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LETTER TO THE EDITOR

On the exact ground states of three-dimensional Ising spin glasses

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Abstract. We present a new method based on linear programming to obtain the exact ground states of three-dimensional Ising spin glasses. Numerical simulations were carried out with the $\pm J$ model, and the Gaussian model with mean μ and variance σ^2. Ferromagnetism disappears in the $\pm J$ model at concentrations of negative bonds near 27%. This occurs, in the Gaussian model, when μ is near 0.6σ.

Numerical simulations of spin glasses have been made during recent years using the Monte Carlo method. At zero temperature this method is quite inefficient to find the true ground states, as the system might be trapped for a very large time in a low-lying excited state. For two-dimensional spin glasses this problem has been solved by an efficient algorithm of combinatorial optimisation in Bieche *et al* (1980). Moreover, the morphology of ground states has been studied by a related method of matching theory in Barahona *et al* (1982). However, in 3D, this problem has been shown to belong to the class of NP-hard problems (Barahona 1982), and this fact suggests that it is very unlikely that an efficient algorithm could exist. Hence, we must expect to obtain an exact solution only for grids of moderate size.

The problem of getting a ground state can be formulated as the quadratic problem

(P1) $\qquad$ Minimise $-\sum J_{ij}S_iS_j$ subject to: $S_i \in \{-1, 1\}$ for any spin i.

Given an assignment of values to the variables $\{S_i\}$, a bond (ij) is said to be satisfied if $J_{ij}S_iS_j > 0$, otherwise it is said to be unsatisfied. Contours having an odd number of negative bonds are called frustrated. Frustrated contours have always at least one unsatisfied bond.

If we define

$$X_{ij} = \begin{cases} 1 & \text{if } (ij) \text{ is unsatisfied,} \\ 0 & \text{if } (ij) \text{ is satisfied,} \end{cases}$$

it is easy to see that (P1) is equivalent to the integer linear programming problem

$$\text{(P2)} \begin{cases} \text{Minimise (1) } \sum |J_{ij}| X_{ij} \text{ subject to:} \\ \text{(2) } \sum_{(ij)\in C} X_{ij} \geq 1 \text{ for any frustrated contour } C, \\ \text{(3) } X_{ij} \in \{0, 1\} \text{ for any bond } (ij). \end{cases}$$

We define (P2′) as (P2), but replacing the integrality condition (3) by (3′) $X_{ij} \geq 0$.

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As is shown in Barahona *et al* (1982), for 2D, (P2′) has always an integer-valued solution, and hence it is a solution of (P2).

For 3D, (P2′) does not necessarily have an integer-valued solution, thus it would give a lower bound of the ground state energy. However, in all the cases we have tried the solution of (P2′) has been integer valued, and hence, a solution of (P2). This fact indicates that (P2′) is a 'tight' relaxation of (P2).

Even when (P2′) is a linear programming problem it cannot be solved directly, because the number of frustrated contours can be tremendously large. We describe below an iterative procedure to solve (P2′), and then show the results obtained with $5\times5\times5$ grids both for the $\pm J$ model and the Gaussian model.

The study of polyhedra associated with combinatorial optimisation problems has been a field of intensive research in the last few years and it has given powerful tools for the solution of these problems. In our case, the frustrated contours define facets of the polyhedron associated with (P2), hence these inequalities are required in any non-redundant description of this polyhedron. In an integer programming sense they are 'strong' cutting planes and can be expected to perform satisfactorily in computation.

We can mention that a similar approach has been successfully applied to the travelling salesman problem in Grötschel (1980) and Padberg and Hong (1980).

The procedure can be described as follows.

Step 1. Solve (P2′) with a subset S of its constraints. Let X be the solution thus obtained.

Step 2. If X does not violate any constraint of type (2) stop, X is the solution of (P2′). Otherwise identify a set of violated constraints of type (2), add this set to S and go to step 1.

