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EXACT GROUND STATE OF FINITE AMORPHOUS ISING SYSTEMS

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Branch and bound algorithms of discrete optimization programming are used to find the exact ground state of Ising systems with random antiferromagnetic exchange coupling constants.

1. Introduction

Apart from a few exceptions many-particle problems cannot be solved without approximations and often the influence of these approximations on the results is not clear. Thus computer simulations of simple theoretical models are useful to compare approximate solutions of infinite systems with exact solutions of finite ones. Of course, the significance of such a comparison depends on a sufficiently large number of particles of the system, which can be simulated on the computer. Unfortunately, already in the simple Ising model ($S = \frac{1}{2}$) the situation does not seem to be very hopeful since 2^N states are necessary for the exact thermodynamics of a N-spin system [1]. In the last few years the so-called Monte Carlo methods [2,3] succeeded in this field using a large number of randomly chosen spin configurations for the calculation of thermodynamical quantities.

In special cases (e.g. amorphous systems with antiferromagnetic interactions, spin glass models) the exact ground state and the exact low temperature behaviour are of interest. Here a method is presented, to calculate the ground state of a finite Ising model with random exchange coupling constants with any sign without explicit knowledge of all 2^N states.

A simple example in section 2 shows the general principle of the method (cf. discrete optimization problems, e.g. ref. [4]). The representation of a very effective strategy follows in section 3. A selection of possible applications of the method and some extensions are discussed in section 4.

2. The branch and bound algorithm – a simple example

Let us consider the zero field Ising Hamiltonian for a finite system

$$\mathcal{H} = -\sum_{i<j}^{N} I_{ij} S_{zi} S_{zj} \qquad (1)$$

with random antiferromagnetic exchange coupling constants $I_{ij} \leqslant 0$. N is the number of spins S_{zi}, each of which can be +1 (↑) or −1 (↓). The lower bound for the minimum of the energy function (1) is obviously given by $E_0 = -\Sigma_{i<j}^{N} |I_{ij}|$. This value is the starting point of a tree, which can be "branched" by putting the spins successively in a fixed direction. The tops of this tree represent all 2^N states with the corresponding energies. The energy in a given branching point E_l can be calculated from the energy of the

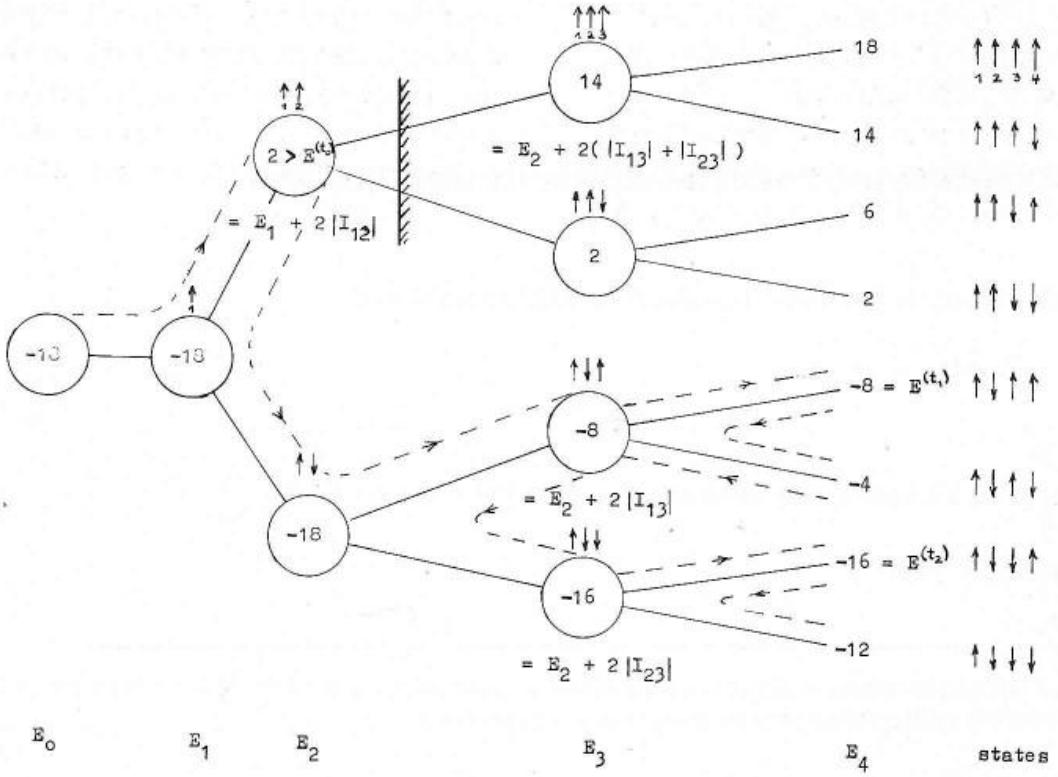

Fig. 1. A simple example for the branch and bound algorithm for $N = 4; I_{12} = -10, I_{13} = -5, I_{23} = -1, I_{24} = -2, I_{14} = I_{34} = 0$; $E^{(t_0)} = -4$ ($\uparrow\downarrow\uparrow\downarrow$); $E^{(t_2)} = -16$ is the exact solution.

previous branching point by

$$E_l = E_{l-1} + 2 \sum_{k(\|l)}^{l-1} |I_{kl}| , \tag{2}$$

where $k(\|l)$ denotes a summation only over such k, for which the spins had been previously fixed in the same direction as the spin l. It is important to note that always

$$E_l \geqslant E_{l-1} , \tag{3}$$

which follows from eq. (2).

