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Coarse graining of a spin-glass state space

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Abstract. The complex structure of a spin-glass state space can be simplified by a coarse-graining procedure, i.e. microscopic states being assembled into larger clusters. An algorithm for the coarse graining of the state space of a short-range Ising spin glass is provided, which is the basis of a coarse-grained dynamics. Different ways for modelling the transition rates in the coarse-grained state space are discussed. A comparison with the dynamics of the microscopic system shows that the dynamics in the coarse-grained state space gives an appropriate approximation.

1. Introduction

The complex energy landscape in the state space of spin glasses is a key feature for their dynamic properties. One important ingredient is the existence of a large number of local minima which are separated by energy barriers of different heights. The relaxation at low temperatures is characterized by a slow transition over these barriers. As in typical spin-glass experiments the thermodynamic equilibrium is not reached on macroscopic timescales, non-equilibrium phenomena can be observed such as aging [1–3] and reinitialization effects [4–7]. Thus for the understanding of such phenomena, the knowledge of the state-space structure is of great importance.

The exact enumeration of the state space of complex systems is in most cases impossible, as the effort required to achieve this increases exponentially with the system size. Even if it were to be possible, the large number of microscopic states would lead to a very complex and detailed structure in the configuration space, which constrains computer simulations of the spin-glass dynamics to small regions in state space.

However, the macroscopic properties of a system should not depend on the microscopic details of its configuration-space structure. This raises the question of whether or not a coarse-grained description of a 'real' state space is possible without neglecting the features of interest. For example, it has already been shown that heuristical model state spaces, where the states are organized on hierarchical trees, show typical features of the dynamics of complex systems [8–14].

Such a coarse-grained energy landscape could then be used for visualizing the structure of the state space and is a more sophisticated basis for simulations of the system dynamics in large systems. The coarse-graining procedure itself will give more insight into the microscopic dynamical mechanisms in complex energy landscapes. Moreover the coarsening of the state space can be used to improve optimization algorithms [15].

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In [16] the complex energy landscape of the $\pm J$ spin-glass model has been simplified by assembling microscopic states into so-called microcanonical clusters. However, the definition of the microcanonical clusters is strongly connected to the existence of discrete energy levels in the model, which do not exist in the more general case of continuously distributed interactions.

In this paper we present two coarse-graining procedures which should be regarded as a first step towards the above-defined goal. One procedure is very simple while the other more complicated one tries to capture more details of the landscape. For both procedures we will first discuss their common part, namely in which way the microstates are clustered. We will refer to this as structural coarse graining. In a second step we will then investigate the relaxation dynamics on the original state space and ways to obtain an appropriate coarse-grained dynamics for the clustered states (dynamical coarse graining). Such a coarse-grained dynamics of course neglects the fast local equilibration, but should reproduce the long-time relaxation over energy barriers at low temperatures.

The quality of the different procedures will be checked by comparing the spectra of the relaxation times of the original, microscopic system with those of the coarse-grained systems. The temperature dependence of the largest relaxation times is checked in more detail.

As an example, we analyse the coarse graining of the configuration space of a short-range Ising spin glass. We note, however, that the coarse-graining algorithm considered and the approximation of the dynamics in the phase space do not depend on this choice of model system.

2. The model

As a realization of a complex system, we consider a short-range $4 \times 4 \times 4$ Ising spin glass with periodic boundary conditions. Every state i refers to a spin configuration with energy

$$E_i = -\sum_{\langle m,n \rangle} J_{m,n} s_m s_n \tag{1}$$

where the summation is performed over all pairs of neighbouring Ising spins s which can have only the values $+1$ and -1. The interaction constants $J_{m,n}$ are uniformly distributed with a zero mean and a standard deviation normalized to unity.

The relaxation dynamics considered is given by thermally activated transitions between the different states of the spin glass. The possible transitions are given by flipping one spin at a time. In technical terms this means that if two states differ by one spin only, they are connected in the state space and are called neighbours. As the thermal fluctuations are random, the dynamics is described by a master equation

$$\frac{\partial p_i(t)}{\partial t} = \sum_j w_{ij} p_j(t) \tag{2}$$

where $p_i(t)$ is the probability of being in state i at the time t and w_{ij} with $i \neq j$ is the rate of transition from state j to state i, while $w_{ii} = -\sum_{j\,(\neq i)} w_{ij}$ is the rate of transition out of state i. The transition rates are such that the stationary probability distribution corresponds to the Boltzmann distribution.

