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# Optimal Cuts in Graphs and Statistical Mechanics

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Abstract—We survey well known problems from statistical mechanics involving optimal cuts of graphs. These problems include finding the ground states for the spin glass problem or for the random field Ising model, as well as finding the lowest energy barrier between the two ground states of a ferromagnet. The relations between the results in graph theory and in physics are outlined. In particular, the solvability of a special max cut problem which arises in statistical mechanics is an easy consequence of a gauge invariance. Throughout the paper, we review some useful algorithms and results. We also give a simple solution of the cutwidth problem in the case of a regular tree.

Keywords—Discrete optimization, Statistical mechanics, Optimal cuts, Ground state properties.

# 1. INTRODUCTION

In statistical mechanics, one is often interested in describing nature at an intermediate level. Models are introduced which are then 'solved' and the comparison with experiments serves as a validation of the model itself. But solving the model is sometimes extremely difficult, and the study of models became itself a field of research. The paradigm of this kind of model is the Ising model [1] introduced to describe the properties of a ferromagnet. But this model turns out to describe also a variety of physical situations. Many generalizations were introduced to describe more realistic situations. For example, the Potts model proves itself to be of considerable interest [2]. Also, to take into account the many 'defaults' always present in a real sample, disordered models have been introduced. For example, the spin glass model has been very popular in the eighties [3]. Disorder leads to much more difficult problems, and even at the mean field level, the spin glass problem can only be solved using an Ansatz. Whereas the low temperature physics of ordered models is usually well understood, the low temperature physics of disordered models leads to very difficult optimization problems as will be discussed at length in this paper. This draws a link between statistical physics and discrete optimization. The connection works in both directions. Using methods of statistical physics in optimization is very useful [4]. In this paper, we will present mainly the opposite direction, i.e., how to use optimization methods for finding ground states. Nevertheless, a simple gauge transformation will be shown to have a nontrivial counterpart in cut-problems.

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The paper is organized as follows: in Section 2, we recall some basic results in graph theory and more precisely in cut-problems. In Section 3, we present known transformations of different statistical mechanics models into discrete optimization problems, the complexity of which are discussed. Different cases are considered: the Random Field Ising Model is investigated in Section 3.2 and the spin glass problem is investigated in Section 3.3. In Section 3.4, a known result of combinatorial optimization is presented as a very simple consequence of a statistical mechanics model. We present in Section 3.5 a generalization to the Potts model. Finally, in Section 4, the problem of finding the lowest energy barrier between two degenerate ground-states of a ferromagnet is shown to be also a known problem in optimization. The case of the Cayley tree is analyzed and solved. We provide a simple proof of a known result of combinatorial optimization.

# 2. DEFINITIONS AND WELL-KNOWN RESULTS ABOUT CUTS IN GRAPH THEORY

We will first give some definitions and present related problems and classical results. From now on, we will consider a graph G with vertex set V and edge set E.

A k-cut of G ( $k \ge 2$ ) is a set C of edges such that there exists a partition of the set of vertices into k disjoint subsets  $A_1, A_2, \ldots, A_k$  with the property that C is equal to the set of edges having their extremities in different sets of the partition. C will be said to be generated by the partition and this will be denoted by  $C = \Omega(A_1, A_2, \ldots, A_{k-1})$ . The most usual and well-known case is the one where k = 2. In the following we will use the word cut instead of 2-cut.

Given a specified set of k vertices  $t_1, \ldots, t_k$  called terminals, a  $(t_1, \ldots, t_k)$ -separating cut or for short a k-separating cut is a k-cut such that no two terminals are in the same component of G - C.

A weight-function of G is a function w which associates to each edge e a weight w(e) which is a real number. The weight w(F) of a set F of edges is the sum of the weights of the edges.

All along this paper we will be concerned with the complexity of combinatorial problems. We refer the reader to [5] and for an introduction to the theory of complexity. We will just give a very quick intuitive explanation of the basic notions. An algorithm is a step-by-step procedure for solving a problem. A polynomial time algorithm is an algorithm which always generates a solution in a running time bounded by a polynomial in the size of the input. The class of problems for which such an algorithm does exist is called P. The class NP is the class of problems for which what is claimed to be the answer can be checked to be the right answer in polynomial time. Of course, P is included in NP. A problem is NP-hard if it has the property that a polynomial algorithm solving it would imply that there is such an algorithm for each problem in NP. A problem in NP which is NP-hard is called NP-complete. So the NP-complete problems are the hardest problems in NP. It is commonly believed that there exists no polynomial algorithm to solve these problems, although there is no proof of this fact.

Now we are able to state the more general version of the problems we will be interested with in most parts of this paper.

