to the maximal energy of the system. Therefore the probability to leave the considered valley increases drastically. The system is no longer trapped in this valley.

This behaviour is not only important from a thermodynamic point of view, but for optimization problems and methods, too [9]. Assuming there exists such a critical temperature, the cooling scheme for simulated annealing methods should be chosen in such a way that the algorithm has found the ground-state valley at a temperature above the critical one. Otherwise, it may happen that the algorithm never finds the true ground-state due to the low probability to jump to other valleys below the critical temperature.

If the local density of states is exactly exponential, the critical temperature is sharply defined. However, if there is no exponential behaviour, the transition might vanish or is at least smeared out. In this paper we try to clarify this situation. We analysed finite two- and

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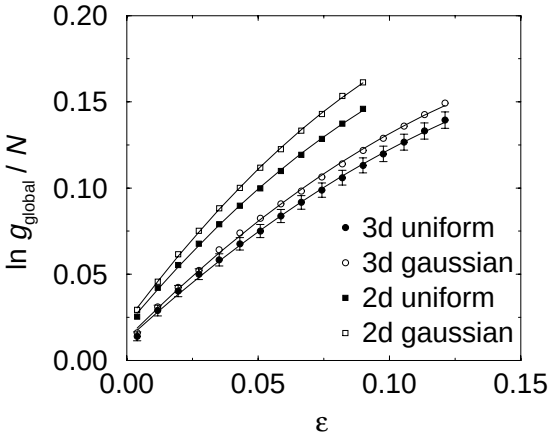

Fig. 1. Global density of states $g_{\mathrm{global}}(\varepsilon)$ for 2d (squares) and 3d (circles) systems with uniform (full symbols) or Gaussian (open symbols) distribution of interactions averaged over different realizations of interactions. The lines correspond to quadratic fits.

three-dimensional systems with respect to their density of states. Starting from the exact knowledge of all energetically low-lying states we calculated at first the global density of states. After sorting the states according to the valley in state space to which they belong, we will discuss various different measures for the local state density. Finally we will compare these different measures.

2 Model and methods

In the following we will present results for two- and three-dimensional Ising-spin systems on square and cubic lattices with randomly chosen interactions between nearest neighbours and periodic boundary conditions. The lattice size is restricted by computational reasons, and is $L = 8$ for the two-dimensional, and $L = 4$ for the three-dimensional case. There is no external field applied to the systems.

We analysed systems with a Gaussian distribution of interactions as well as systems with a uniform distribution. A disadvantage of the Gaussian distribution of interactions, in particular for local structure investigations of the state space, is the possibility of extremely large local fields. These fields can lead to a crossing of all energy barriers by just a single spin flip. This unphysical drawback can be overcome by using a uniform distribution, which is in this sense a counterpart to the Gaussian one. It restricts the maximal strengths of interactions and thus the maximal local field.

In order to allow the comparison of both distributions the first two moments have been set equal. As usual the mean is set to zero and the standard deviation is normalized to unity. If this choice leads to a very similar state-space structure, both system classes could be used alternatively.

The basis of the state-space analysis is an exact determination of all energetically low-lying states up to a given cut-off energy by the method of recursive branch-and-bound [10]. The main idea of this method is to search the binary tree of all states. The search can be restricted by finding lower bounds for the minimal reachable energy inside a subtree. If this lower bound is higher than the energy of a suboptimal state already found, it is not necessary to examine the corresponding subtree. A first good suboptimal state can be found by recursively solving smaller subproblems. By adding an energy offset to the calculated lower bounds it is possible to calculate not only the ground states, but all states below a given cut-off energy too.

The obtained states were ordered by increasing energy using a distributed sort algorithm. Starting from the ground state and successively increasing the maximal energy of the considered states all states are sorted according to their valley in the configuration space. For a chosen energy, two states are sorted to the same valley, if one state can be reached from the other *via* a series of single spin flips without exceeding the chosen energy. Thus the definition of a valley depends on this energy. Each valley can be addressed by the state with minimal energy inside the valley. Note, that a valley is joined with a more low-lying valley, if the considered energy becomes larger than the barrier between both valleys. Furthermore it should be noted here, that the definition of a valley of course depends on the definition of neighbouring spin configurations. As it is done in most investigations we restricted ourself to consider only single spin flip processes.

