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2000 J. Phys. A: Math. Gen. 33 657

(http://iopscience.iop.org/0305-4470/33/4/301)

J. Phys. A: Math. Gen. **33** (2000) 657–674. Printed in the UK PII: S0305-4470(00)04259-1

A new method for analysing ground-state landscapes: ballistic search

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Received 12 May 1999, in final form 22 November 1999

Abstract. A 'ballistic-search' algorithm is presented which allows the identification of clusters (or funnels) of ground states in Ising spin glasses even for moderate system sizes. The clusters are defined to be sets of states, which are connected in state-space by chains of zero-energy flips of spins. The technique can also be used to estimate the sizes of such clusters. The performance of the method is tested with respect to different system sizes and choices of parameters. As an application the ground-state funnel structure of two-dimensional $\pm J$ spin glasses of systems up to size $L = 20$ is analysed by calculating a huge number of ground states per realization. A $T = 0$ entropy per spin of $s_0 = 0.078(5)k_B$ is obtained.

1. Introduction

The calculation of the energetic minima of spin glass systems (for reviews on spin glassess see [1]) remains the paradigm for difficult optimization problems in physics. Usually, only one of the states exhibiting the lowest energy is calculated, even if a system is characterized by many minima having all the same lowest energy. In [2] an algorithm is presented, which allows one to analyse large numbers of ground states and enables one to identify all ground-state funnels of Ising spin glass systems efficiently. Moreover, it is possible to analyse all funnels without having all ground states available. In this paper the algorithm is presented in detail. Since the algorithm has a random nature, one has to show that the method is in fact reliable. This will be the main part of this paper.

The algorithm is applicable to Edwards–Anderson (EA) $\pm J$ spin glasses. They consist of N spins $\sigma_i = \pm 1$, described by the Hamiltonian

$$H \equiv -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j. \tag{1}$$

The sum $\langle i, j \rangle$ runs over all pairs of neighbours. The spins are placed on a d-dimensional lattice of linear size L with periodic boundary conditions in all directions. Systems with quenched disorder of the interactions (bonds) are considered. Their possible values are $J_{ij} = \pm 1$ with equal probability. To reduce the fluctuations, a constraint is imposed, so that $\sum_{\langle i,j \rangle} J_{ij} = 0$. Since the Hamiltonian exhibits no external field, reversing all spins of a *configuration* (also called *state*) $z = \{\sigma_i\}$ results in a state with the same energy, called the *inverse* of z. In the following, a spin configuration and its inverse are regarded as one single state.

The study of ground-state landscapes helps us to understand the nature of random systems [3]. But the calculation of the minima of H turns out to be a hard computational

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problem: it is only for the special case of two-dimensional systems with periodic boundary conditions in no more than one direction and without external field that a polynomial-time algorithm is known for obtaining exact ground states [4]. For more than two dimensions or in the presence of a magnetic field the problem belongs to the class of the NP-hard tasks [5], i.e. only algorithms with exponentially increasing running time are available. The simplest method works by enumerating all 2^N possible states and has obviously an exponential running time. Even a system size of 4^3 is too large. The basic idea of the so-called *branch-and-bound* algorithm [6] is to exclude those parts of state space where no low-lying states can be found, so that the complete low-energy landscape of systems of size 4^3 can be calculated [7].

A more sophisticated method called *branch-and-cut* [8,9] works by rewriting the quadratic energy function: then a minimum of a linear function is to be found, but an additional set of inequalities must hold for all feasible solutions. Since not all inequalities are known *a priori*, the method iteratively solves the linear problem, looks for inequalities which are violated, and adds them to the set until the solution is found. Since the number of inequalities grows exponentially with the system size, the same holds for the computation time of the algorithm. Anyway, with branch-and-cut small systems up to 8^3 are feasible.

The method utilized here is able to calculate true ground states [10] up to sizes 14^3. For two-dimensional systems, sizes up to 50^2 can be treated. Additionally, in contrast to the methods mentioned earlier, the algorithm used here is able to calculate many statistically independent ground states for each realization of the randomness. The method is based on a special genetic algorithm [11, 12] and on the cluster-exact approximation (CEA) method [13]. This technique is explained briefly in the next section.

But it is not only the computer time needed for the calculation of one ground state which may increase exponentially with the system size. For the $\pm J$ spin glass the number of ground states D, called the *ground-state degeneracy*, grows exponentially with N as well. This is due to the fact that there are always *free* spins, i.e. spins which can be turned over without changing the energy of the system. A state with f independent free spins allows for 2^f different configurations all having the same energy. The quantity suitable to describe this behaviour is the ground-state entropy

$$S_0 \equiv k_B \langle \ln D \rangle \tag{2}$$

where $\langle \cdots \rangle$ denotes the average over different realizations of the bonds. Since the number of free spins is extensive, the entropy per spin $s_0 \equiv S_0/N$ is non-zero for the $\pm J$ spin glass.

As the ground-state degeneracy increases exponentially, it seems to be impossible to obtain all ground states for systems unless they are not very small. To overcome this problem in this work all *clusters* (also called *funnels*) of ground states are calculated. A cluster is defined in the following way: two ground-state configurations are called *neighbours* if they differ only by the orientation of one free spin. All ground states which are accessible through this neighbour relation are defined to be in the same cluster.

The method presented here, called *ballistic search* (BS), is able to obtain all ground-state funnels without knowing all ground states. Additionally one can estimate the size of the funnels. Consequently, it is possible to calculate directly the ground-state entropy per spin even for systems exhibiting a huge $T = 0$ degeneracy. Furthermore, the number of funnels and their size distribution as a function of system size are of interest on their own: for the infinite-ranged Sherrington–Kirkpatrik (SK) Ising spin glass a complex configuration-space structure was found using the replica-symmetry-breaking mean-field (MF) scheme by Parisi [14]. If the MF approximation is valid for finite-dimensional spin glasses as well, then the number of ground-state funnels must diverge with increasing system size. On the other hand, the droplet-scaling picture predicts that, basically, one ground-state funnel dominates

the spin-glass behaviour [15–19]. To address this issue a cluster analysis was performed for small three-dimensional systems of one size $L = 4$ [7]. In [20] two-dimensional spin glasses of sizes up to 5×5 were investigated. As a first application of BS, an analysis of the size dependence of the number of clusters for $d = 3$ (up to $8 \times 8 \times 8$) is presented in [2], revealing an exponential increase as a function of the number of spins.