THE MAX k-CUT PROBLEM. Given a graph G, an integer weight function w, and an integer k, find a k-cut in G of maximum weight.

With the preceding assumptions, it is clear that this problem is equivalent to the one of finding a k-cut of minimum weight by replacing each weight w(e) by -w(e). It is NP-complete since, as will be seen later, subproblems of it are, but there are also subproblems known to be in P. All these subproblems depend on the following four criteria.

- The value of k. The case when k is fixed can be easier. Also as will be seen later, the case k=2 is sometimes easier.
- The values of the weights. One can consider the case where all weights are positive (respectively, negative). Note that the max k-cut problem and the min k-cut problems are

then not anymore equivalent. A special case is the one where all weights are equal to one: this means that for fixed k we are interested by the cardinality of the k-cuts.

- Must the k-cut be a k-separating cut? Notice that one can transform a minimum (respectively, maximum) k-separating cut problem into a minimum (respectively, maximum) k-cut problem by adding an edge of sufficiently small (respectively, large) weight between each pair of terminals. Of course this cannot be done keeping the property that all the weights are positive (respectively, negative). Conversely, any k-cut problem can be solved by solving  $\binom{n}{k}$  k-separating cut problems. This means that for fixed k, the k-separating cut problem is at least as difficult as the k-cut problem even in the case of positive weights.
- Does the partition  $A_1, \ldots, A_k$  have to be proper? Note, that in the case of the search for a min k-cut in a graph with positive weights, allowing empty  $A_i$ 's would give rise to a trivial solution of zero weight. But if the weights are not restricted it is not anymore trivial to find a solution. Note that if empty  $A_i$ 's are allowed, then any optimal k-cut problem can be transformed into an optimal k-separating cut problem by adding k new vertices  $t_1, \ldots, t_k$  to G.

We will now give some well-known results. First we will see how different the max k-cut and the min k-cut problems are in terms of complexity in the simple case where k=2 and all weights are positive.

THEOREM 1. [6]. The max cut problem is NP-hard in the case where all weights are positive. In fact the max cut problem is NP-hard even in the case where all weights are equal to 1 [7] and if in addition, no vertex has degree exceeding 3 (see [8]). But we have the following.

THEOREM 2. [9,10]. The max cut problem is solvable in polynomial time in the case of a planar graph for any weight function.

This result can be extended to graphs not contractible to  $K_5$  [11] or weakly bipartite [12]. We will see in the next section other tractable cases. In the case of the min cut, the well-known "Max flow-Min cut" theorem of Ford and Fulkerson gives the following.

THEOREM 3. [13]. The min cut problem is solvable in polynomial time if all weights are positive.

Indeed a min cut separating two given vertices s and t can be found in such a graph by using a max flow algorithm. One replaces each edge xy of the graph by two directed edges  $\overrightarrow{xy}$  and  $\overrightarrow{yx}$  of capacities equal to w(xy). By the theorem due to Ford and Fulkerson [13], the maximum value of a flow from s to t is equal to the minimum value of a cut separating s from t in the original graph. Moreover, given a maximum flow, such a cut is easy to find. There are a lot of polynomial algorithms to solve this problem (see [14]). Now, a min cut can be found by applying  $\binom{n}{2}$  max flow as noticed above. Even n-1 are sufficient: from one arbitrarily fixed vertex to each other vertex. Recently new algorithms [15,16] were discovered which compute a min cut without using maximum flows. So the min cut problem is easy to solve in the case of positive weights; this remains true for a k-cut,  $k \geq 3$  [17,18].

THEOREM 4. [18]. For any fixed k, the min k-cut problem is solvable in polynomial time if all weights are positive.

If k is not fixed but part of the input, the problem becomes NP-hard [18]. Also, we have the following.

THEOREM 5. [19]. For any  $k \geq 3$ , the min k-separating cut problem is NP-hard. This is true even if all weights are equal to 1.

# 3. CUTS IN STATISTICAL PHYSICS

We will now see how k-cuts occur in statistical physics.

The Ising model was initially devised to describe the magnetic properties of matter. In this model the spins responsible for magnetism are supposed to be localized on the atoms of a regular

crystal. In appropriate energy unit the energy of a spin configuration  $\{\sigma\} = \{\sigma_1, \dots, \sigma_n\}$  (n is the number of spins) is

$$\mathcal{H}(\{\sigma_i\}) = -\sum_{ij} J_{ij}\sigma_i\sigma_j,$$

where  $\sigma_i = \pm 1$  and  $J_{ij}$ , the coupling constant between spins i and j, is a real number. The spins can also interact with an external uniform magnetic field and with local fields. The energy takes the most general form:

$$\mathcal{H}(\{\sigma_i\}) = -\sum_{ij} J_{ij}\sigma_i\sigma_j - \sum_i H\sigma_i - \sum_i h_i\sigma_i.$$