3 Results

The global density of states $g_{\mathrm{global}}(\varepsilon)$ (GDOS) is defined as the number of states with energy ε per spin above the ground state. Figure 1 shows the logarithm of the global density of states normalized to the number of spins N in the system for the 2d and the 3d systems with Gaussian and uniform distribution. The results are averaged over 20 different realizations of disorder for the Gaussian distribution, and over 50 samples for the uniform distribution. The errorbars give an idea of the sample to sample fluctuations.

The GDOS is significantly higher for the 2d systems compared to the 3d systems. This is obviously caused by the different coordination numbers, as can be seen in Figure 2. The GDOS for the Gaussian distribution is slightly higher than for the uniform distribution. Nevertheless, there seems to be no qualitative difference between the two curves.

For all systems the GDOS clearly increases subexponentially with energy. To quantify this behaviour it is possible to make an ansatz of the form

$$g(\varepsilon) \propto \exp\left(c + \alpha\varepsilon + \gamma\varepsilon^{\delta}\right) \tag{1}$$

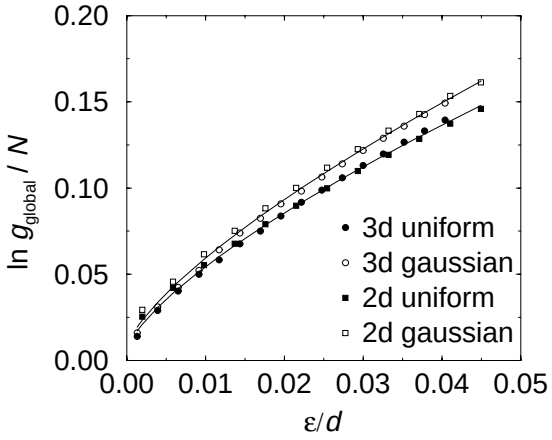

Fig. 2. Global density of states g_{global} *versus* energy per bond for 2d (squares) and 3d (circles) systems with uniform (full symbols) or Gaussian (open symbols) distribution of interactions averaged over different realizations of interactions. The lines correspond to power fits.

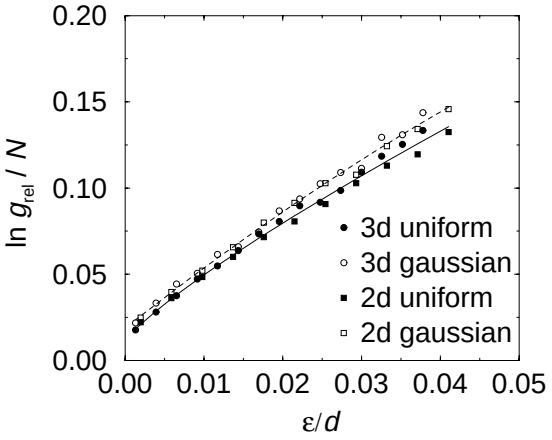

Fig. 3. Relatively measured LDOS g_{rel} *versus* energy per bond for 2d (squares) and 3d (circles) systems with uniform (full symbols) or Gaussian (open symbols) distribution of interactions averaged over different configuration space valleys and different realizations of interactions. The dashed and the full line correspond to a quadratic fit and a power fit, respectively.

for small energies ε above the minimal energy. The occupation probability in equilibrium then reads

$$p(\varepsilon) \propto \exp\left[c + (\alpha - \beta)\,\varepsilon + \gamma\varepsilon^{\delta}\right], \tag{2}$$

where β denotes the inverse temperature. The extremal value of such a distribution is reached for

$$\varepsilon_{\mathrm{ext}} = \left(\frac{\beta - \alpha}{\gamma\delta}\right)^{1/(\delta-1)}. \tag{3}$$

The only singular point in equation (3) is at $\beta = \alpha$. In the linear case $\gamma = 0$ the maximum of equation (2) jumps at this value of β from the maximal energy of the system for high temperatures to the minimal energy for low temperatures.