The paper is organized as follows. First the procedures used in this work are presented in detail. Then the behaviour of the algorithms is tested with respect to different system sizes and parameters. It is shown that BS works reliably. In section 4 a variant of BS is presented, which allows us to estimate the size of clusters, if only a small number of ground states are available per funnel. Next, as an application, the algorithm is utilized to investigate the ground-state cluster structure of two-dimensional $\pm J$ spin glasses. In particular, the dependence of the number of clusters and the number of ground states on N are evaluated. The last section summarizes the results.

2. Algorithms

In this section all necessary algorithms for studying the ground-state clusters are presented. For the calculation of the ground states the CEA method is used, which is explained briefly. If all ground states of a system are available a straightforward method to identify all clusters can be used. But if the system size gets larger, the degeneracy grows extremely; thus it is impossible to obtain all ground states of a realization. In the main part the BS method is presented, which allows us to determine the cluster structure, even if only a tiny subset of all ground states is available. Additionally, the BS algorithm is much faster for the case where all ground states have been calculated.

The basic method used here for the calculation of spin-glass ground states is the CEA algorithm [13], which is a discrete optimization method designed especially for spin glasses. In combination with a genetic algorithm [11, 12] this method is able to calculate true ground states [10] in three-dimensions for systems of sizes up to $L = 14$ on standard workstations. A detailed description of the method can be found in [10]. Here the basic ideas of genetic CEA are summarized.

The concept of *frustration* [21] is important for its understanding. A system is called frustrated, if it is not possible to find a configuration, where all bonds contribute with negative values to the energy. One says it is not possible to *satisfy* all bonds. The CEA method constructs iteratively and randomly a nonfrustrated subset of spins within the system. Spins adjacent to many unsatisfied bonds are more likely to be added to the subset. During this construction a local gauge transformation of the spin variables is applied so that all interactions between subset spins become ferromagnetic [13]. The spins not belonging to the subset act like local magnetic fields on the subset spins. Therefore, the ground state of the subset is not trivial. Since the subset gives raise only to ferromagnetic interactions, an energetic minimum state for its spins can be calculated in polynomial time by using graph theoretical methods [22–24]: an equivalent network is constructed [25], the maximum flow is calculated [26, 27] and the spins of the subset are adjusted to their orientations leading to a minimum in energy regarding the subset. Therefore, the energy is decreased for the total system or remains the same. By iterating this process a few times the total energy of a system is decreased quite efficiently, but obtaining ground states turned out to be very hard.

To increase the efficiency of CEA it is combined with a genetic algorithm [12]. Genetic algorithms are biologically motivated. An optimal solution is found by treating many instances of an optimization problem in parallel, keeping only better instances and replacing bad ones by new ones (survival of the fittest). With an appropriate choice of few simulation parameters,

usually more than 90% of all genetic CEA runs end up with a true ground state. Configurations with a higher energy are not included in further calculations.

Using this method one does not encounter ergodicity problems or critical slowing down as in algorithms which are based on Monte Carlo methods. Moreover, it is possible to calculate many statistically independent configurations (replicas). Genetic CEA was already utilized to examine the ground-state landscape of two-dimensional [28] and three-dimensional [29] $\pm J$ spin glasses by calculating a small number of ground states per realization. Furthermore the existence of a spin-glass phase for nonzero temperature was confirmed for the three-dimensional spin glass [10]. Finally, the method was applied to the $\pm J$ random-bond model to investigate its $T = 0$ transition from ferromagnetism to spin-glass behaviour [30], which takes place by increasing the fraction of antiferromagnetic bonds starting from a ferromagnet.

Once many ground states are calculated the straightforward method to obtain the structure of the clusters works as follows: the construction starts with one arbitrarily chosen ground state. All other states, which differ from this state by one free spin, are said to be its neighbours. They are added to the cluster. These neighbours are treated recursively in the same way: all their neighbours which are yet not included in the cluster are added. After the construction of one cluster is complete, the construction of the next one starts with a ground state, which has not been visited so far.

The running-time of the construction of the clusters is only a linear function of the degeneracy D (O(D)), similar to the Hoshen–Kopelman technique [31], because each ground state is visited only once. Unfortunately, the detection of all neighbours, which has to be performed at the beginning, is of O(D^2), because all pairs of states have to be compared. Since for $L = 5$ systems it is possible that they exhibit more than 10^5 ground states, this algorithm is not suitable for larger sizes than $L = 5$.

So far we have seen how ground states can be calculated with the genetic CEA method and how the cluster structure can be established with a simple but slow algorithm if all ground states are available. Now, the BS method is presented. The main idea is to analyse the cluster structure with having only a small subset of all ground states available, thus much larger systems can be treated.

The basic tool is a *test*, which tells whether two ground states are in the same cluster or not. Assume that it is known that some ground states belong to the same cluster. Now we know that another state z belongs to the cluster as well, if the test tells us that z is in the same cluster as *any* of the states already treated. The main feature of the test is that it can be performed for states which are not direct neighbours in phase space. This is the reason why only a small subset of all ground states is needed.

The test works as follows. Given two independent replicas $\{\sigma_i^\alpha\}$ and $\{\sigma_i^\beta\}$ let Δ be the set of spins, which are different in both states: $\Delta \equiv \{i | \sigma_i^\alpha \neq \sigma_i^\beta\}$. Now BS tries to build a path in configuration space of successive flips of free spins, which leads from $\{\sigma_i^\alpha\}$ to $\{\sigma_i^\beta\}$. The path consists of states which differ only by flips of free spins from Δ (see figure 1). For the simplest version iteratively a free spin is selected randomly from Δ, flipped and removed from Δ. Therefore, a straight path in built in phase space. This is the reason why the search for a path is called *ballistic*. This test does not guarantee finding a path between two ground states which belong to the same cluster. It may depend on the order of selection of the spins whether a path is found or not, because not all free spins are independent of each other. Thus, a path is found with a certain probability p_f, which depends on the size of Δ. Later on, the behaviour of p_f is analysed. It will be shown that it can be easily ensured that p_f is large enough such that all clusters are identified correctly.