We are here interested in the zero temperature behavior of the system, where only the configurations of lowest energy contribute. The connection between zero temperature statistical physics and discrete optimization is now clear since we look, among the  $2^N$  configurations, for those of minimum energy. In most physical situations the coupling constants  $J_{ij}$  and the local fields  $h_i$  are random variables and the model is said to be disordered. Moreover, it is often not possible to satisfy all the coupling constants  $J_{ij}$ . (A positive  $J_{ij}$  is said to be satisfied if  $\sigma_i = \sigma_j$ ; in case  $J_{ij}$  is negative it is satisfied if  $\sigma_i \neq \sigma_j$ ; a  $J_{ij}$  which is not satisfied is said to be frustrated.) Take for example a triangle with one negative and two positive coupling constants. Disorder and frustration have a lot of experimental consequences [20]. If we believe that real samples are at equilibrium, it means that nature somehow manages to actually find the configurations of minimum energy. This idea has been exploited in the so-called simulated annealing methods [21] to solve complex optimization problems.

Let us now state the problem in terms of graph theory. Consider a graph  $R = (V \cup \{s, t\}, E \cup F)$  with weight w in the following way:

- to each spin is associated a vertex; so let  $V = \{1, 2, \dots, n\}$ ;
- to each two spins i and j which interact, associate an edge ij in E of weight  $w(ij) = J_{ij}$ ;
- to each spin i such that  $h_i + H > 0$ , associate an edge si in F of positive weight  $w(si) = h_i + H$ :
- to each spin i such that  $h_i + H < 0$ , associate an edge it in F of positive weight  $w(it) = -h_i H$ .

The goal is to minimize the following expression among all possible  $\{\sigma\} = \{\sigma_1, \dots, \sigma_n\}$  where  $\sigma_i = \pm 1$ 

$$\mathcal{H}(\{\sigma\}) = -\sum_{ij \in E} w(ij)\sigma_i\sigma_j - \sum_{si \in F} w(si)\sigma_i - \sum_{it \in F} -w(it)\sigma_i. \tag{1}$$

Note, that there is a one-to-one correspondence between the configurations  $\sigma$  and the bipartitions P, N of the vertices of R such that  $s \in P$  and  $t \in N$ :  $P = \{i; \sigma_i = +1\} \cup \{s\}$  and  $N = \{i; \sigma_i = -1\} \cup \{t\}$ . Let us also remark that in order to minimize the function  $\mathcal{H}$  in case where  $J_{ij}$  is positive (respectively, negative),  $\sigma_i$  and  $\sigma_j$  will tend to take the same (respectively, different) value in an optimal solution. Similarly, if  $h_i$  is positive (respectively, negative),  $\sigma_i$  will tend to be positive (respectively, negative).

Furthermore we have

$$\mathcal{H}(\{\sigma\}) = -\sum_{ij \in E} w(ij) - \sum_{si \in F} w(si) - \sum_{it \in F} w(it) + 2\left(\sum_{ij \in E, \sigma_i \neq \sigma_j} w(ij) + \sum_{si \in F, \sigma_i = -1} w(si) + \sum_{it \in F, \sigma_i = +1} w(it)\right). \tag{2}$$

The first part of this equation is a constant and the second part that we would like to minimize is nothing else than the weight of the (s,t)-separating cut generated by the bipartition P,N

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associated to  $\{\sigma\}$ . By Theorem 1, the general problem is NP-complete since it contains the min-cut problem with negative weights on the edges (in case there are negative interactions and no magnetic fields). Nevertheless depending on physics hypothesis, the weights can take values in different sets, the graph can have special properties, and depending on it we will see that the problem can be sometimes tractable.

#### 3.1. The Pure Ferromagnetic Case

Here the interactions are all ferromagnetic, that is, all the  $J_{ij}$  are positive. There is no magnetic field  $h_i$ , but possibly an external field H. This case is trivial. Indeed, it is clear that in that case all  $\sigma_i$  will take the same value whose sign will be the same as the sign of H. If we add local magnetic fields, the problem is still tractable, as explained in the next section.

# 3.2. The Ferromagnetic Random Field Ising Model (RFIM)

Now again the interactions are all ferromagnetic, that is, all the  $J_{ij}$  are positive but local magnetic fields are allowed. In that case R is a graph where all edges have a positive weight in which we want to find a minimum (s,t)-separating cut. As noticed in the previous chapter, this is an easy problem which can be solved by computing a maximum flow from s to t. An efficient algorithm for solving this problem is the one of Goldberg and Tarjan [22]. It has been used to study the RFIM on a cubic lattice [23,24]. In general, this algorithm runs in  $O(n^3)$ , but it is empirically found that on a cubic graph it runs in  $O(n^{4/3})$  [24]. On a workstation for a  $90 \times 90 \times 90$  cubic lattice, it is possible to find one configuration of lowest energy among the  $2^{729000} \sim 10^{218700}$  configurations in one hour of cpu time.