An example for this very simple branch and bound strategy is illustrated in fig. 1 with $N = 4$. Because of the two-fold degeneracy of the problem (1) a restriction on the states with $S_{z1} = +1$ is possible. We start with the calculation of an admissible energy value $E^{(t_0)}$ for an arbitrary spin configuration and follow the branches in the given way (——→—). If we reach a branching point with $E_l \geqslant E^{(t_0)}$ the remaining branch can be cut because of the condition (3) (cf. E_2 in the upper part of fig. 1). If we reach sometimes the top of the tree (E_N) and $E_N < E^{(t_0)}$ is fulfilled, then we replace $E^{(t_0)}$ by the new comparison value $E^{(t_1)} = E_N$ and so on. The last found comparison value is the exact energy minimum of eq. (1).

3. Improved branch and bound technique

The generalization of the problem (1) is

$$\min_{\boldsymbol{S}_z \in M} (-\boldsymbol{S}_z^{\mathrm{T}} \boldsymbol{I} \boldsymbol{S}_z - \boldsymbol{H}^{\mathrm{T}} \boldsymbol{S}_z)$$

$$M = \{\boldsymbol{S}_z | \boldsymbol{S}_z \in R^N, S_{zi} = -1 \text{ or } 1\} , \tag{4}$$

where $\boldsymbol{S}_z$ is the vector with the components S_{zi} ($i = 1, \ldots, N$) and $\boldsymbol{I}$ is the triangular matrix of the exchange coupling constants ($I_{ij} \gtrless 0$). The components H_i of the vector $\boldsymbol{H}$ can be considered as proportionally to additional local field elements (the special case of an external field can be included in the problem by putting all of them equal).

First an algorithm is considered, which yields a heuristic approach of this problem. In every successive step k one component S_{zk} will be fixed. Thereby new contributions for the linear part are obtained and we get an analogous problem with reduced dimen-

sion. The product $S_{zk}H_k$ is called the "pivot" and after N steps the sum over all pivots is the value of the function for the approximate solution $S_z^{(0)}$.
Algorithm: For $l = 1$ step 1 until N do: Determine k so that $\max_i |H_i| = |H_k|$, take $S_{zk} := -\text{sign } H_k$.
This algorithm gives after $O(N^2)$ operations a good heuristic solution. It is the starting point for the exact calculation using a branch and bound algorithm with lower bounds: The algorithm for the heuristic approach contains N alternatives, which imply again problems of the same type, but with corresponding lower dimensions.