If however $\gamma \neq 0$ and $\delta > 1$ the subexponential behaviour of the DOS as found in our data leads to a negative coefficient γ. Then it can easily be seen that the energy of the maximum of equation (2) is positive and finite for high temperatures, and goes down with decreasing temperature. At and below $T = 1/\alpha$ the occupation probability is highest for $\varepsilon_{\mathrm{ext}} = 0$. If the linear term in $g(\varepsilon)$ vanishes ($\alpha = 0$) and $0 < \delta < 1$, the maximum energy goes continuously from the maximal energy of the system down to the minimal one with decreasing temperature. Thus there is no sign of a critical behaviour caused by the DOS.

As a result of the above discussion we chose two different ansatzes for fitting functions in the analysis of our numerical data. For $\delta = 2$ equation (1) simplifies to a quadratic polynomial ansatz, which we call in the following the quadratic fit. The choice $\alpha = 0$ leads to a fitting ansatz without any linear term, which will be called power fit.

The quadratic fits shown in Figure 1 fit the data quite well. The ratio of the linear and the quadratic coefficient corresponds for the 3d systems to an energy of about 0.47 per spin. The inverse linear coefficients correspond to a temperature of $T \sim 0.5$ in 2d and $T \sim 0.65$ in 3d. The errors of these fit parameters have been estimated. For the energy per spin it is of the order 0.05 per spin, the error for the temperature can be estimated to 0.05. The lines in Figure 2 are power fits, which seem to fit the data quite well, too. The Gaussian and the uniform distribution differ only in the coefficients c and γ. The exponents δ are about 0.72 for both distributions. The error is of the order 0.05.

The local DOS (LDOS) is given by the number of states inside a valley at a given energy. In order to average the LDOS, it is necessary to clarify the measuring procedure. We discuss here three different possibilities.

The first one is to start at a high temperature and to perform a steepest descent algorithm. The LDOS of the valley the system was trapped in, can then be measured relative to the minimal energy of this valley. The averaging will be done over different runs and different realizations of interactions. We will call the measure defined in this way the relatively measured LDOS (RLDOS) and denote it by g_{rel}.

The second possibility assumes that the ground-state of the system is known already. Then the local density of states can be measured relative to the ground-state energy instead of the minimal energy of the valley found. We will call this variant the absolutely measured LDOS (ALDOS) and denote it by g_{abs}. If the averaging procedures for g_{rel} and g_{abs} are restricted to the ground-state valley, both variants are equivalent and result in the averaged local density of ground-state valleys (GLDOS), which will be denoted by g_{gs}.

It should be noted here, that in practice the averaging will be performed not over different runs, but over all valleys found up to the cut-off energy. This may cause a systematic error due to valleys with local minima higher

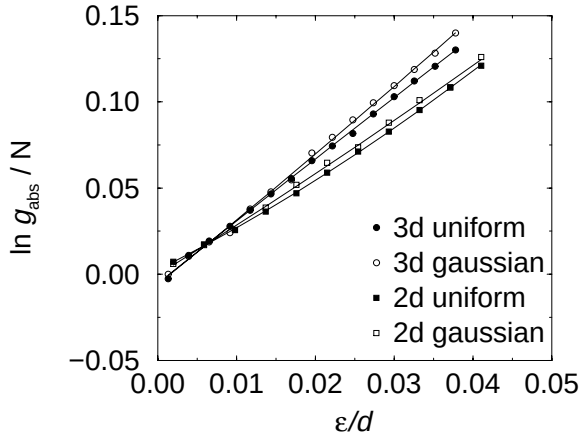

Fig. 4. Absolutely measured LDOS $g_{\rm abs}$ *versus* energy per bond ε/d for 2d (squares) and 3d (circles) systems with uniform (full symbols) or Gaussian (open symbols) distribution of interactions averaged over different realizations of interactions and different valleys. The lines correspond to quadratic fits.

