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An Algorithm for Finding the First Excited State in the Random-Field Ising Model

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We present an efficient algorithm for finding the first excited state of the random-field Ising model based on the equivalence of its Hamiltonian with the capacity of cuts of a certain network. Some preliminary results in the two-dimensional case with a Gaussian distribution of random fields are presented.

Key Words: Gaussian random-field Ising model; exact ground states; excited states.

1. INTRODUCTION

Many physical properties of real systems are determined by the amount of disorder (vacancies, impurities, dislocations, etc.) present. Among others, some important examples can be found in magnetism, superconductivity, and structural phase transitions. For many years the study of such disordered systems has been a challenging problem and has attracted large attention. One of the simplest models proposed to describe such systems is the random-field Ising model (RFIM). It is defined on a finite regular lattice with N sites indexed from $i = 1 \dots N$. At each lattice site one defines a spin variable taking values $S_i = \pm 1$. The Hamiltonian reads

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - \sigma \sum_{i=1}^{N} h_i S_i, \tag{1}$$

where the first sum extends over nearest-neighbor pairs, $J > 0$ is a ferromagnetic exchange coupling (we will take $J = 1$ as a unit of energy), h_i are Gaussian random fields with zero mean and standard deviation 1, and $\sigma (\geq 0)$ is a parameter that controls the amount of disorder present in the system.

The statistical properties of systems presenting a free energy with many minima are very difficult to calculate. The difficulty is greater when these properties must be studied at very

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low temperatures. The conventional Monte Carlo method suffers from the problem that the system becomes trapped in a metastable state and cannot escape in a reasonable computing time. A first approach to overcome this difficulty and to understand the role of disorder in this model has been the study of its behavior at $T = 0$. The aim of this approximation is to decouple the thermal fluctuations from disorder. The study of the exact ground state of the RFIM has been possible due to the existence of a well-established equivalence between the problem of finding the ground state of the Hamiltonian (1) and the problem of finding the cut with minimum capacity of a network [1–3]. Using this mapping, many numerical efforts have been devoted to the understanding of how the ground state properties change when the amount of disorder σ is changed for the 2d [4, 5] and 3d [6] Gaussian RFIM. In this paper we propose an algorithm that allows us to go one step forward and study the properties of the first excited state (FES) of the Hamiltonian (1). The idea behind this is to gain insight into the understanding of the properties of the system at low temperatures. It should be mentioned that recently a similar study of low-energy excitations has been applied to the study of two similar models (the random bond Ising model and the diluted antiferromagnet in a field model) [7].

The paper is organized as follows; in Section 2 we revisit the equivalence to the minimum cut problem; in Section 3 the mathematical basis of the algorithm for finding the FES is presented; and in Section 4 some preliminary results, corresponding to a two-dimensional square lattice with periodic boundary conditions, are presented.

2. EQUIVALENCE WITH CUT CAPACITIES IN A NETWORK

In this section we revisit the equivalence between finding the ground state of the Hamiltonian (1) and finding the cut with minimum capacity in a network. This equivalence was established 25 years ago by Picard and Radcliff [1]. A brief explanation is given below to provide the notation.

One considers a network $\mathcal{N}$ based on a di-graph $G = [V, E]$ [9]. The set of vertices V has $N + 2$ elements associated with the N sites of the square lattice plus a source u and a sink v. These vertices are indexed from 0 to $N + 1$. The vertex with index 0 corresponds to the source u, vertices with index 1 to N correspond to the sites $i = 1, \ldots, N$ of the lattice, and the vertex with index $N + 1$ corresponds to the sink v. The set of directed edges E has $3N$ elements. Each edge corresponds to an ordered pair of vertices (i, j) and has an associated capacity $c(i, j) > 0$. The edges and capacities are defined as follows:

- For each pair $\langle i, j \rangle$ of nearest-neighbor sites of the lattice, a directed edge departing from the vertex with lowest index and reaching the vertex with highest index is defined.[1] The capacity of that edge is taken to be $c(i, j) = 4$ $(i < j)$.
- For each lattice site i with $h_i > 0$ an edge departing from the source u and reaching the corresponding vertex is defined. Its capacity is taken to be $c(0, i) = 2\sigma h_i$.
- For each lattice site i with $h_i < 0$ an edge departing from the corresponding vertex and reaching the sink v is defined. Its capacity is taken to be $c(i, N + 1) = -2\sigma h_i$.