There are also algorithms to study all minimum cuts [25–28].

#### 3.3. The Spin Glass Model

In that particular case there are no magnetic fields, which means that in R the vertices s and t are isolated. So we are led to the problem of finding a minimum cut in a graph with arbitrary weight function, and we have seen that this problem is NP-hard (Theorem 1). But now the structure of the graph can help. For example, the case of a planar grid (square lattice) is of particular interest, and there is a polynomial algorithm [9,10] for computing a minimum cut in a planar graph. It is based on the idea of a matching between some faces of the graph. This idea was introduced for the first time in the context of statistical mechanics by Toulouse [20]. In fact, the problem turns out to be a Chinese Postman problem in a planar graph [29]. It can be solved using the matching algorithm of Edmonds [30]. The search for configurations of minimum energy for the spin glasses has been carried out by several authors [31–33]. To be more realistic some generalizations of the previous problem are possible: adding an external magnetic field to a square lattice or considering a tridimensional grid (cubic lattice) makes the problem NP-complete [11].

As noticed in the previous section, there are other particular kinds of graphs than the planar ones for which one knows how to compute a minimum cut for arbitrary weights, but these are not classical models for the physicists. Nevertheless, we will see in the next section another tractable case.

#### 3.4. Gauge Transformation and Consequences

As already noticed, the problem is that one does not know how to compute a minimum cut in the case of negative weights. This occurs each time we have negative  $J_{ij}$ . Nevertheless, as noticed long ago by the physicists, there is sometimes a possibility to transform a case with antiferromagnetic interactions (negative  $J_{ij}$ ) into a completely ferromagnetic case (all  $J_{ij}$  positive). This can be done by the well-known gauge transformation explained below [34]. Let us suppose

that there is a bipartition A, B of the vertices of V (the spins) such that all weights of edges inside A or B are positive and all weights of edges with one extremity in A and the other in B are negative. This is equivalent to saying that one can associate to each vertex i a value  $\epsilon_i$  in the set  $\{+1, -1\}$  in such a way that  $J_{ij} = |J_{ij}|\epsilon_i\epsilon_j$ . In this case we have

$$\mathcal{H}(\sigma) = -\sum_{ij \in E} |J_{ij}| \epsilon_i \epsilon_j \sigma_i \sigma_j - \sum_{i \in V} h_i \sigma_i$$

$$= -\sum_{ij \in E} |J_{ij}| (\epsilon_i \sigma_i) (\epsilon_j \sigma_j) - \sum_{i \in V} (h_i \epsilon_i) (\epsilon_i \sigma_i).$$
(3)

Let  $\tau_i = \epsilon_i \sigma_i$  for i = 1, ..., n, we have  $\tau_i \in \{+1, -1\}$  and the function to be minimized is  $\mathcal{H}'(\tau) = -\sum_{ij \in E} |J_{ij}| \tau_i \tau_j - \sum_{i \in V} (h_i \epsilon_i) \tau_i$ . This is the Hamiltonian of a ferromagnetic Random Field Ising Model, and as seen before we know how to solve it. Furthermore, from any optimal configuration  $\tau$ , one obtains an optimal configuration for the original case  $\sigma = \epsilon \tau$ .

It is interesting to see to which min cut algorithm the gauge transformation leads.

#### GAUGE ALGORITHM.

- Input: a graph  $R = (A \cup B \cup \{s, t\}, E)$  with a weight function w on the edges such that—no vertex in  $A \cup B$  is adjacent to both s and t—an edge is of negative weight if and only if it has one extremity in A and the other in B.
- Output: a bipartition P, N inducing a min (s, t)-separating cut of R.
- 1. Build from R a graph  $R' = (A \cup B \cup \{s, t\}, E')$  with weight function w' by—keeping all edges e with one extremity in A or both extremities in B with a weight equal to |w(e)|—replacing each edge sb with  $b \in B$  by an edge bt of weight w(sb)—replacing each edge bt with  $b \in B$  by an edge sb of weight w(bt).
- 2. Find a bipartition P', N' generating a min (s,t)-separating cut in R' by any polynomial algorithm. Set  $P = (P' \cap A) \cup (N' \cap B) \cup \{s\}$  and N is the complement of P.