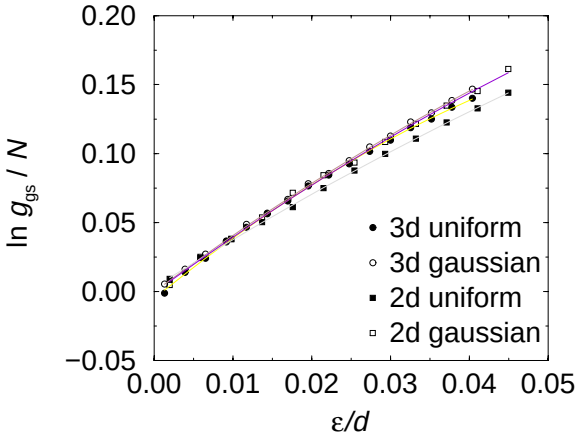

Fig. 5. Local density of states in the ground-state valleys $g_{\rm gs}$ *versus* energy per bond ε/d for 2d (squares) and 3d (circles) systems with uniform (full symbols) or Gaussian (open symbols) distribution of interactions averaged over different realizations of interactions and different valleys. The lines correspond to quadratic fits.

than the cut-off energy. Obviously, this effect could only be important for $g_{\rm rel}$.

As for the GDOS, the RLDOS as a function of the energy per bond ε/d is quite equivalent for 2d and 3d systems (Fig. 3). However, for energies higher than 0.02 per bond there seem to be systematic deviations. In both dimensions $g_{\rm rel}$ is slightly higher for the Gaussian distribution. Both fitting ansatzes fit the numerical data quite well, as can be seen by the examples given in Figure 3. The linear coefficients of the quadratic fits correspond to critical temperatures of about 0.85 in the 3d case. The ratio between the linear and the quadratic coefficients is equivalent to an energy of about 0.6 (2d) and 0.9 (3d). The alternative power fit results in an exponent $\delta \sim 0.85$ for both distributions.

For the absolutely measured DOS it is not possible to map the results for 2d to the results in 3d by taking into account the different coordination numbers (Fig. 4). The planar systems result in a lower ALDOS compared to the cubic systems. Moreover the power fits lead to exponents δ, which are very close to unity. The only exception is the 2d uniform distributed system with $\delta \sim 1.17$. The quadratic fits result in ratios between the linear and the quadratic coefficients larger than 1.0 per spin (2d Gaussian), and larger than 2.0 per spin (3d), which is almost the inverse ground-state energy per spin. The exception is again the 2d uniform distributed system with a ratio of about 0.3 per spin. All in all the ALDOS grows almost exponentially with energy, and the linear coefficients correspond to temperatures of about 0.82 in 3d and 0.71 or 0.87 for 2d systems with Gaussian or uniform distribution, respectively.

For the averaged LDOS of the ground-state valleys the 2d uniform distributed case seems to be an exception too (Fig. 5). It is not clear, whether this is really an effect or just a problem of the statistical errors. The $g_{\rm gs}$ *versus* energy per bond curves for the other cases agree quite well. The power fits lead to an exponent δ between 0.77 and 0.89. According to the ratio of the linear and the quadratic term of the quadratic fits, the deviations from the linear behaviour are of the order unity for energies between 0.6 and 0.9 per spin. The linear terms correspond to temperatures of about 0.5 (2d) and 0.65 (3d), which agree with the GDOS values.

In Figure 6 the different DOS measures are compared for the 3d uniform distributed case. With increasing energy all valleys are joined successively with more low-lying valleys. If there is essentially only the ground-state valley left, the different DOS measures become equivalent. This seems to be the case at an energy of about 0.13 per spin. For all lower energies the global DOS, which counts the states in all existing valleys, is certainly larger than the DOS of the ground-state valleys. Because $g_{\rm abs}$ is averaged over the ground-state valley and more high-lying valleys and $g_{\rm abs}$ is always lower than the ground-state valley DOS $g_{\rm gs}$, for absolutely measured energies the local DOS of the high-lying valleys is smaller than the GLDOS. On the other hand the relatively measured RLDOS $g_{\rm rel}$, which measures the DOS relatively to the minimal energy of a valley, is always larger than the GLDOS. Therefore the more high lying valleys must have larger local densities of states than the ground-state valley measured relatively to the minimal energy of these valleys.