The algorithm for the identification of clusters using BS works as follows: the basic idea

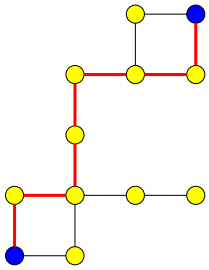

Figure 1. Ballistic search: a path in configuration-space of free spins is constructed between two ground states (dark nodes) belonging to the same cluster. Depending on the order the spins are flipped the path may be found or not. Nodes represent ground states, edges represent flips of free spins. Please note that this figure is only schematic, the configuration space has N dimensions.

is to let a ground state represent that part of a funnel which can be reached using BS with a high probability by starting at this ground state. If a cluster is large it has to be represented by a collection of states, so that the whole cluster is 'covered'. For example, a typical cluster of a $L = 8$ spin glass consisting of 10^{17} ground states is usually represented by only some few ground states (e.g. two or three). A detailed analysis of how many representing ground states are needed as a function of cluster and system size can be found in the next section. At each time the algorithm stores a set of m clusters $A = \{A(r)|r = 1, \ldots, m\}$ each consisting of a set $A(r) = \{z^{rl}\}$ of representing configurations $z^{rl} = \{\sigma_i^{rl}\}$ $(l = 1, \ldots, |A(r)|)$. At the beginning the cluster set is empty. Iteratively all available ground states $z^j = \{\sigma_i^j\}$ $(j = 1, \ldots, D)$ are treated: The BS algorithm tries to find paths from z^j or its inverse to all representing configurations in A. Let F be the set of cluster numbers, where a path is found. Now three cases are possible (see figure 2):

- No path is found: $F = \emptyset$.
  A new cluster is created, which is represented by the actual configuration treated: $A(m + 1) \equiv \{z^j\}$. The cluster is added to A: $A \equiv A \cup \{A(m + 1)\}$.
- One or more paths are found to exactly one cluster: $F = \{f_1\}$. Thus, the ground state z^j belongs to one cluster. Consequently, nothing special happens, the set A remains unchanged.
- z^j is found to be in more than one cluster: $F = \{f_1, \ldots, f_k\}$. Since a path is found from z^j to several states, they all belong in fact to the same cluster. Thus, all these clusters are merged into one single cluster, which is now represented by the union $\tilde{A}$ of the states, which have represented before all clusters affected by the merge:

$$\tilde{A} \equiv \bigcup_{j=1}^{k} A(f_j) \qquad A \equiv \{\tilde{A}\} \cup A \setminus \bigcup_{j=1}^{k} \{A(f_j)\}.$$

This procedure is conducted for all available states. Please note that the merging mechanism ensures automatically that larger clusters are represented by more states than smaller clusters. Later we will see that the number of states necessary to 'cover' a cluster grows only slowly with the cluster size. Thus, systems exhibiting a large degeneracy can be treated.

The whole loop is performed two times. The reason is that a state which links two parts of a large cluster (case 3) may appear in the sequence of ground states before states appear belonging to the second part of the cluster. Consequently, this linking state is treated as being part of just one single smaller cluster and both subclusters are not recognized as one larger cluster (see figure 4). During the second iteration the 'linking' state is compared with all other representing states found in the first iteration, i.e. the large cluster is identified correctly. With one iteration, the problem appears only if few ground states per cluster are available. Nevertheless, two iterations are always performed, so the difficulty does not occur.

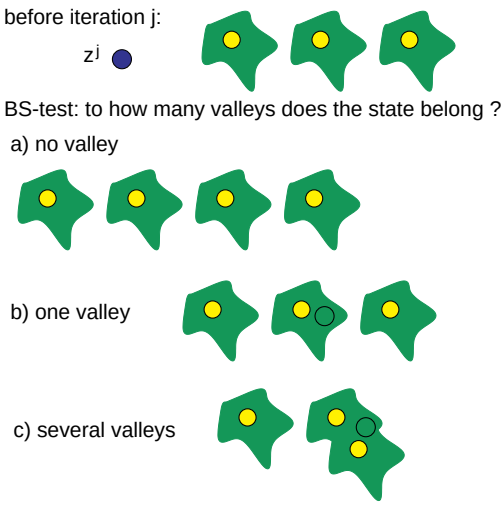

Figure 2. Algorithm for the identification of all clusters: several ground states (circles) 'cover' parts of clusters (filled areas). During the processing of all states a set of clusters is kept. When state z^j is treated, it is tested using BS to how many of the already existing clusters the state belongs. Three cases can occur: (*a*) the ground state is found to belong to no cluster, (*b*) it is found in exactly one cluster and (*c*) it is found in several clusters. In the first case a new cluster is found, in the second one nothing changes and in the third case several smaller clusters are identified as subsets of the same larger cluster.

Now a small example of how the algorithm works is given. Assume that we have six ground states $z^1, \ldots, z^6$. Initially we have an empty set of clusters. The development of the set of clusters is shown in figure 3. The state z^1 surely belongs to a cluster, thus in a first step a cluster with z^1 as representative is created. Now assume that the BS test fails for z^2 and z^1. Thus, a second cluster is created. For z^3 a path is found in phase space to z^2, but not to z^1. Therefore, the cluster structure does not change in this step. Ground state z^3 is represented by an open circle in the figure. This means that it is not stored in the cluster data structure. In the next step, a path is found from z^4 to z^1 and to z^2. Consequently, all states encountered so far belong to the same cluster. Both clusters are merged and now represented by z^1 and z^2. For z^5 a path to z^2 but not to z^1 is found. Nevertheless, this means that z^5 belongs to the cluster as well. Finally, for z^6 no path is found to either z^1 or z^2. Therefore, z^6 belongs to another cluster, which is created in the last step.

The BS-identification algorithm has the following advantages: since each ground-state configuration represents many ground states, the method does not need to compare all pairs of states. Each state is compared only with the representing configurations. For the system sizes usually encountered, this value is only slightly larger than the number of funnels itself. Thus, the computer time needed for the calculation grows only a little faster than $O(Dn_C)$, where n_C is the number of clusters. Consequently, large sets of ground states, which appear already for small system sizes, can be treated. Furthermore, the ground-state funnel structure of even larger systems can be analysed, since it is sufficient that there are only a small number of ground states per cluster available. One has to ensure that really all clusters are found, which is simply done by calculating enough states. A study of how many states are needed for different sizes L is presented in the next section.