Step 1 can be carried out with a linear programming package such as IBM's MPSX or CDC's APEX. There are standard procedures to revise the solution when a set of constraints is added.

Step 2 involves a combinatorial problem that can be solved in polynomial time. To describe the method we will use some graph theoretic terminology that can be found in Berge (1962) and Harary (1969).

First, we describe the heuristic method we have utilised. The grid is seen as a graph G, the weight X_{ij} is given to the bond (ij), and a minimum-weighted spanning tree T is found. When a bond in $G-T$ is added to T a cycle is formed; if this cycle is a frustrated contour the sum of the weights of its bonds is computed and compared with 1. In all the cases we have tried this procedure has given a large set of violated constraints. Furthermore, if we fix as satisfied the bonds in T, we obtain a spin configuration that can be a good approximation to the ground state, and can give a good upper bound to the ground state energy. On the other hand, the solution X gives a lower bound to this energy. The size of the interval defined by these bounds decreases when the computation advances. If these two bounds coincide, the ground state is attained.

Now, we will describe an exact method to carry out step 2. First, at the middle of each positive bond, a vertex is added. It is easy to see that there is a one-to-one correspondence between frustrated contours and cycles of odd cardinality in the new graph. As each positive bond has been transformed into two bonds, the weight of the new bonds must be one half of the weight of the original one. In Grötschel and Pulleyblank (1981) is described a polynomial method that utilises the matching algorithm to find a minimum-weighted odd cycle. We have not used this procedure because our heuristic method takes less computation time.

In order to essay this method we have tried three samples of n impurities randomly distributed in a cube of edge size 10^{-5} cm. The interactions are calculated as

$$J(r_{ij}) = \cos(2.4 \times 10^8 r_{ij})/r_{ij}^3,$$

where r_{ij} is the distance between the impurities. We have found the ground states considering only the m greatest interactions. In table 1 are shown for different values of n and m the number of iterations of the algorithm (number of times that step 1 and step 2 must be executed), and the total number of frustrated contours needed.

Table 1.

n	m	Iterations	Frustrated contours
100	435	6	3028
125	510	6	2473
150	601	10	5055

Then we have tried with $5 \times 5 \times 5$ grids with periodic boundary conditions, and $\pm J$ interactions. Table 2 shows the number of iterations of the algorithm and the total number of frustrated contours needed, for different values of X, the concentration of negative bonds.

Table 2.

X	Iterations	Frustrated contours
0.10	2	712
0.20	5	1631
0.25	27	4869
0.30	19	5253

In figure 1 the ground state energy (per spin) is plotted as a function of X. In figure 2 the magnetisation is plotted as a function of X. It can be noted that ferromagnetism disappears for X near 0.27.

Finally we have tried with the Gaussian model with mean μ and variance σ^2, in $5 \times 5 \times 5$ grids with periodic boundary conditions. Table 3 shows the number of iterations and the number of frustrated contours for $\mu = 0, 0.3\sigma, 0.6\sigma, 0.9\sigma$.

Table 3.

μ	Iterations	Frustrated contours
0	15	4096
0.3σ	16	3897
0.6σ	10	4090
0.9σ	3	1165

In figure 3 the ground state energy (per spin) divided by σ is plotted as a function of μ.

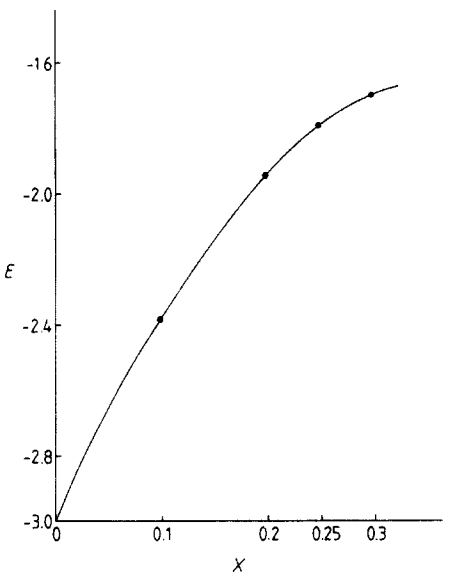

Figure 1.