From what precedes it is clear that R corresponds to the expression  $\mathcal{H}(\sigma)$  and that R' corresponds to the expression  $\mathcal{H}'(\tau)$ . So any bipartition P,N obtained from P',N' as in Step 2 in the algorithm corresponds to the transformation of  $\tau$  into  $\sigma$ , where  $\sigma$  and  $\tau$  correspond, respectively, to P,N and P',N'. Furthermore, we have that  $2w(\Omega(P)) = \mathcal{H}(\sigma) + \sum_{e \in E} w(e)$  and  $2w'(\Omega(P')) = \mathcal{H}'(\tau) + \sum_{e \in E} |w(e)|$ . Since  $\mathcal{H}'(\tau) = \mathcal{H}(\sigma)$ , we obtain that  $w(\Omega(P)) = w'(\Omega(P)) + \sum_{e \in E; w(e) < 0} w(e)$ .

By simple arguments we can even enlarge a little bit the class of graphs for which the min cut problem is polynomially solvable despite some negative weights. Let us call a gauge graph any graph  $R = (V \cup \{s,t\}, E)$  which has the property that: there is a bipartition A, B of V such that the set of edges with negative weights in the subgraph G induced by V is exactly equal to the cut generated by A, B. (There is no restriction for the edges with one extremity equal to s or t.)

THEOREM 6. The min cut problem is polynomially solvable for gauge graphs.

PROOF. We use two claims.

CLAIM 1. It is sufficient to show that one is able to find in polynomial time a min (s,t)-separating cut in gauge graphs.

Indeed, suppose this is true and we want to find a min cut in a gauge graph  $G = (V \cup \{s, t\}, E)$ . We need to know the weight of a cut which does not separate s and t. This can be done by computing a min (s', t')-separating cut in the graph R' obtained from R by identifying vertices s and t in s', and creating a new vertex t' joined by edges of weight zero to all other vertices. Such a min cut in R' may correspond to a nonproper bipartition of the vertices of G, but as noticed above, this is not absurd in the case of edges with negative weights. By our hypothesis, such a cut can be found, since G' is gauge too.

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CLAIM 2. It is sufficient to show that one is able to find in polynomial time an (s,t)-separating cut in gauge graphs where edges incident to s or t are of positive weights and no vertex in V is adjacent to both s and t.

Indeed, suppose this is true and we want to find a min (s,t)-separating cut in a gauge graph  $R = (V \cap \{s,t\}, E)$ . For each vertex  $v \in V$  let w(sv) and w(vt) be the weights of, respectively, the edges sv and vt (a nonedge is considered as an edge of weight zero). We construct from R a new graph R' with weights w' by the following procedure:

- for each vertex v such that w(sv) w(vt) is positive, delete vt and set w'(sv) = w(sv) w(vt),
- for each vertex v such that w(sv) w(vt) is negative, delete sv and set w'(vt) = w(vt) w(sv).

(All other edges and weights remain the same as in R.) It is clear that R' has the required properties. Furthermore, let P, N be a bipartition of the vertices of R separating s and t, and let C and C' be the weights of the corresponding cuts in, respectively, G and G'. We have:  $C' = C - \sum_{v;w(sv)-w(vt)>0} w(vt) - \sum_{v;w(vt)-w(sv)>0} w(sv)$ . So to minimize C is the same as to minimize C'.

From the preceding two claims we obtain the proof of our theorem since a graph with the properties indicated in Claim 2 corresponds exactly to the case solvable by the Gauge Algorithm.

Note that the class of gauge graphs is related to other classes of graphs for which the min cut problem is known to be polynomially solvable [35,36].

#### 3.5. Generalization of the Ferromagnetic RFIM to the Potts Model

Here we want to minimize:

$$\mathcal{H}(\{\sigma\}) = -\sum_{ij} J_{ij}(q\delta_{\sigma_i\sigma_j} - 1) - \sum_{i} h_i(q\delta_{\epsilon_i\sigma_i} - 1), \tag{4}$$

where  $\sigma_i$  is a Potts spin variable which can attain q different values  $(\sigma_i = 1, 2, ..., q)$ ,  $\delta_{ij} = 1$  if i = j and 0 otherwise;  $J_{ij} \geq 0$ ;  $h_i \geq 0$ . The random field variables  $\epsilon_i$  favour the state  $\sigma_i = \epsilon_i$ . As in the case of the RFIM one can associate a graph  $R = (V \cup \{s_1, s_2, ..., s_q\}, E)$  to this model [37]:

- to each spin is associated a vertex; so let  $V = \{1, 2, \dots, n\}$ ,
- to each two spins i and j which interact, associate an edge ij in E of weight  $w(ij) = J_{ij} \geq 0$ ,
- to each spin i such that  $\epsilon_i=j$ , associate an edge  $s_ji$  in E of weight  $w(s_ji)=h_i\geq 0$ .