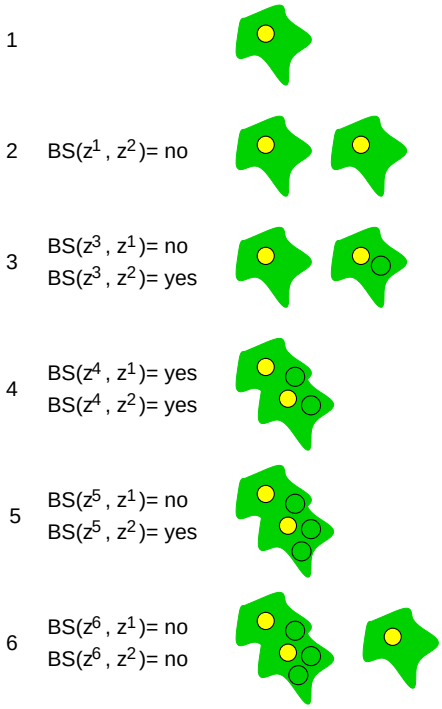

Figure 3. Example run of the BS cluster-identification algorithm. Six ground states are processed. For details, see the text.

3. Numerical tests

Since the BS cluster algorithm does not guarantee finding all clusters, numerical tests on two- and three-dimensional systems were performed. Here, the tests for three dimensions are presented, because for this type of system results are already available [2]. For two dimensions the algorithm behaves similarly. Results concerning the number of ground states and the number of funnels for $d = 2$ are presented later.

For system sizes $L = 3, 4, 5, 6$ and 8, large numbers of independent ground states were calculated using genetic CEA. Usually 1000 different realizations of the disorder were considered. Table 1 shows the number of realizations n_R and the number of independent runs r per realization for different system sizes L. For small systems sizes (and for 100 realizations of $L = 5$) many runs plus an additional local search were performed to calculate all existing ground states. For the larger sizes $L = 5, 6, 8$ the number of ground states is too large, so it is only possible to try to calculate at least one ground state per cluster. We will see later that for most of the realizations it is highly probable that all existing clusters were found using genetic CEA.

But first we concentrate on another issue: the ground states were grouped into clusters using the BS algorithm. To interpret the following results correctly, one should keep in mind that for detecting one ground state being part of a cluster it is sufficient to find just one path to any of the other states of the cluster. The question under consideration now is, how large is the probability that, for ground states belonging to the same cluster, the BS test finds a path?

To investigate this question the following test was performed. Many thousand times pairs of ground states were selected, which belong to the same cluster. The probability for selecting

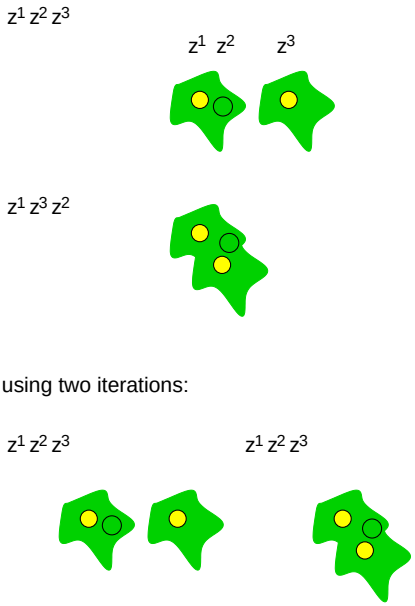

Figure 4. Example showing that the order in which the states are treated may affect the result. Consider three states z^1, z^2, z^3, all belonging to the same cluster. Assume that BS finds a path between (z^1, z^2) and (z^2, z^3), but not between (z^1, z^3). In the first case two clusters are found (false), in the second case one cluster (correct). To always obtain the correct result, two iterations are needed.

Table 1. Three-dimensional $\pm J$ spin glasses. For each system size L: number n_R of realizations, number r of independent runs per realization.

L	n_R	r
3	1000	1000
4	1000	10^4
5	100	10^5
5	1000	3000
6	1000	5000
8	192	2×10^4

a pair was proportional to the size of the cluster. (How to estimate the size of a cluster, if not all ground states are available, is shown in the next section.) This guarantees that each ground state contributes to the result with its proper thermodynamical weight. The outcome of this test depends on the assumption that the construction of the clusters has been performed correctly. Later we will see that this has indeed been the case with a very high probability. Let p_f be the probability that BS finds a direct path in configuration space connecting two given states. The result is expected to depend on the number of spins, which are different in both states, i.e. on the length l_{path} of the path. The result is shown in figure 5 for system sizes $L = 3, 4, 5, 6, 8$. The probability decreases with increasing length of the path. Thus, finding a successful path becomes more difficult, which is to be expected, since the number of possible paths increases exponentially with l_{path}. On the other hand, by increasing the system size, it is more likely to find a connecting path. This is caused by the fact that the number of isolated free spins increases, which in fact can be flipped in any order. To investigate the dependence on L the

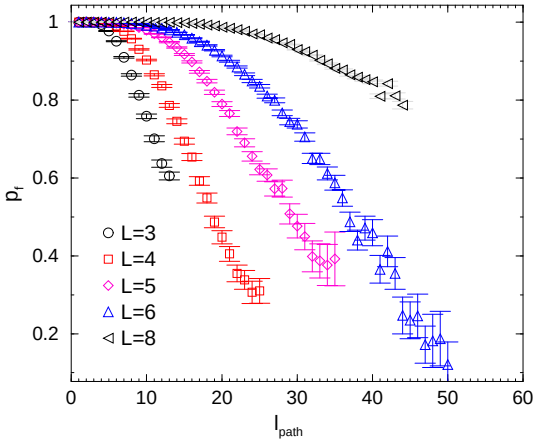

Figure 5. Probability p_f that BS finds a path of free flipping spins between two ground states belonging to the same funnel of three-dimensional $\pm J$ spin glasses. p_f is shown as a function of the number l_{path} of spins, which are different in the two states for lattice sizes $L = 3, 4, 5, 6, 8$.