A cut X is any subset of V such that $0 \in X$ and $(N + 1) \notin X$. Thus, a cut defines a partition of $V = X \cup \overline{X}$. The capacity of a cut is the sum of the capacities of the edges leaving X and reaching $\overline{X}$. We introduce, for each vertex, a variable x_i that equals 1 if

[1] In fact, the direction of the edge can be arbitrarily defined.

$i \in X$ and 0 otherwise. With this definition $x_o = 1$ and $x_{N+1} = 0$ for any cut. Any cut X is equivalent to a configuration of these variables $\{x_i\}$. The capacity of a cut X can be written as

$$C(X) = \sum_{\text{edges}}^{i,j} c(i, j)x_i(1 - x_j)$$

$$= \sum_{i=1}^{N} \{c(0, i)(1 - x_i) + c(i, N + 1)x_i\} + \sum_{\langle i,j \rangle} c(i, j)x_i(1 - x_j). \tag{2}$$

Each cut can be related to a configuration of spins $\{S_i\}$ through the correspondence

$$S_i = 2x_i - 1 \Leftrightarrow x_i = \frac{1 + S_i}{2}, \tag{3}$$

and so $S_i = +1$ if $i \in X$ and $S_i = -1$ if $i \notin X$. With these definitions the capacity of a cut can be related to the energy of the configuration $\{S_i\}$ via

$$C(X) = \sum_{i=1}^{N} \left\{ c(0, i)\frac{1 - S_i}{2} + c(i, N + 1)\frac{1 + S_i}{2} \right\} + 4 \sum_{\langle i,j \rangle} \frac{1 + S_i}{2}\frac{1 - S_j}{2}$$

$$= \sum_{h_i>0} 2\sigma h_i \frac{1 - S_i}{2} + \sum_{h_i<0} -2\sigma h_i \frac{1 + S_i}{2} + \sum_{\langle i,j \rangle} 1 + \sum_{\langle i,j \rangle} (S_i - S_j) - \sum_{\langle i,j \rangle} S_j S_i$$

$$= -\sum_{\langle i,j \rangle} S_j S_i - \sigma \sum_{i=1}^{N} h_i S_i + \frac{z}{2} N + \sigma \sum_{i=1}^{N} |h_i|, \tag{4}$$

where z is the lattice coordination number. Note that $C(X)$ differs from the Hamiltonian (1) by a constant value ($\frac{z}{2}N + \sigma \sum_{i=1}^{N} |h_i|$) which is independent of the configuration $\{S_i\}$. Thus, the capacity of each cut $\{x_i\}$ is related to the energy of the corresponding configuration $\{S_i\}$. This reduces the problem of finding the configuration with minimum energy $\mathcal{H}$ to finding the cut of minimum capacity X^{min} of the corresponding network. There are several efficient algorithms that solve the problem of finding the maximum flow and the minimum cut of a network [10]. Hereafter, we will suppose that any of these algorithms may be used.

Our interest here is to find the first excited state. Thus, we should find the cut with capacity nearest the minimum X^{nm}. The algorithm presented in the next section is deterministic and can be applied to any lattice of any spatial dimension, provided that no frustration appears. It can also be extended to models with longer range interactions. The algorithm is related to the so-called sensitivity analysis technique in the context of linear programming [8].

3. FINDING THE CUT WITH CAPACITY NEAREST THE MINIMUM

Let us consider a general network $\mathcal{N}$ based on a di-graph $G = [V, E]$ and capacity function c. Without losing generality we will assume that all the edges of E have a capacity larger than zero. We will denote the cut with minimum capacity (or min-cut) of $\mathcal{N}$ as X^{min}. There is an implicit association between any cut X of $\mathcal{N}$ and the set of edges leaving X and reaching $\bar{X}$. This set of edges is denoted as $(X, \bar{X})$. For any element w of $(X, \bar{X})$, it is said that w is an edge of the cut X and that the cut X contains w.

Let us consider the set of all possible cuts of the network $\mathcal{N}$: $\mathcal{S}^{\mathcal{N}}$. Any edge w of E divides $\mathcal{S}^{\mathcal{N}}$ into two subsets: the set of cuts containing w ($\mathcal{S}_w^{\mathcal{N}}$) and the set of cuts not containing w ($\bar{\mathcal{S}}_w^{\mathcal{N}}$).