A configuration  $\{\sigma\}$  corresponds to an  $(s_1, s_2, \ldots, s_q)$ -separating cut C in R and

$$\mathcal{H}(\{\sigma\}) = -(q-1)\sum_{ij\in E} w(ij) + qw(C). \tag{5}$$

So from Theorem 5 the problem of finding a configuration of minimum energy is NP-hard.

# 4. CUTWIDTH AND LOWEST ENERGY BARRIERS

It is well known that the low temperature behavior of a spin glass is closely related to the topology of the configuration space. In particular, the existence of many free energy valleys has many consequences, such as, for example, a critical slowing down of the dynamics. Loosely speaking it means the system is trapped in some free energy valley, and that configurations of the same energy will not be reached in a finite time. The time needed to go from one ground-state to another ground-state is the ergodic time and is always finite on a finite lattice (even though it can be extremely large) but can diverge in the thermodynamical limit. The behavior of this time in the thermodynamical limit is controlled by the divergence of energy barrier between ground

states. We show in this section that, in a special case, the determination of the energy barrier is a combinatorial optimization problem which has already been solved.

Disorder and frustration usually induce complicated configuration space with high energy barriers. Nevertheless, it has been suggested that glassy behavior could also be found in ordered systems [38,39]. The main ingredient for spin glass behaviour could be the existence of a very large number of local minima of free energy, separated by high energy barriers. To test this idea, it has also been suggested to study the Ising model on a regular lattice of a surface of positive curvature. The simplest case of such lattice is the Cayley tree (also called Bethe tree) where all coupling constants  $J_{ij}$  have the same value. It is shown in [38] that in this case the barriers are not high enough to ensure a real spin glass behaviour, and this relies on the formula in Theorem 8 demonstrated below. Nevertheless a spin-glass-like behaviour is seen as a finite size effect. In this context it was important to know the largest value of the energy of a configuration between the two ferromagnetic ground states of a Cayley tree (we remind the reader that these two ground states are  $\sigma_i = +1$  for all i and  $\sigma_i = -1$  for all i). Two spin configurations are neighbors in the space configuration if they differ by exactly one spin. This definition is somewhat arbitrary but it corresponds to the single spin flip and is commonly used. We consider then all the paths of neighbor configurations from one ferromagnetic ground state to the other, and we look for the highest energy of a configuration along this path, that we call the barrier of the path. The problem is to find the lowest barrier among all the possible paths. In other terms, we look for a linear order on the spins such that starting from one of the ground states and flipping the spins in this order, the largest energy we get during the process is minimized. This problem turns out to be known in the context of discrete optimization as the cutwidth problem. We switch now to the graph theory language to solve the question. A labeling of a graph G = (V, E) is a one to one mapping L of the vertices of the graph to the first n = |V| positive integers  $\{1, 2, \dots, n\}$ . The cutwidth  $c_L(G)$  of a labeling L is then defined to be

$$c_L(G) = \max_i (|\Omega(\{v : L(v) \le i\})|),$$

and the cutwidth of G is  $C(G) = \min\{c_L(G) : L$  is a labeling of  $G\}$ . We will equivalently consider a labeling as a sequential process of marking the vertices of the graph: at time t the vertex v of label L(v) = t is marked; the cutwidth of the labeling is the maximum size of a cut induced by the marked vertices during this process. A labeling L such that  $c_L(G) = c(G)$  is called optimal. The problem of computing the cutwidth (also called minimum cut linear arrangement problem) [40] is NP-complete for general graphs [5]. Yannakakis has defined an  $O(n \log n)$  algorithm to determine the cutwidth of a tree [41] and Lengauer [42] determined an explicit formula of the value of the cutwidth of complete k-ary trees. The algorithms proposed by Yannakakis and Lengauer are quite complicated and we will give here a simple method for the case of Cayley trees. These are regular trees defined below.

- $T_{h,d}$  is a tree with a root at level 0 and each vertex of level i has d sons of level i+1, for  $i=0,1,\ldots,h-1$ : the vertices of level h have no sons.
- $-T_{h,d}^*$  is a tree with a root at level 0, this root has d+1 sons of level 1 and each vertex of level i and d sons of level i+1, for  $i=1,2,\ldots,h-1$ : the vertices of level h have no sons.

We give now some useful definitions and properties.

A labeling L of a tree T rooted in r will be called *strong* if it is optimal and  $|\Omega(\{v: L(v) \leq i\})| < c(T)$  for i < L(r). (The cutwidth is not reached before r is marked.)

A labeling L of a tree T rooted in r will be called minus if it is optimal and  $|\Omega(\{v: L(v) \leq L(r)\})| < c(T)$ . (The cutwidth is not reached at the time r is marked.)

