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The Ground-State Energy of the $\pm J$ Spin Glass. A Comparison of Various Biologically Motivated Algorithms

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We compare various evolutionary strategies to determine the ground-state energy of the $\pm J$ spin glass. We show that the choice of different evolution laws is less important than a suitable treatment of the "free spins" of the system. At least one combination of these strategies does not give the correct results, but the ground states of the other different strategies coincide. Therefore we are able to extrapolate the infinite-size ground-state energy for the square lattice to -1.401 ± 0.0015 and for the simple cubic lattice to -1.786 ± 0.004.

KEY WORDS: Spin glass; ground-state energy; evolutionary algorithms; genetic algorithms; mutation; Monte Carlo simulation.

1. INTRODUCTION

Genetic algorithms are in widespread use for computing optimal solutions of complex problems by means of the evolutionary principles of genetic mixing and genetic mutation respectively.[1,2] Generally these principles can be subdivided into two classes: first, methods where only one genetic code—a population containing one member—is manipulated i.e., the following generations are created by mutation of the genetic code of the actual generation, and second, methods where the population consists of two or more members which may in addition exchange genetic information between each other.

Both strategies were tested in various ways to determine the ground-state energy of the Edwards–Anderson spin glass by biologically motivated algorithms. In principle all the authors agree by initially calculating one or more random configurations of the spin glass which build the initial

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population and afterward manipulating the system by mutations—random flipping of one or more spins without respect to the spin energy—and/or genetic mixing, i.e., mixing of spin sequences of two (or more) members of the population. Further, the manipulated members of the population check if their energy may be lowered through spin flips. Repeating this process several times allows one to generate a population of low-energy configurations. Recent calculations,[3,4] however, showed that it may be more efficient to allow in addition random flipping to the free spins of the system—flipping of these spins does not change the spin energy.

2. IMPLEMENTATION

Generally we examine two different evolutionary algorithms:

(A) *Only Mutation Method.* Only one initial spin configuration is calculated and subsequent generations are created by mutations of this generation. We introduce 10% mutations for each new generation, i.e., 10% of the spins are flipped without regard to energy changes. Afterward the new generation is "equilibrated"—the system is updated in a regular way and all spin flips that lower the configuration energy are carried out.

(B) *Genetic Method.* A random set of spin configurations is calculated initially—we chose a population of 1000 members—and afterward new generations are created by a combination of genetic exchange and mutation. Two "parents" are chosen randomly out of the population and a child is created by randomly mixing half of the spins (the genes) of each parent. This child replaces one of its parents—i.e., each pair may only create one common child. In addition to the genetic exchange process the child receives 10% mutations and afterward all spin flips that lower the configuration energy are carried out (regular updating).

Each of these methods may be extended by the additional rule that free spins whose flipping does not influence the energy of the system ("$E=0$ spins") perform random flipping. We call those methods 1-methods, i.e., A1, B1; and methods where the free spins are fixed, we call 2-methods, A2, B2. For 2-methods the number of sweeps through the lattice to find those spin configurations which lower the energy by flipping is a well-determined finite number, which can be recognized by the algorithm itself. At some time no further flippable spins are detected during one whole sweep, i.e., the spin configuration arrives at an optimal configuration and will not change during further sweeps—on the other hand, for 1-methods any time $E=0$ spins may flip and the algorithm cannot stop. We restrict the maximum number of sweeps for 1-methods to L^2, which means that a mutation is able to influence the whole lattice in a random-walker-like manner.

To calculate the average ground-state energy of the finite-size $\pm J$ spin glass we consider various samples with random configurations of the spin couplings J_{ij}, at least 136 samples for the biggest L, and up to several 10,000 samples for the smallest system sizes. The ground-state energy of each configuration and the average number of generations necessary to reach the ground-state energy are calculated by the following termination criterion: the algorithm calculates new generations continually and we consider between 32 and 136 samples simultaneously on different nodes of the parallel processor. If a member of a new generation shows a configuration energy less than the lowest energy calculated so far, this energy is taken to be the temporary ground-state energy of that sample, i.e., that node of the processor. Further, the number of generations evolved so far is saved. If the algorithm reaches 10 times (for the $d=3$ spin glass, 100 times) this number of generations and cannot further lower the configuration energy of any sample on any node, then we consider that all the samples have reached their ground-state energies. The average number of generations necessary to reach the ground-state energy is calculated as the average of the number of those generations on each node where the last successful improvement of the configuration energy was registered. That is, the algorithm terminates on all nodes at the 750th (7500th) generation if one node calculates an energy improvement for its sample at the 75th generation and further no node calculates any energy improvements up to the 750th (7500th) generation. Afterward every node is asked for the generation where the last energy improvement was calculated—of course all these numbers are less than or equal to 75—and the average of this number is considered to be the average generation number necessary to calculate the ground-state energies.