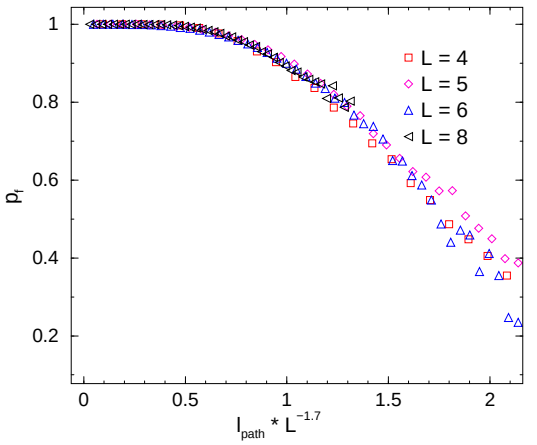

Figure 6. Finite-size scaling plot of $p_f(L, l_{\text{path}})$ (see figure 5). A scaling behaviour of $p_f(L, l_{\text{path}}) = \tilde{p}(L^{-\lambda} l_{\text{path}})$ is assumed. Using $\lambda = 1.7$ the data points for $L = 4, 5, 6, 8$ fall onto one curve near the origin $l_{\text{path}} = 0$.

following finite-size behaviour is assumed (λ being a scaling exponent):

$$p_f(l_{\text{path}}, L) = \tilde{p}_f(L^{-\lambda} l_{\text{path}}). \tag{3}$$

By plotting $p_f(l_{\text{path}}, L)$ against $L^{-\lambda} l_{\text{path}}$ with correct parameter λ the datapoints for different system sizes near $l_{\text{path}} = 0$ should collapse onto a single curve. The best results were obtained for $\lambda = 1.7$. In figure 6 the resulting scaling plot is shown. Now assume that two ground states differ by a certain fraction of spins. Thus, the absolute number of spins being different increases with L^3. Since the length of a path for a fixed value of p_f increases only with $L^{1.7}$, it becomes indeed more and more difficult to find a path with increasing system size L.

So far the behaviour of the BS has been investigated. But what does it mean for the cluster-identification algorithm? We are interested in the question of whether all clusters are

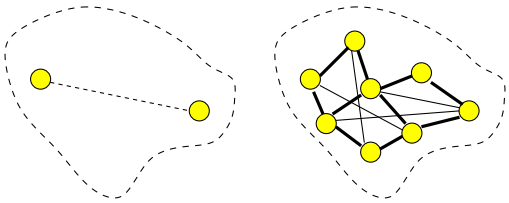

Figure 7. By increasing the number of available states per cluster, the probability increases that they are identified as members of the same cluster. Circles denote states, the thickness of the line represents the probability that a path is found by the BS.

identified correctly. This can be formulated as a generalized percolation problem.

- Consider
  — A set $B = \{z^1, \ldots, z^K\}$ of objects
  — A distance function $d(z^a, z^b)$
  — A probability $p_{\text{bond}}(d)$, that a bond is created between two elements from B, The probability depends on the distance d between the elements and decreases monotonically with d.
- The quantity of interest is the probability p_1 that *all* objects belong to the same cluster, i.e. the probability that there is only one cluster.

One can identify B with a set of ground states belonging all to the same cluster, $d(z^a, z^b)$ with l_{path} and $p_{\text{bond}}(d)$ with the probability p_f that a path is found. Then the quantity p_1 is the probability that all ground states are identified correctly by the BS clustering algorithm as being members of the same cluster. Since the average distance between different states decreases for a given cluster by increasing the number K of states, p_1 should increase with K. The reason is that more bonds are likely to be created (see figure 7). It should be possible to determine $p_1(K)$ for different functions $d(z^a, z^b)$ and $p_{\text{bond}}(d)$, at least numerically. But here a different approach is selected. Since all ground states and funnels are available, $p_1(K)$ can be evaluated directly. For each realization, each lattice size L and each number $K \in [2, 20]$, a set of K different ground states was selected 50 times randomly from one cluster. Again each ground-state funnel was chosen with a weight proportional to its size. The BS clustering method was applied and it was verified whether just one cluster was found. The result is shown if figure 8. As the system size increases, larger clusters occur, which are harder to identify. But it can be seen that even two ground states are sufficient most of the time to identify a cluster correctly. To be almost sure, a value of $p_1 > 0.999$ is expected to be sufficient, which means that $K = 10$ is enough for $L = 3$ and, as found by further analysis, $K = 40$ for $L = 8$.

In fact, for the largest ground-state funnels found in this work there are usually many more ground states available than needed for identifying a cluster correctly with a probability of 99.9%. Consequently, our results for the probability p_f and p_1 are very reliable. Furthermore, whenever the number of ground states is too small, it is always possible to generate additional states by performing $T = 0$ Monte Carlo simulations, i.e. selecting spins randomly and flipping them if they are free. Consequently, we can be sure that the funnels, which were used for the preceding analysis, were obtained correctly.

Another question is, whether for a given realization there are some ground-state funnels, for which no ground states are found using just a restricted number of runs of genetic CEA. This problem does not occur for the smallest sizes, because it is possible to calculate all states of lowest energy using that method. But even for $L = 6$ there are realizations already exhibiting more than 10^6 ground states, making it impossible to obtain all of them directly. The genetic

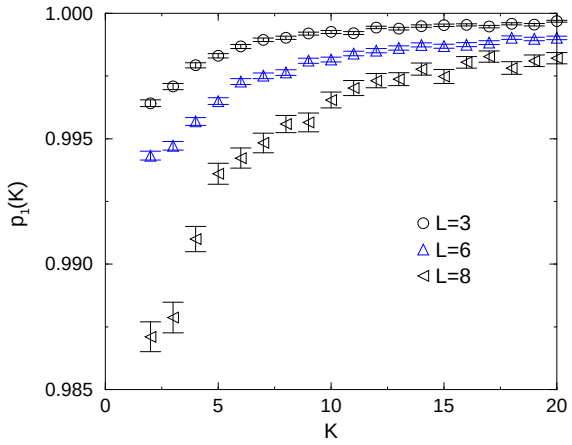

Figure 8. Probability p_1 that a sample of K ground states belonging to the same cluster is indeed identified by the BS clustering algorithm as one single cluster as a function of K for different system sizes L ($d = 3$).