For this spin-glass model the total number of states ($>10^{19}$) exceeds the computational possibilities for an exact enumeration by far. Thus we concentrate on the most interesting part of the state space which, in the case of low-temperature relaxation, is comprised of the energetically low-lying states. Therefore we determine all states below a certain cut-off energy using a branch-and-bound algorithm.

3. The structural coarse graining

The aim of the structural coarse graining is to assemble sets of microscopic states into larger clusters. In order to obtain a good approximation for the dynamical properties of the system on macroscopic timescales, it is important that the inner relaxation in a cluster is faster than the interaction with the surrounding clusters. In this case the clusters can be considered to be in internal equilibrium on larger timescales. To fulfil this condition for all temperatures, a cluster must not contain any energy barriers, because such barriers would lead to diverging relaxation times in the zero-temperature limit.

Thus the central aim of this paper is to discuss algorithms that guarantee that there are no internal energy barriers inside a cluster. Furthermore, to make the algorithm independent of the underlying model it should only use general structural information of the system, i.e. neighbourhoods and energies. It should not make use of any particular structural information of the model or any dynamical information such as transition rates.

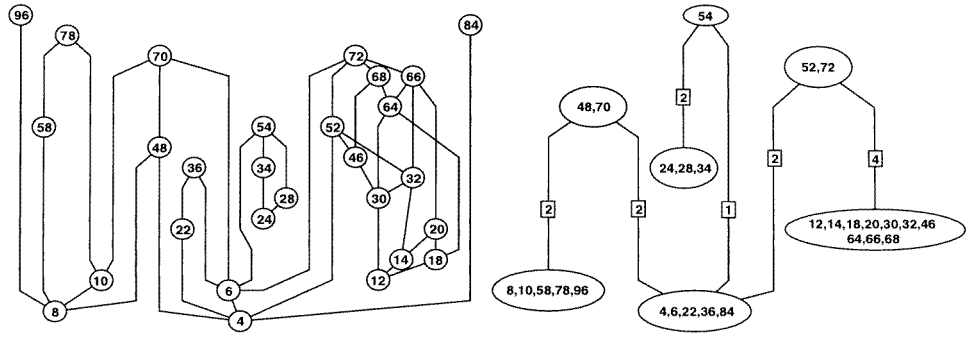

Figure 1. Left: microscopic states with connections. Right: the coarse-grained state space obtained from the microscopic states using the algorithm. The number in a square at a connection is the number of corresponding microscopic connections.

The algorithm for constructing clusters from a microscopic state space is not completely defined by the above conditions. With the additional restriction that such an algorithm should result in clusters with maximal size, we arrived at the following procedure.

(i) Sort all states in ascending order in energy.
(ii) Start with one of the lowest-energy states and
  – create a cluster to which this state belongs;
  – the reference energy of the cluster is the energy of this state;
  – create a new valley to which the cluster and the state belong.
(iii) Consider one of the states with equal energy, or if not present, the state with the next higher energy.
(iv) If the new state is
  (a) not a neighbour to states considered yet ⇒
    – create a new cluster to which the new state belongs;
    – the reference energy of the cluster is the energy of the new state;
    – create a new valley to which the new cluster and the new state belong;
  (b) a neighbour to states which belong to different valleys (such states are here called barrier states; e.g. 48 or 52 in figure 1) ⇒
    – link the connected valleys to one new large valley;

– create a new cluster to which the new state belongs;
– the new cluster belongs to the new large valley;

(c) a neighbour to states which belong to one valley and
(c1) one cluster (e.g. state 6 in figure 1) ⇒ the state is added to this cluster;
(c2) different clusters (e.g. state 72 in figure 1) ⇒ the state is added to the cluster with the highest reference energy;

(v) go to step (iii) until all states have been considered.

This procedure was applied to our example spin-glass model. In figure 1 (left) the structural coarse graining has been applied to a small subsystem with 28 states for demonstration purposes. The resulting coarse-grained system is shown in figure 1 (right), where the numbers inside a cluster are the numbers of the states which are 'lumped' into the cluster.