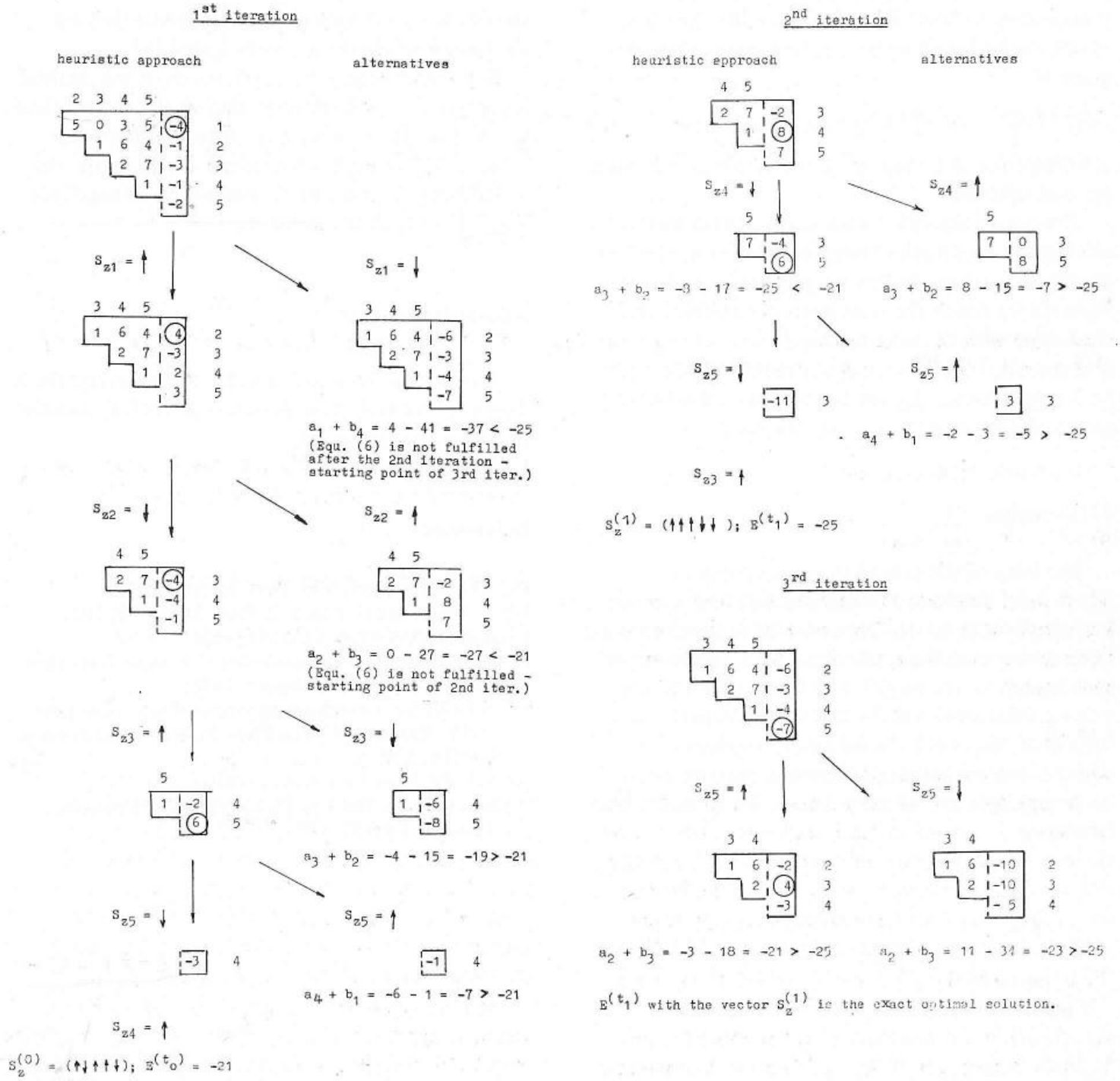

Fig. 2. Example for $N = 5$: The first triangular matrix contains the $-I_{ij}$ until column $j = 5$, the last column is the linear part with the components $-H_i$.

For $\boldsymbol{S}_z \in M$ we get the simple bound

$$-\boldsymbol{S}_z^{\mathrm{T}} \boldsymbol{I} \boldsymbol{S}_z - \boldsymbol{H}^{\mathrm{T}} \boldsymbol{S}_z \geqslant -\sum_{i<j} |I_{ij}| - \sum_i |H_i| \,. \tag{5}$$

Such bounds can be used for the reduced alternative problems, too.

Let a_l be the sum over all pivots so that l of the S_{zi} are known and $N-l$ are unknown. b_{N-l} is the bound of the remaining problem. $\boldsymbol{S}_z^{(t)}$ is the vector representing the best known value of the function, which was be found up to a certain stage of the program. If

$$-S_z^{(t)\mathrm{T}} I S_z^{(t)} - H^{\mathrm{T}} S_z^{(t)} \leqslant a_l + b_{N-l} \tag{6}$$

is fulfilled for all l, then $S_z^{(t)}$ is the vector of the exact optimal solution.

This search algorithm with lower bounds has to calculate in backtrack strategy because of the limited computer memory. In this strategy we look for the highest l for which the criterion is not fulfilled and start there with the next iteration.

Example ($N = 5$): The triangular matrix until column $j = 5$ contains the $-I_{ij}$, the last column is the linear part with the components $-H_i$, see fig. 2.

4. Discussion

The Ising model is used in various fields of physics and biophysics to describe two-level systems in a simple way. In the framework of computer simulations the represented method can help to discuss just such aspects of the model, which are related to the exact ground state and the exact low temperature behaviour. Especially, in the case of random exchange coupling constants including negative ones, up to now no other access is known for an exact treatment.

Using the algorithm of section 2 in ref. [5] the ground state of an amorphous Ising model with antiferromagnetic interactions for $N = 40$ spins on the basis of a fixed dense random packing structure is calculated. It is easy to see, that we can get all states with energies lower than a given one (say $E^{(t_0)}$ in the notation of section 2), if we consider this $E^{(t_0)}$ as an upper bound of our search strategy. Using the 1355 lowest states of a $N = 24$ spin glass model (random Gaussian distribution of coupling constants) some thermodynamical properties are investigated [6].

Some further possible applications of the method are obvious, e.g. the introduction of an external field (cf. section 3), the treatment of models with spin values $S > \frac{1}{2}$ (more-level-systems), furthermore, the use of Ising models with "conservation of total spin ΣS_{zi}" [7] for all temperatures.

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References

[1] K.G. Wilson, Rev. Mod. Phys. 47 (1975) 773.
[2] K. Binder and H. Rauch, Z. Phys. 219 (1969) 201.
[3] K. Binder, Z. Phys. B26 (1977) 339.
[4] H.A. Taha, Integer programming (Academic Press, New York, San Francisco, London, 1975).
[5] S. Kobe, in: Amorphous magnetism II (eds. R.A. Levy and R. Hasegawa; Plenum Press, New York and London, 1977) p. 529.
[6] S. Kobe, Phys. Lett. 65A (1978) 55.
[7] B.L. Gelmont and A.L. Efros, Prisma Zh. Eksperim. i Teor. Fiz. 25 (1977) 77.