CEA method calculates a ground state with a probability p_C, which increases on average with the size $|C|$ of the cluster it belongs to [32]. Thus, ground states belonging to small funnels have a small probability p_C of being found using a finite number of runs. This probability is not extremely small, since p_C increases slower than the size of a cluster $|C|$ [32], i.e. for $|C_1| < |C_2|$

$$\frac{p_{C_1}}{|C_1|} > \frac{p_{C_2}}{|C_2|} \tag{4}$$

but it is still small enough that some funnels may have been missed. Since p_C increases with $|C|$, the probability that a cluster is *not* found at all takes the largest values for the smallest clusters, i.e. for a cluster of size 1. This probability is denoted here with $\overline{p}_1$. Consequently, $\overline{p}_1$ is an upper limit for the probability that a certain cluster is missed. Now $\overline{p}_1$ is estimated.

Consider a list of K ground states $z^1, \ldots, z^K$ ($z^j = \{\sigma_i^j\}$), in the order they were obtained in the calculation using genetic CEA. Thus, on average, states from larger funnels appear earlier in the list than states from smaller funnels. A state which is calculated several times is stored in the list just once. For each state the number of times h_j it has occurred is recorded, let $h \equiv \sum_j h_j$. For small systems, where the number of existing ground states is small compared with the number of runs, usually $h_j > 1$. Now we look at the smallest cluster $C_{\min}$, which was found using the procedure. The relative frequency, that a ground state from $C_{\min}$ is found, is approximately $p_{\min} = \sum_{j \in C_{\min}} h_j / h$. It follows from (4) that $p_1 > p_{\min}/|C_{\min}|$. Thus, we have for the probability $\overline{p}_1$ that a cluster of size 1 is not found during h different runs

$$\overline{p}_1 = (1 - p_1)^h < \left(1 - \frac{p_{\min}}{|C_{\min}|}\right)^h. \tag{5}$$

Consequently, it is possible to estimate for each single configuration the likelihood that a small cluster may have been missed. For the smaller sizes, where it was claimed that all ground states were found using a large number of runs, typical values $\overline{p}_1 < 10^{-10}$ were found. A small cluster was missed with $\overline{p}_1 > 0.01$ only for three realizations of $L = 3$ and never for $L = 4, 5$. Thus, it is highly probable that all ground states were found for the smaller sizes $L = 3, 4, 5$.

For larger sizes, the number of states obtained per cluster is small compared with the size of the cluster. The estimate (5) gives always a large value. Consequently, another method of estimating the quality of the results has to be applied: the progression of the BS cluster algorithm is observed during the processing of the ground states $z^1, \ldots, z^K$. Each state which causes a new cluster to be created or some clusters to be merged is called an *event*. Since there is only a finite number n_C of clusters and each cluster is represented by a finite number of configurations there is only a finite number of events. For the systems sizes encountered here, the number of events is only slightly larger than n_C, because most of the clusters are represented by just one ground state. In principle, if the last event is known, no further ground states have to be processed. Since the last event is not known for system sizes $L > 5$, one can only assume that the last event has already occurred, if no new event is found for a long time, while treating more and more states z^j. At each step let

$$Q(j) \equiv \frac{j}{\text{number of the last event before } z^j}. \tag{6}$$

The fraction Q measures the relative length of sequences, where no event occurs. For j beyond the last event, $Q(j) \to \infty$. The longest sequence found before the last event, $Q \equiv \max_{j \leqslant \text{last}} Q(j)$, describes how many states are needed to find all clusters without knowing the last event.

Using the number of runs of the genetic CEA algorithms given above, a value of Q larger than 4 was never observed for $L = 3$. This means that one can be sure that all funnels have been identified, if the number of ground states processed is four times larger than the number of the state constituting the last event. For $L = 4$ the largest Q found was 3 and for $L = 5$ it was observed that $Q < 2.5$ for all realizations. For larger sizes Q is not known, so $Q(K)$ is used instead. Assume that the last event has already occurred, then by including more and more states into the analysis, $Q(K)$ grows linearly and the confidence increases that really no further event is to be expected. We believe that if the number K of ground states is more than four times the number of the last event in $z^1, \ldots, z^K$, i.e. $Q(K) > 4$, one can be quite sure that all funnels have been found, because $Q \leqslant 4$ for all small sizes. Even if $Q(K) = 2$, it seems very likely that no cluster has been missed, since Q seems to decrease by going to larger sizes. For $L = 5, 6$ $Q(K) < 4$ was found for only about 8% of the realizations, and $Q(K) < 2$ only for 2% ($L = 5$) respectively 5% ($L = 6$). Consequently, nearly all clusters have been identified. $Q > 4$ holds for 75% of all $L = 8$ realizations ($Q > 2$ for 85%), i.e. here a small number of funnels may have been missed for 25% of all realizations, while for the majority of the realizations really all funnels have been detected. Only by increasing massively the number of available ground states per realization, is a substantial improvement for the largest size treated in this work possible.

On the other hand, if physical properties have to be evaluated, the results are very reliable even for $Q(K) \approx 2$, because each cluster contributes with a weight proportional to its size. As mentioned before, the probability that genetic CEA returns a certain ground state increases with cluster size. Consequently, only small clusters are omitted and the result is affected only slightly.

4. Size of a cluster

Once all clusters are identified their sizes have to be obtained to calculate the entropy. A variant of BS is used to perform this task. Starting from a state $\{\sigma_i\}$ from a cluster C, free spins are flipped iteratively, but each spin not more than once. During the iteration additional free spins may be generated and other spins may become fixed. When there are no more free spins left

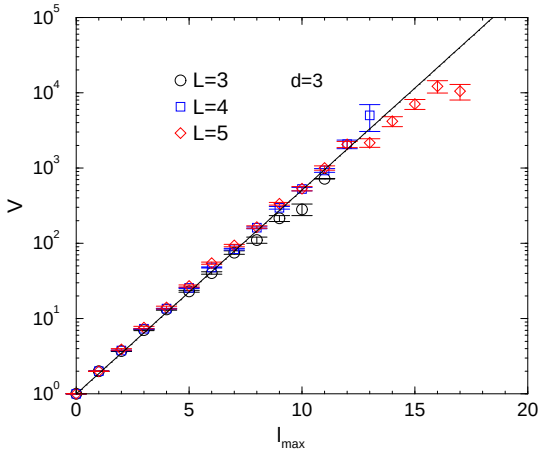

Figure 9. Average size V of a cluster as a function of average dynamic number $l_{\max}$ of free spins (see the text) for three-dimensional $\pm J$ spin glasses of system sizes $L = 3, 4, 5$, where all ground states have been obtained. A $V = 2^{0.9 l_{\max}}$ dependence is found, indicated by a line.

the process stops. Thus, one has constructed a straight path in state space from the ground state to the border of the funnel C. The number of spins that has been flipped is denoted by $l'_{\max}$. By averaging over several trials and several ground states of a cluster, one obtains an average value $l_{\max}$, which is a measure for the size of the cluster.