The reflected labeling RL of a labeling L is such that RL(v) = n - L(v) + 1. A labeling L will be called reflected strong if RL is strong. It is clear that

•  $c_L(G) = c_{RL}(G)$ ; consequently, if L is optimal then RL is optimal too,

- if L is strong then RL is minus,
- RRL = L.

Given a labeling L of a tree T with root r and a vertex w not in T, we denote by  $L^w$  the labeling of  $T \cup \{w\}$  such that:

- $L^w(v) = L(v)$  for  $c \in T$  such that  $L(v) \leq L(r)$ ;
- $L^w(w) = L(r) + 1;$
- $L^w(v) = L(v) + 1$  for  $v \in T$  such that L(v) > L(r).

(The vertices of T are marked in the same order as in L, w is marked just after the root of T.) To determine the cutwidth of  $T_{h,d}^*$  we first determine the cutwidth of  $T_{h,d}$  and some properties of the optimal labelings of  $T_{h,d}$ .

CLAIM 3. For  $h \ge 1$ ,  $d \ge 2$ , we have:

$$c(T_{h+1,d}) \ge c(T_{h,d}) + \left\lfloor \frac{d-1}{2} \right\rfloor. \tag{6}$$

Moreover, if d is even and the equality holds in (6), then there exists a strong labeling for  $T_{h,d}$  and no strong labeling for  $T_{h+1,d}$ .

PROOF OF THE CLAIM. Let  $T=T_{h+1,d},L$  be any labeling of T, and r be the root of T. This root is adjacent to the root of d subtrees isomorphic to  $T_{h,d}$ . When the vertices of T are marked with respect to L, the vertices of each of these subtrees are marked. So, by the definition of the cutwidth, each of these subtrees will once reach or surpass the value of its cutwidth, and since they are disjoint this time will be different for each. We number them  $T_1, T_2, \ldots, T_d$  in the order each of them reaches or surpasses the value  $c(T_{h,d})$  when using the labeling L on T, and denote by  $t_1, \ldots, t_d$  the time when they reach it. Now consider  $T_{\lfloor (d-1)/2 \rfloor + 1}$  at the time  $t^* = t_{\lfloor (d-1)/2 \rfloor + 1}$ . If r is already marked then since  $T_{\lfloor (d-1)/2 \rfloor + 2}, \ldots, T_d$  did not reach yet their cutwidth, they will count for at least 1, and  $|\Omega(\{v: L(v) \leq t^*\})| \geq c(T_{h,d}) + \lceil (d-1)/2 \rceil$ . If r is not yet marked, then each  $T_1, \ldots, T_{\lfloor (d-1)/2 \rfloor}$  will contribute for at least 1 since they must have marked vertices by hypothesis and so  $|\Omega(\{v: L(v) \leq t^*\})| \geq c(T_{h,d}) + \lfloor (d-1)/2 \rfloor$ . From what precedes we obtain that if d is even then equality holds in (6) only if:

- -r is not marked at time  $t^*$  and so L cannot be strong, and
- the root of T and the root  $T_{\lfloor (d-1)/2 \rfloor+2}$  are already marked at time  $t_{\lfloor (d-1)/2 \rfloor}+2$  and so a strong labeling for  $T_{h,d}$  must exist.

CLAIM 4. If there exists a strong labeling for  $T_{h,d}$   $(h \ge 1, d \ge 2)$  then  $c(T_{h+1,d}) = c(T_{h,d}) + \lfloor (d-1)/2 \rfloor$ . Moreover, if d is odd there exists a strong labeling of  $T_{h+1,d}$ ; if d is even there is no strong labeling for  $T_{h,d}$  but there exists a minus labeling,  $c(T_{h+2,d}) = c(T_{h+1}) + d/2$  and there exists a strong labeling for  $T_{h+2,d}$ .

PROOF OF THE CLAIM. Let L be a strong labeling for  $T_{h,d}$  and let  $T_1, \ldots, T_d$  be the d trees to which the root r of  $T_{h+1}$  is adjacent.

If d is odd, then use sequentially RL for  $T_1, T_2, \ldots, T_{(d-1)/2-1}$ , then use  $(RL)^r$  for  $T_{(d-1)/2} \cup r$ , then sequentially use L for  $T_{(d+1)/2}, \ldots, T_d$ . One verifies that thus we obtain a labeling  $L_{h+1}$  such that  $c_{L_{h+1}}(T_{h+1}) = c(T_{h,d}) + \lfloor (d-1)/2 \rfloor$  and  $L_{h+1}$  is strong.