3. RESULTS

First of all we have to state that, in agreement with calculations of Stauffer,[6] method A2 does not calculate the correct ground-state energy of the $\pm J$ spin glass. The ground-state energies calculated by this algorithm are much higher than those of all the other methods A1, B1, and B2. As shown by Stauffer, even for $L \to \infty$ the extrapolation of the ground-state energies does not agree with the expected spin-glass ground state. For that reason we will not consider strategy A2 any further.

Figure 1 shows that the average ground-state energies calculated by methods A1, B1, and B2 agree for all examined system sizes L for the $d=2$ spin glass. These results are confirmed by a more complex genetic 2-strategy used in ref. 5. Thus the data in Fig. 1 give the dependence of the average ground-state energy of the $d=2$ spin glass on the system size L.

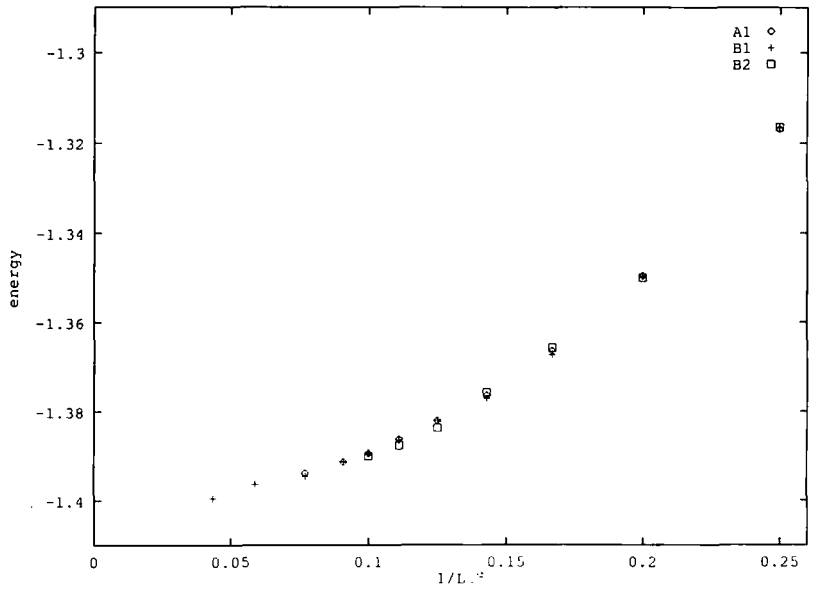

Fig. 1. Ground-state energy versus linear system size L for various strategies.

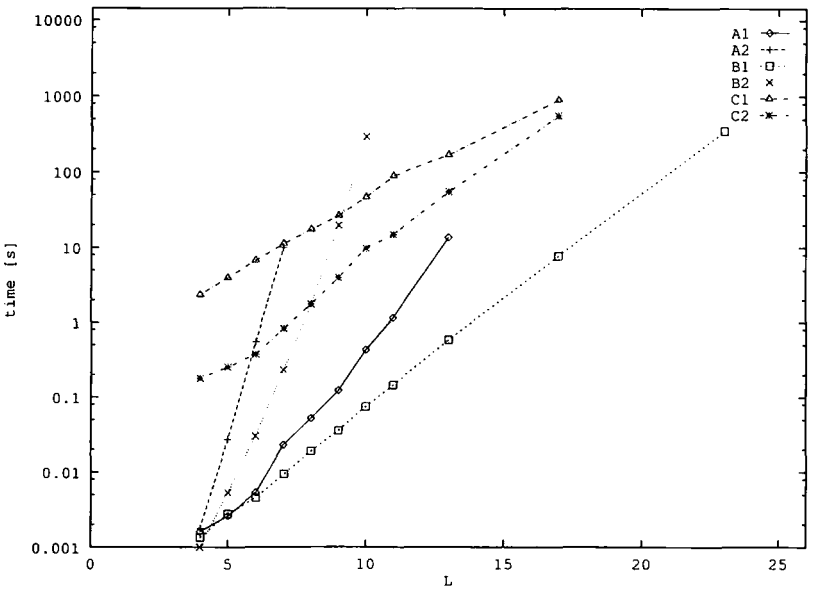

Fig. 2. The average time necessary to find the ground-state energy.