For system sizes $L = 3, 4, 5$ all ground states were available (for 100 realizations for $L = 5$) and the cluster sizes are known exactly. Figure 9 displays the average size V of a cluster as a function of $l_{\max}$. An exponential dependence is found, yielding

$$V = 2^{\alpha l_{\max}} \tag{7}$$

with $\alpha = 0.90(5)$. The deviation from the pure exponential behaviour for the largest clusters of each system size should be a finite-size effect.

One might think that instead of successively turning spins over, one could simply count the static number of free spins. But it turns out that the quantity $l_{\max}$ describes the size of a cluster better. The reason is that by flipping spins additional free spins are created and deleted. Consider, for example, a one-dimensional chain of N ferromagnetic coupled spins with antiperiodic boundary conditions. Each ground state consists of two linear domains of spins. In each domain all spins have the same orientation. For each ground state there are just two free spins, but all $2N$ ground states belong to the same cluster. The possibility of similar ground-state topologies is taken into account using the definition given above.

5. Results

The data presented in the preceding sections show that earlier results [2] for three-dimensional spin glasses are reliable, where an exponential increase of the degeneracy and the number of ground-state funnels was found. In this section a similar analysis of the ground-state landscape of two-dimensional systems is performed. It will be shown that qualitatively the behaviour is the same as for $d = 3$.

For system sizes $L = 5, 7, 10, 14, 20$ large numbers of independent ground states were calculated using genetic CEA, up to 10^4 runs per realization were performed. Since many runs are needed to describe the ground-state landscape as completely as possible, no runs for

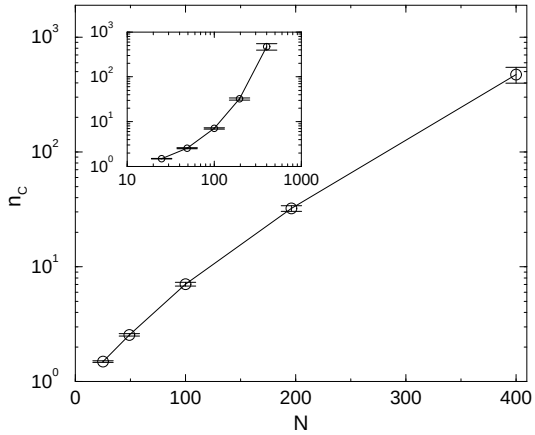

Figure 10. Number n_C of ground-state clusters for two-dimensional $\pm J$ spin glasses as a function of system size N. The inset shows the same data using a double-logarithmic scale. Lines are guides to the eye only.

larger systems were conducted, although it is possible to obtain true ground states easily up to $L = 50$. Usually 1000 different realizations of the disorder were considered, except for $L = 20$, where only 92 realizations could be treated. For the small systems sizes $L = 5, 7$ many runs plus an additional local search were performed to calculate *all* ground states. For the larger sizes $L = 10, 14, 20$ the number of ground states is too large, so we restrict ourselves to calculate at least one ground state per cluster. The probability that some clusters were missed is higher for two dimensions than for the $d = 3$ case, because the ground-state degeneracy grows faster with the system size: for small systems sizes $L \leqslant 10$ it is again highly probable that all funnels have been obtained. For $L = 14$ some small funnels may have been missed for about 30% of all realizations, while for $L = 20$ this fraction rises to even 60%. This is due to the enormous computational effort needed for the largest systems. For the $L = 20$ realizations a total computing time of more than 2 CPU years was consumed on a cluster of Power-PC processors running with 80 MHz.

The ground states were grouped into clusters using the BS algorithm. The number of states per funnel was sufficiently large, so that only with a probability of less than 10^{-3} some configurations from a large cluster may be mistaken for belonging to different funnels. In figure 10 the average number n_C of clusters is shown as a function of the number N of spins. By visualizing the results in a double-logarithmic plot (see inset) one realizes that n_C seems to grow faster than any power of N. The larger slope in the linear–logarithmic plot for small systems may be a finite-size effect. Additionally, for $L = 20$ there is a large probability that some small funnels are missed, explaining the smaller slope there. Consequently, the data presented here favour an exponential increase of $n_C(N)$.

For the small system sizes the number of ground states in each cluster could be counted directly. For the larger sizes the variant of the BS method was used to estimate the size of each cluster. The average size V of a cluster as a function of $l_{\max}$ is displayed in figure 11. Similar to the results presented in the preceding section, an exponential dependence is found, yielding $V = 2^{\alpha l_{\max}}$ with $\alpha = 0.85(5)$.

By summing up all cluster sizes for each realization the ground-state degeneracy D is obtained. Here we have to be careful when using relation (7). The largest contribution to the ground-state degeneracy comes from the biggest clusters. Because the path of the spins being

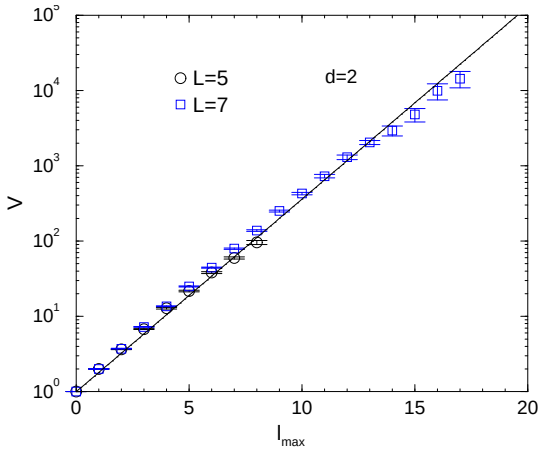

Figure 11. Average size V of a cluster as a function of average dynamic number $l_{\max}$ of free spins (see the text) for two-dimensional $\pm J$ spin glasses of system sizes $L = 5, 7$, where all ground states have been obtained. A $V = 2^{0.85 l_{\max}}$ dependence is found, indicated by a line.