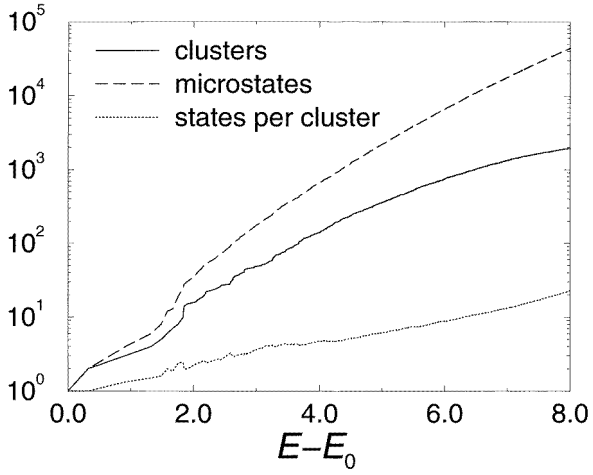

Figure 2. The number of microscopic states with an energy below $E - E_0$ (dashed line) and the number of clusters resulting from the coarse-graining procedure which start at energies below $E - E_0$ (solid line). The dotted curve displays the ratio of the number of microstates below $E - E_0$ to the number of clusters started below this energy.

In figure 2 the total number of microscopic states and of clusters is plotted versus $E-E_0$, where E is the energy of the microscopic state and E_0 is the energy of the global minimum. In the energy range considered, the number of clusters increases more slowly than that of the microscopic states. The mean number of microstates 'lumped' into one cluster increases exponentially, as we can see from the dotted curve. Thus the coarse-graining algorithm becomes more and more effective for larger energies and thus for larger systems.

Figure 3 shows the dependence of the cluster size (the number of microscopic states which are 'lumped' into the cluster) on the minimum energy of the cluster. It can be clearly seen that on average the cluster size decreases with increasing energy. The number of microscopic states inside the clusters which start at small energies is large compared to the number of microscopic states which are located at such energies (see figure 2). This leads to the conclusion that the maximum difference of energies of the microscopic states inside a cluster is large. The clusters are 'long' on the energy axis. The clusters starting at higher energies become smaller, because their parts above the cut-off energy are not considered in the calculation.

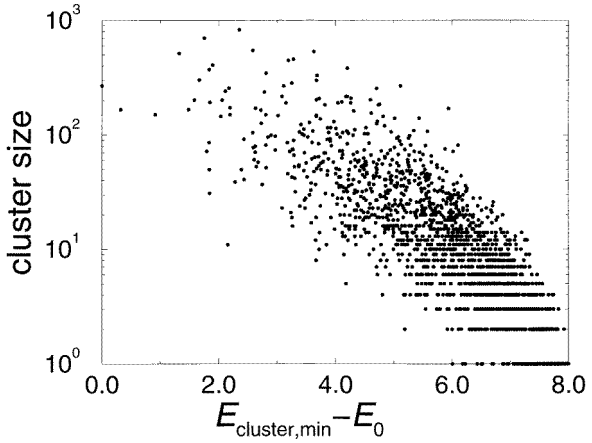

Figure 3. The number of states in a cluster versus its minimum energy.

4. The dynamical coarse graining: transition rates

Now that the topology of the coarse-grained state space is defined, the appropriate transition rates of the coarse-grained system have to be determined. To find the structure of these rates let us start with the exact calculation of the probability of a transition between two neighbouring clusters starting from the microscopic picture. The probability flux from the states belonging to cluster C_ν to the states belonging to cluster C_μ is given by

$$J_{\mu\nu} = W_{\mu\nu} P_\nu = \sum_{j\in C_\nu, i\in C_\mu} w_{ij}\, p_j \tag{3}$$

where P_ν is the total probability of being in cluster C_ν, i.e. the sum of the probabilities of all states in cluster C_ν, and $W_{\mu\nu}$ is the rate of transition from cluster C_ν to cluster C_μ. Again we assume that the internal relaxation inside the clusters is fast compared to the relaxation between different clusters. For the timescale of interest all clusters are in internal equilibrium, i.e. $p_j \propto \exp(-\beta E_j)$. The microscopic transition rates have the form $w_{ij} = w_0 \exp(-\beta \max(E_i - E_j, 0))$. Thus the coarse-grained transition rate is

$$W_{\mu\nu} = \left(\sum_{j\in C_\nu, i\in C_\mu} t_{ij} \exp(-\beta \max(E_i, E_j)) \right) \Big/ \left(\sum_{i\in C_\nu} \exp(-\beta E_i) \right) \tag{4}$$

where t_{ij} equals one if the states i and j are neighbouring and is zero otherwise.