If d is even, then use RL sequentially for  $T_1, \ldots, T_{d/2}$ , then mark r, then use L sequentially for  $T_{d/2+1}, \ldots, T_d$ . It is easy to verify that thus we obtain a labeling  $L_{h+1}$  such that  $c(L_{h+1}) = c(T_{h,d}) + \lfloor (d-1)/2 \rfloor$  and  $L_{h+1}$  is minus.

From Claim 3 we know that there is no labeling for  $T_{h+1,d}$ , so by Claim 3 again  $c(T_{h+2,d}) \ge c(T_{h+1,d}) + \lfloor (d-1)/2 \rfloor + 1 = c(T_{h+1,d}) + d/2$ .

Now, let  $L_{h+1}$  be any minus labeling of  $T_{h+1,d}$  and let  $T'_1, \ldots, T'_d$  be the d isomorphic trees adjacent to the root r' of a tree  $T_{h+2,d}$ . By using sequentially  $L_{h+1}$  on  $T'_1, \ldots, T'_{d/2-1}$ , then using  $L^{r'}_{h+1,d}$  to  $T_{d/2}$ , and using sequentially  $L_{h+1}$ , we obtain a labeling  $L_{h+2,d}$  of  $T_{h+2,d}$  such that  $c(L_{h+1}) = c(T_{h+1,d}) + d/2$  and  $L_{h+2,d}$  is strong.

To determine  $c(T_{h,d})$ , it remains to study the case of small values of h. If d is odd there is a strong labeling for  $T_{1,d}$  and  $c(T_{1,d}) = \lfloor (d-1)/2 \rfloor + 1$ . For an even d it is easy to see that:

- there is no strong and no minus labeling for  $T_{1,d}$  and  $c(T_{1,d}) = d/2$ ,
- there is a minus labeling but no strong labeling for  $T_{2,d}$  and  $c(T_{2,d}) = d$ ,
- there is a strong labeling for  $T_{3,d}$  and  $c(T_{3,d}) = 3d/2$ .

So from the previous claims we obtain the following theorem.

THEOREM 7. The cutwidth of the tree  $T_{h,d}$  is given by

$$c(T_{h,d}) = \left\lceil \frac{h(d-1)}{2} \right\rceil + 1, \qquad (h, d \ge 2).$$

If d and h are even, then there is a minus labeling but no strong labeling for  $T_{h,d}$ . In all other cases a strong labeling for  $T_{h,d}$  exists.

Now it remains to determine the cutwidth of  $T_{h,d}^*$ .

THEOREM 8. The cutwidth of the tree  $T_{h,d}^*$  is given by

$$c(T^*_{h,d}) = \left\lceil \frac{(h-1)(d-1)}{2} \right\rceil + \left\lfloor \frac{d}{2} \right\rfloor + 1, \qquad (h,d \geq 2).$$

PROOF OF THEOREM. We just have to show that  $c(T_{h,d}^*) = c(T_{h-1,d}) + \lfloor d/2 \rfloor$ ,  $(h \geq 2, d \geq 2)$ . Let  $T^* = T_{h,d}^*$  and r be the root of  $T^*$ . This root is adjacent to the root of d+1 subtrees isomorphic to  $T_{h-1,d}$ . The same proof as the one of Claim 3 gives that  $c(T^*) \geq c(T_{h-1,d}) + \lfloor d/2 \rfloor$ ,  $(h \geq 2, d \geq 2)$ . If d is odd, there exists by Theorem 7 a strong labeling for  $T_{h-1,d}$  and as in proof of Claim 4 we get a labeling  $L^*$  of  $T^*$  such that  $c_{L^*}(T^*) = c(T_{h-1,d}) + \lfloor d/2 \rfloor$ ,  $(h \geq 2, d \geq 2)$ . If d is even, there exists by Theorem 7 a minus labeling  $L_{h-1}$  for  $T_{h-1,d}$ . Let  $T_1, \ldots, T_{d+1}$  be the d+1 trees to which r is adjacent. Use sequentially L for  $T_1, T_2, \ldots, T_{d/2}$ , then use  $L^r$  for  $T_{d/2+1} \cup \{r\}$ , then sequentially use L for  $T_{d/2+2}, \ldots, T_{d+1}$ . One verifies easily that thus we obtain a labeling  $L^*$  such that  $c_{L^*}(T^*) = c(T_{h-1,d}) + \lfloor d/2 \rfloor$ . Note that from our proofs we obtain recursive algorithms to produce optimal labelings for  $T_{h,d}$  and  $T_{h,d}^*$ .

We summarize this section noting that the number of sites of a tree is an exponential function of the variable h, and consequently, the energy barrier between the two ground-states of a ferromagnet on a regular tree diverges like the logarithm of the number of sites.

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