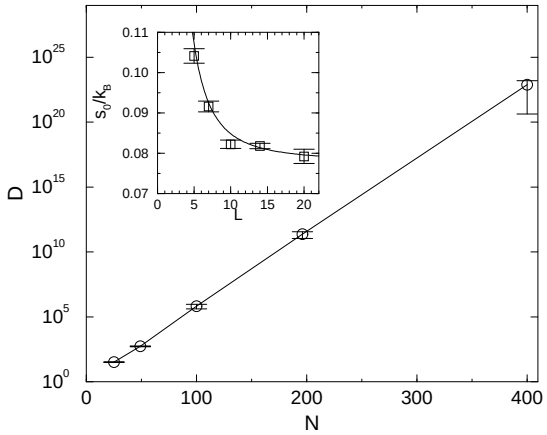

Figure 12. Number D of ground states for two-dimensional $\pm J$ spin glasses as a function of system size N (with $\alpha = 0.8$). The number of states grows exponentially with the number of spins. Lines are guides to the eye only. The inset displays the ground-state entropy per spin as a function of L. The line shows a fit extrapolating s_0 to the infinite system which yields $s_0(\infty) = 0.078(2)k_B$.

flipped may span the whole system, finite-size effects occur and the biggest clusters are smaller than the size given by (7). This is clearly visible in figure 11: please note the logarithmic scale, i.e. the size of the largest clusters is considerably smaller than $2^{0.85 l_{\max}}$. To take this effect into account, for estimating D, a slightly smaller value of $\alpha = 0.8$ is used, where the relation is correct for the largest clusters. The degeneracy averaged over all realizations is shown in figure 12 as a function of N. The exponential growth is obvious.

The result for the average ground-state entropy per spin is shown in the inset of figure 12. By fitting a function of the form $s_0(L) = s_0(\infty) + a * L^{-\beta}$ a value of $s_0(\infty) = 0.078(2)k_B$ is obtained.

The result for the entropy does not suffer from the fact that some ground-state funnels may have been missed for $L = 14, 20$: the probability for finding a cluster by applying genetic

CEA grows with the size of the cluster [32]. This implies that the clusters which may have been missed are relatively small, so the influence on the result is negligible. The largest source of uncertainty is caused by the assumption that the size of a cluster grows like $2^{\alpha l_{\max}}$. The error of the constant α enters linearly into the result of the entropy. To estimate the influence of this approximation, s_0 was calculated using estimated cluster sizes as well for the three smallest systems sizes, where the entropy had been obtained exactly. For both cases the results were equal to the exact values within error bars. The final result quoted here is $s_0 = 0.078(5)$.

In [33] $s_0 \approx 0.075 k_B$ was estimated by using a recursive method to obtain numerically exact free energies up to $L = 18$. The result of $s_0 \approx 0.07 k_B$ found in [34] is even slightly lower. The value found by a Monte Carlo simulation $s_0 \approx 0.1 k_B$ [35] for systems of size 80^2 is much larger. The deviation is presumably caused by the fact that it was not possible to obtain true ground states for systems of that size, i.e. too many states were visited. Recent results are more accurate: by applying the replica Monte Carlo method [36] a value of $s_0 = 0.071(7)$ was obtained. A transfer matrix calculation [37] resulted in $s_0 = 0.0701(5)$. By using a Pfaffian method $s_0 = 0.0704(2)$ [38] respectively $s_0 = 0.0709(4)$ [39] was obtained. The most recent values are smaller than the entropy found in this work. The reason may be that larger systems could be treated (up to $L = 256$ in [38, 39]), while here an extrapolation has been performed with systems of size $L \leqslant 20$. At least, the value $s_0[L = 22] = 0.079(1)$ is comparable with the value of $s_0[L = 32] = 0.0780(8)$ found in [38]. Additionally, the fact that for the other works the number of antiferromagnetic bonds fluctuates from sample to sample while it is kept fixed here may have an influence as well. This was tested by calculating ground states for small systems ($L \leqslant 10$), where each bond has a probability 0.5 of being (anti-)ferromagnetic. In this case the entropy turned out to to 5–10% below the values found above. For large system sizes, which are out of range for the method presented here, this effect should decrease.

The entropy found for $d = 2$ is considerable higher than for the three-dimensional $\pm J$ spin glass, where $s_0(\infty) = 0.051(1) k_B$ was obtained using the same method applied here [2].

6. Conclusion

The BS method has been presented, which allows the fast identification of very large clusters, appearing, for example, in the calculation of the ground-state landscape of $\pm J$ spin glasses. Furthermore, it is possible to calculate clusters of systems when only a small fraction of all their states is available. The method should be extendable to similar clustering problems, especially for analysing results from simulations at finite temperature. A variant of the technique is used to estimate the size of the clusters.

Since the BS algorithm does not guarantee finding a path in configuration space between two ground states which belong to the same cluster, extensive numerical tests were performed. It was shown that by increasing the number of available states, it is possible to reduce the probability that a cluster is not identified correctly. Additionally, it is possible to estimate the probability that small clusters are not found. Consequently, the new technique enables us to analyse the complete funnel structure for two-dimensional $\pm J$ spin glasses up to $L = 20$ and for three-dimensional systems up to $L = 8$. Thus, systems exhibiting up to 10^{17} ground states can be treated efficiently.

For $d = 2$ an analysis of the ground-state landscape has been presented. The number of funnels and the ground-state degeneracy increases exponentially with the system size. The ground-state entropy per spin was found to be $s_0 = 0.078(5) k_B$. This is slightly higher than the values found elsewhere. But it should be stressed that the intention of the method presented here is to study the cluster structure of the ground states. Consequently, only systems of medium size can be treated, which does not allow for precise results for the entropy. Nevertheless, the

result for the entropy does not depend on the way a cluster is defined. The specific definition given here is only a tool which allows the treatment of systems exhibiting a huge ground-state degeneracy. Results for three-dimensional systems can be found in [2].

Acknowledgments

The author thanks K Battacharya for interesting discussions. He is grateful to P Müller for critically reading the manuscript. He was supported by the Graduiertenkolleg 'Modellierung und Wissenschaftliches Rechnen in Mathematik und Naturwissenschaften' at the *Interdisziplinäres Zentrum für Wissenschaftliches Rechnen* in Heidelberg and the *Paderborn Center for Parallel Computing* by the allocation of computer time. The author obtained financial support from the DFG (*Deutsche Forschungs Gemeinschaft*).

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