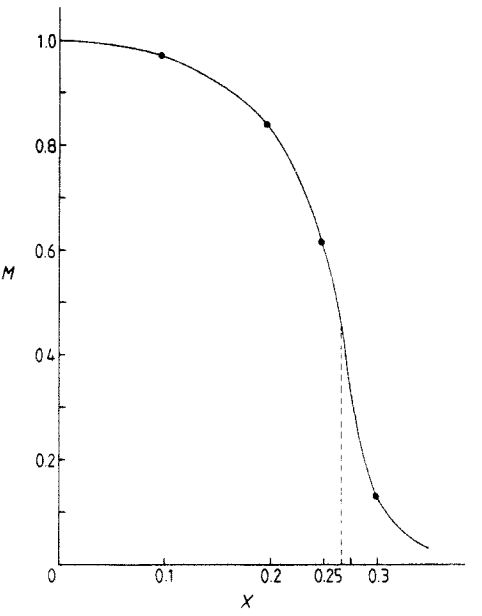

Figure 2.

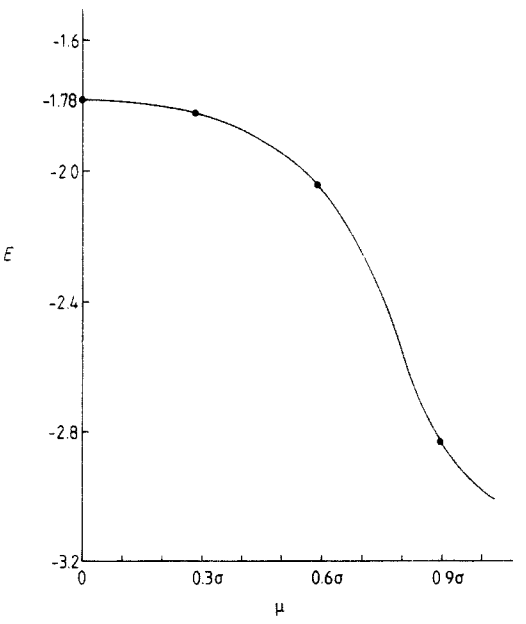

Figure 3.

Figure 4 shows the magnetisation as a function of μ. Ferromagnetism disappears for values of μ near 0.6σ.

As we can see, this method appears as a useful tool to get the ground state for samples of moderate size. To our knowledge this is the only non-trivial method that guarantees that the solution obtained is a true ground state.

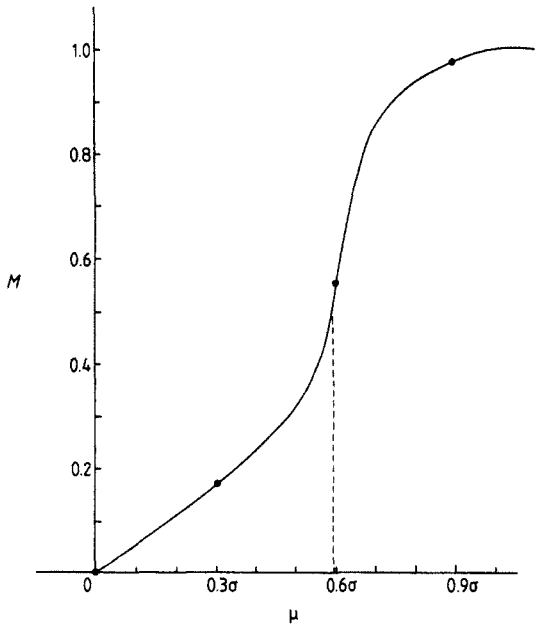

Figure 4.

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