4 Summary

We investigated the global and the local DOS for square and cubic Ising spin glass systems with a Gaussian and with a uniform probability distribution of interactions, respectively. The quantitative differences between the 2d and the 3d systems are mostly caused by their different coordination numbers. Although the first two moments

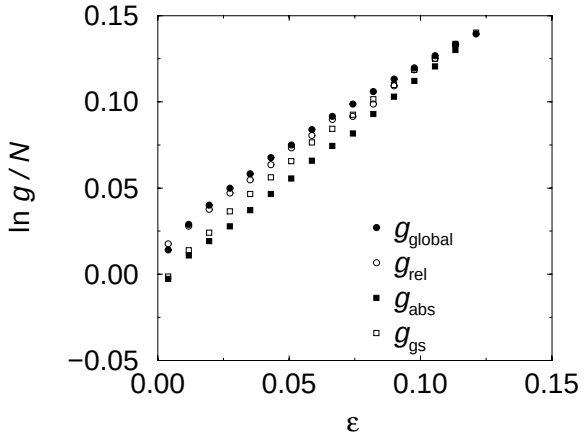

Fig. 6. Comparison of the different DOS measures for the 3d uniform distributed case.

of the chosen distributions of interactions were set equal, the DOS for the Gaussian systems is slightly higher than for the uniform distributed systems. However there is no significant qualitative difference. Therefore it should be possible to use both distributions alternatively for investigations of the state-space structure.

From the direct comparison of the different DOS measures it follows, that at a given absolute energy most of the valleys have a lower LDOS than the ground-state valley. On the other hand, the more high lying valleys have a higher LDOS measured relatively to the minimal energy of the considered valley. Thus we get a picture of the state space with small energetically low-lying valleys which have high energy barriers and wide energetically high-lying valleys with low energy barriers.

The existence of a large ground-state valley in the system could explain, why simple heuristic and approximative optimizing algorithms are often able to find very good sub-optimal states in problems of this kind. In a first approximation the probability to find the ground-state valley of a system by a random search at a given energy is defined by the ratio between the DOS of the ground-state valley and the global DOS. In Figure 6 this ratio is for high energies close to unity and decreases for lower energies. Therefore a simple search algorithm can easily find the true ground-state valley at high energies (or high temperatures). With decreasing energy or temperature the chance to hit the right sub-valley decreases. Thus the algorithm will find sub-optimal solutions, but not necessarily the optimal state.

A second feature of the state space picture seen here is, that for valleys which start at a high energy the RLDOS grows faster with energy than for valleys which start at a lower energy. As the LDOS should determine most of the non-equlibrium thermodynamic properties seen in real or computer experiments, these properties will depend on the energy range at which the system is investigated. This should be kept in mind while approximating ground-state or low-temperature properties by the investigation of energetically high-lying valleys.

The more detailed quantitative analysis of the DOS shows that only the absolutely measured local DOS g_{abs} grows almost exponentially. All other measures for the local DOS and the global DOS grow clearly subexponentially. In all these cases the applied two trial fits with a quadratic and a power ansatz, respectively, describe the numerical data for the logarithm of the DOS quite well.

For the quadratic fits the corrections to the linear behaviour become of the order unity for energies of about 0.5 per spin. The linear coefficients correspond to temperatures, which are for the 3d systems in the region of the transition temperature found for the Gaussian systems [11]. However, although there should only be a zero-temperature transition in 2d, the temperatures resulting from the quadratic fits are about 0.5. The power fits differ in the absolute terms and the coefficients of the power terms. The exponents are with values about 0.7 significantly different to a linear behaviour. Therefore there is at least no sharply defined transition temperature, below which a system is trapped in a valley.

The question whether the form of the local DOS leads to a transition at all remains unclear. To decide this, a further analysis of the occupation probability of a valley with respect to the distribution of energy barriers of this valley would be necessary. Furthermore the barrier distribution combined with the density of local minima will give a better understanding of the physical meaning and the connections between the different LDOS measures.

It should be noted here that the definition of the different DOS measures does not depend on the underlying model. Therefore the quantitative analysis of these properties should also give a better insight into the state space structure of similar physical and optimization problems.

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