Figure 2 shows the average time in seconds on a single iPSC860 processor required to find the ground state of the spin- glass system depending on the genetic strategy and the system size L. We include the data of a more complex genetic algorithm similar to that of ref. 5, calling these strategy C, i.e., C1 and C2, depending on the law for the free spins—which yield the same ground-state energies as shown in Fig 1. The C strategies are not really comparable to the A and B versions because these methods calculate a whole subset of genetic manipulations to replace all 1000 members of the old generation at once. For small system sizes this means calculating many more configurations than necessary to find the ground-state configuration. In particular, version C1 generates the ground-state energy within the first generation for nearly all systems examined. For the bigger system sizes version C1 is more efficient than version C2; however, for all calculated systems version B1 is faster than both C strategies. Decreasing the number of members of the population may improve the efficiency of the C strategies, but very small populations do not give correct results.

Comparing versions A1, A2, B1, and B2, it can be seen that the different treatment of the $E=0$ spins influences the performance of the algorithm much more than the choice of the genetic strategy. Although the 1-methods need much more time to calculate the "optimal configuration" for each created child, i.e., to recognize those spins which have to be flipped —L^2 sweeps instead of less than 10 for 2-methods, while in addition the calculation of random numbers for the $E=0$ spins is necessary—these methods are much faster than the comparable 2-methods because fewer generations have to be calculated. For the C strategy this effect is not seen at small system sizes because the number of generations cannot be reduced to less than 1. In addition, the very simple only-mutation strategy (A), which was explicitly wrong for the 2-method, calculates correct results for the 1-method.

All the curves show *average* times necessary to calculate minimum energies; often 10 or even 100 times this time is needed to reach the ground-state energies. Our simulations were computed on the Intel Paragon parallel computer at KFA Jülich, using perfect, i.e., replication parallelization to calculate many samples. The maximum computing time available for a single system was 4 hr.

In Fig. 3 the ground-state energy of the square spin glass is plotted against the system size L^2 for $L=4$ up to $L=23$ calculated with strategies A1 and B1. Extrapolation of these data gives an infinite-size ground state of -1.401 ± 0.0015, which agrees with the results of refs. 5 and 7–9. Finally Fig. 4 shows the data for the $D=3$ spin glass computed with strategy B1 and $L=3$ up to $L=8$. We extrapolate the ground state of the infinite cubic

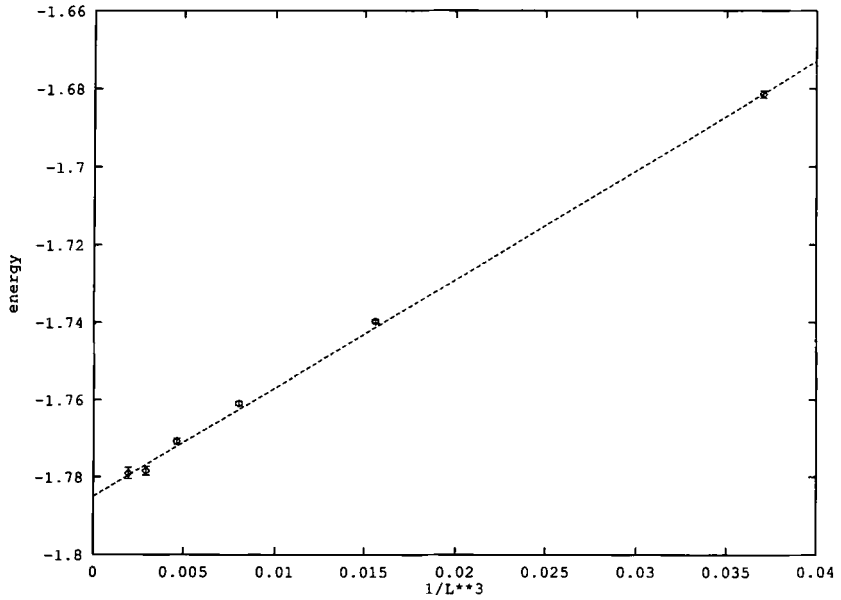

Fig. 3. Extrapolation of the ground-state energy for the $D = 2$ spin glass.