The roughest simplification (here referred to as procedure A) would be to consider all states of a cluster as one state with a certain energy $\hat{E}_i$ which is chosen as the mean energy of the microscopic states. Following this idea, the sums in equation (4) can be simplified to

$$\hat{W}_{\mu\nu} = \frac{\hat{T}_{\mu\nu} \min(\exp(-\beta(\hat{E}_\mu - \hat{E}_\nu)), 1)}{\hat{n}_\nu} \tag{5}$$

where $\hat{T}_{\mu\nu}$ is the number of connections between cluster C_ν and cluster C_μ, and $\hat{n}_\nu$ is the number of states assembled in cluster C_ν.

A better approximation can be achieved if each cluster is modelled by a two-level system, which is in internal equilibrium (procedure B). Here the two sums in (4) become two sums over two terms each. Instead of the four parameters $\hat{T}_{\mu\nu}$, $\hat{E}_\mu$, $\hat{E}_\nu$, and $\hat{n}_\nu$ describing

a connection between two nodes in procedure A, we here obtain eight parameters (twice this set, for the higher and lower levels). Due to the higher number of free parameters, further conditions can be introduced, e.g. that the coarse-grained transition rates match the microscopic ones at certain temperatures or that the first derivatives of the transition rates with respect to the temperature are equal.

Here the parameters have been chosen such that the coarse-grained transition rates match the microscopic ones in the two limiting cases $T \to 0$ and $T \to \infty$. This results in the following procedure.

The state with the minimal energy in a cluster is assigned to the lower level, while the rest of the states of the cluster are assigned to the higher level. In the case where there is more than one state with minimal energy, all of them are assigned to the lower level. The numbers of microstates in the levels are denoted by $\hat{n}^L$ and $\hat{n}^H$, respectively. The levels are assigned the mean energies of the enclosed microstates and labelled by $\hat{E}^H_\nu$ and $\hat{E}^L_\nu$, respectively.

Each connection between two microstates is assigned the energy of the energetically higher end-point. Thus the microconnections between two clusters can also be assigned to two coarse-grained connections. Here we assign the microconnections with the minimal energy to the lower connection, while the rest of the connections are assigned to the higher connection. The numbers of microconnections in the coarse-grained connection are denoted by $\hat{T}^L_{\mu\nu}$ and $\hat{T}^H_{\mu\nu}$, respectively. The coarse-grained connections are assigned the mean energies of the enclosed connections and labelled by $\hat{E}^H_{\mu\nu}$ and $\hat{E}^L_{\mu\nu}$, respectively.

In this case, equation (4) simplifies to

$$\hat{W}_{\mu\nu} = \frac{\exp(-\beta \hat{E}^L_{\mu\nu})}{\exp(-\beta \hat{E}^L_\nu)} \frac{\hat{T}^L_{\mu\nu} + \hat{T}^H_{\mu\nu} \exp(-\beta(\hat{E}^H_{\mu\nu} - \hat{E}^L_{\mu\nu}))}{\hat{n}^L_\nu + \hat{n}^H_\nu \exp(-\beta(\hat{E}^H_\nu - \hat{E}^L_\nu))}. \tag{6}$$

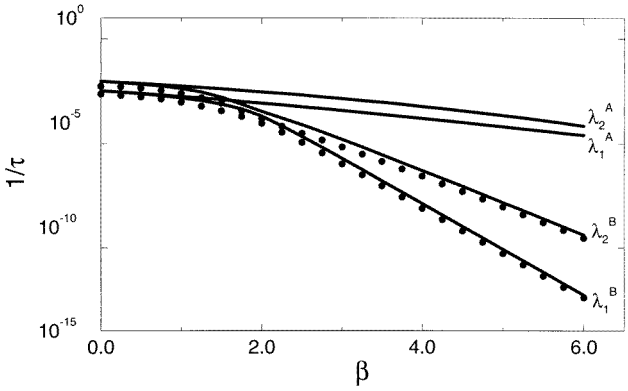

Figure 4. The negative eigenvalues of the transition matrix which correspond to the two largest relaxation timescales are plotted versus the inverse temperature β. The dotted curve refers to the microscopic system with 3971 states. The solid lines show the two negative eigenvalues for the coarse-grained system with 371 clusters, where the dynamics was approximated by procedure A (λ^A) and procedure B (λ^B).

In figure 4 the inverse of the two largest (finite) relaxation times for the coarse-grained and the microscopic system are plotted. These inverse relaxation times τ correspond to the negative eigenvalues of the respective transition matrices. The solid lines show the first two eigenvalues for procedure A (λ^A_1 and λ^A_2) and procedure B (λ^B_1 and λ^B_2), respectively. The

dotted curve corresponds to the microscopic system.