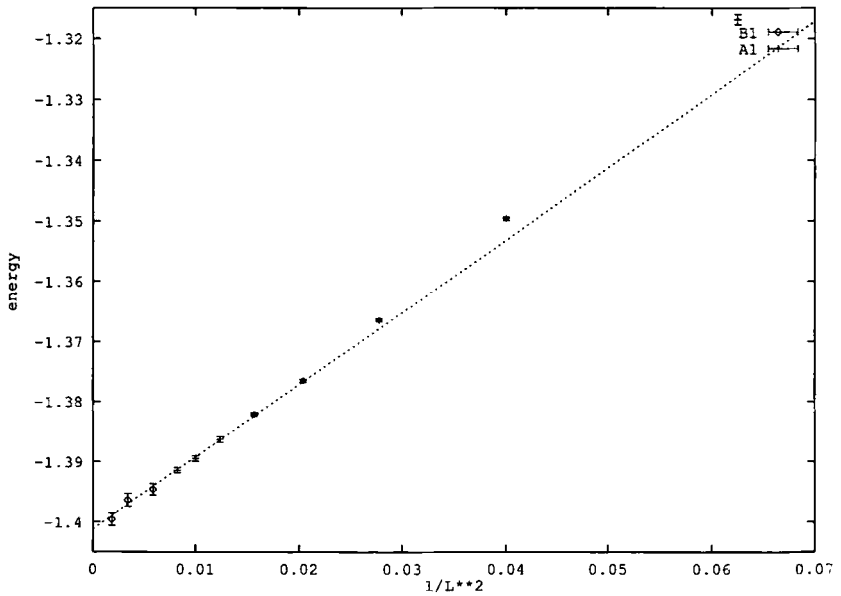

Fig. 4. Extrapolation of the ground-state energy for the $D = 3$ spin glass.

Table I. Ground-State Energies of the $\pm J$ Spin Glass, Using Method B1

L	$D=2$	$D=3$
3	—	-1.68138 ± 0.00089
4	-1.31666 ± 0.00127	-1.73973 ± 0.00058
5	-1.34975 ± 0.00060	-1.76101 ± 0.00054
6	-1.36728 ± 0.00073	-1.77059 ± 0.00078
7	-1.37714 ± 0.00089	-1.77842 ± 0.00111
8	-1.38217 ± 0.00053	-1.77901 ± 0.00147
9	-1.38649 ± 0.00053	—
10	-1.38961 ± 0.00043	—
11	-1.39142 ± 0.00042	—
13	-1.39464 ± 0.00097	—
17	-1.39641 ± 0.00109	—
23	-1.39959 ± 0.00101	—
⋮	⋮	⋮
∞	-1.4010 ± 0.0015	-1.786 ± 0.004
Ref. 5	-1.400 ± 0.005	-1.765 ± 0.01
Ref. 7	-1.394 ± 0.007	-1.786 ± 0.003
Ref. 8	-1.407 ± 0.008	—
Ref. 9	-1.4024 ± 0.0012	—

spin glass to be -1.786 ± 0.004, which is in excellent agreement with the simulation data of ref. 7. Table I gives a list of the ground-state energies of the systems and the probable statistical errors depending on the system size.

4. SUMMARY

Introducing random flipping for the free spins of the system during the biologically motivated configuration search as used by Rodrigues and de Oliveira generally gives better performance calculating the ground-state energies of the $\pm J$ spin glass, independent of the basic evolutionary strategy. For the A and B strategies this fact can be seen obviously from Fig. 2; the C strategy is assumed to show similar behavior for the bigger system sizes, depending on the size of the population. We think that the introduction of random flipping for the free spins reduces the time necessary to calculate the ground-state energies of the spin-glass systems much more than the optimization of the basic evolutionary strategy. For example, we tested some variations of the genetic strategy for the B1 method—a selection rule for the parents according to their "fitness," a selection not of single spins, but of spin sequences, i.e., spin chains during

the gene-mixing process, respectively—and dit not see drastic improvements for the time behavior of the algorithm.

Based on this result we were able to use a very simple genetic algorithm to determine the ground-state energies of the square and simple cubic spin glasses with relatively small computational expense.

Most of the computer time was spent calculating many samples of different random configurations of J_{ij} couplings to increase the accuracy of the average values for the small systems. The computation time to reach the ground-state energy is less than 4 hr with an iPSC860 processor even for the biggest system examined. On the other hand, the calculation of the energies of a large number of samples is necessary to get precise date for the small systems. This makes possible high-quality extrapolations—the data of various samples show considerable fluctuations.

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NOTE ADDED IN PROOF

With a parallel implementation following A. Berengoltz and J. Adler (to be published) we improved our results to -1.401 ± 0.001 and -1.787 ± 0.003 for the square and simple cubic lattice, respectively.

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