It can be seen that procedure A is quite good for high temperatures, i.e. small β, but gives a too fast relaxation for low temperatures. This behaviour is due to the fact that at low temperatures most of the probability is situated in the low-energy part of the cluster and only the connection between the low-lying states contributes to the probability flux while in the procedure all connections are considered with a uniform weight. Thus the strength of the connection is overestimated and the relaxation is too fast. A much better agreement over a wide range of temperatures is obtained with procedure B.

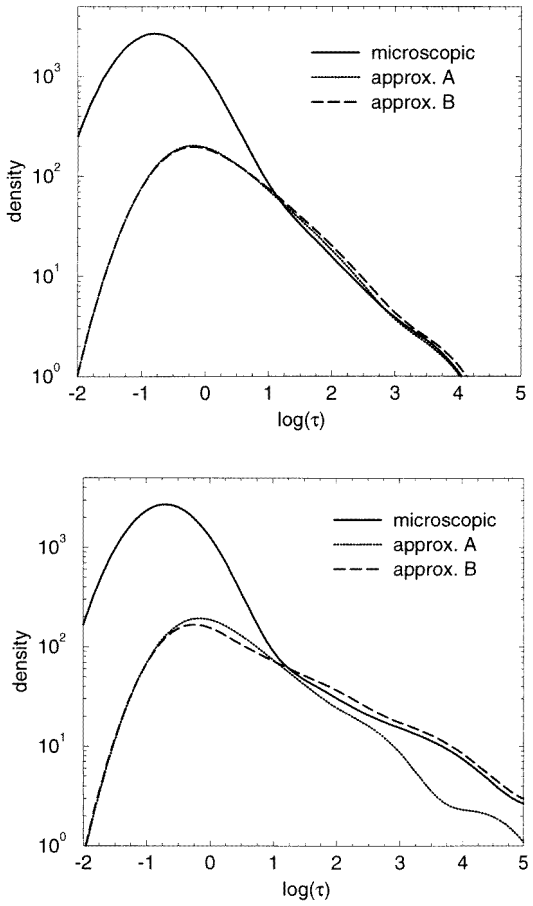

Figure 5. Smoothed relaxation time densities versus the logarithm of the relaxation time for $\beta = 1$ (top) and $\beta = 4$ (bottom) for the microscopic system and the two procedures.

While in the previous paragraph the temperature dependence of the two largest relaxation times has been analysed, we now consider the whole set of relaxation times for different temperatures. Figure 5 shows the density of relaxation times for $\beta = 1$ and $\beta = 4$. The spectra have been computed with a resolution of 0.2 on the logarithmic τ-scale.

In the case of high temperatures (figure 5 (top)) we see a good agreement of the two procedures compared to the case for the original microscopic system in the range of large relaxation times. For short times the microscopic system has many more eigenvalues, which are neglected in the coarse-grained system. Thus the dynamics in the coarse-grained state

space is a good approximation of the dynamics in the microscopic system for slow processes, which are the important ones for the analysis of low-temperature relaxation phenomena.

For lower temperatures (figure 5 (bottom)) the density of relaxation times for procedure A is shifted towards lower values of the relaxation time, i.e. the relaxation is too fast. This observation has already been made from figure 4. Procedure B is also, for lower temperatures (larger β), a good approximation for slow processes.

5. Conclusion

We have provided an algorithm for the coarse graining of complex state spaces. This technique is independent of the choice of model and can be used not only for Ising spin-glass models, as demonstrated, but also for other complex systems such as Lennard-Jones systems and proteins. Coarse graining is not only a means for making the simulation of the dynamics of large complex systems possible, but is also of importance for the visualization of the high-dimensional state spaces of complex systems.

The aim was to construct an algorithm which leads to coarse-grained clusters without any energy barrier inside. The resulting structural coarse graining leads to a sizable reduction of the system size and thus also in the computational effort needed for obtaining a dynamic description. This is implemented by an additional coarsening of the dynamics, for which we provided two procedures. In procedure A, a connection between two clusters was represented by four parameters while a cluster was represented by only two parameters: its mean energy and the number of assembled microstates. Due to the large size of the clusters on the energy axis, the true barrier heights cannot be reproduced in an appropriate fashion. This drawback can be overcome by a more sophisticated modelling. In procedure B, the clusters are modelled by a two-level system which keeps track of the energetical size of the cluster. With this procedure the dynamics of the coarse-grained system is a good approximation for the slow-relaxation modes over a wide range of temperatures.

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