Let $\bar{w}$ be an edge of X^{min} (min-cut of $\mathcal{N}$). We define the network $\mathcal{N}_{\bar{w}}^{\delta}$ based on the same di-graph G, with capacity function $c_{\bar{w}}^{\delta}$ by augmenting the capacity of the edge $\bar{w}$ by an amount $\delta(>0)$ and keeping all the other capacities equal to those of $\mathcal{N}$. That is,

$$\begin{aligned} c_{\bar{w}}^{\delta}(\bar{w}) &= c(\bar{w}) + \delta \\ c_{\bar{w}}^{\delta}(w) &= c(w) \qquad \forall (E \ni) w \neq \bar{w}. \end{aligned} \tag{5}$$

Now, we will focus on the problem of finding the min-cut of $\mathcal{N}_{\bar{w}}^{\delta}$ that depends on the value δ. Let us consider a general cut X of the network $\mathcal{N}$. Obviously, X is also a well-defined cut of $\mathcal{N}_{\bar{w}}^{\delta}$ and its capacity in this network satisfies

$$C_{\bar{w}}^{\delta}(X) - C(X) = \begin{cases} 0 & \text{if } \bar{w} \notin (X, \bar{X}) \\ \delta = c_{\bar{w}}^{\delta}(\bar{w}) - c(\bar{w}) & \text{if } \bar{w} \in (X, \bar{X}). \end{cases} \tag{6}$$

This means that when the capacity of the edge $\bar{w}$ is increased the capacity of all the cuts containing $\bar{w}$ augments by the same amount while all the other cuts maintain their capacity. In other words, all the cuts of set $\bar{\mathcal{S}}_{\bar{w}}^{\mathcal{N}}$ have the same capacity in $\mathcal{N}_{\bar{w}}^{\delta}$ as in $\mathcal{N}$, while all the cuts of set $\mathcal{S}_{\bar{w}}^{\mathcal{N}}$ have a larger capacity in $\mathcal{N}_{\bar{w}}^{\delta}$ than in $\mathcal{N}$. Moreover, all the cuts of set $\mathcal{S}_{\bar{w}}^{\mathcal{N}}$ increase their capacity by the same amount (δ). This implies that whatever the value of δ is, X^{min} is the cut of set $\mathcal{S}_{\bar{w}}^{\mathcal{N}}$ with minimum capacity[2] (both in $\mathcal{N}_{\bar{w}}^{\delta}$ and in $\mathcal{N}$). Let $X_{\bar{w}}^{min}$ be the cut of set $\bar{\mathcal{S}}_{\bar{w}}^{\mathcal{N}}$ with minimum capacity in $\mathcal{N}$. Since the capacity of the cuts of this set does not change with δ, $X_{\bar{w}}^{min}$ is also the cut with minimum capacity of set $\bar{\mathcal{S}}_{\bar{w}}^{\mathcal{N}}$ in $\mathcal{N}_{\bar{w}}^{\delta}$, whatever the value of δ. Thus, for any value of δ, the two candidates to be the min-cut of $\mathcal{N}_{\bar{w}}^{\delta}$ are X^{min} and $X_{\bar{w}}^{min}$; if δ is large enough, $C_{\bar{w}}^{\delta}(X_{\bar{w}}^{min})$ will be lower than $C_{\bar{w}}^{\delta}(X^{min})$. Hence

$$\text{min-cut of } \mathcal{N}_{\bar{w}}^{\delta} = \begin{cases} X^{min} & \text{if } \delta < C\left(X_{\bar{w}}^{min}\right) - C(X^{min}) \\ X_{\bar{w}}^{min} & \text{if } \delta > C\left(X_{\bar{w}}^{min}\right) - C(X^{min}). \end{cases} \tag{7}$$

Obviously, the cut with capacity nearest the minimum (X^{nm}) must differ from the cut with minimum capacity by, at least, one edge. Thus, there exists (at least) one edge w of X^{min} so that X^{nm} is in $\bar{\mathcal{S}}_w^{\mathcal{N}}$. Moreover, X^{nm} must coincide with X_w^{min}. This allows us, with the help of any max-flow min-cut algorithm applied to $\mathcal{N}_{\bar{w}}^{\delta}$ for each edge $\bar{w}$ of the network, to reduce the number of candidates to be X^{nm} to an affordable number. To find X^{nm} it is sufficient to minimize $C(X_{\bar{w}}^{min})$ over all edges $\bar{w}$ of X^{min}:

$$C(X^{nm}) = \min_{\bar{w} \in (X^{min}, \bar{X}^{min})} C\left(X_{\bar{w}}^{min}\right) \tag{8}$$

$$X^{nm} = X_w^{min} \quad \text{so that } \forall \bar{w} \in (X^{min}, \bar{X}^{min}) \qquad C\left(X_w^{min}\right) \leq C\left(X_{\bar{w}}^{min}\right) \tag{9}$$

In fact, the equal sign in Eq. (9) only holds for $w = \bar{w}$. A formal algorithm to find the cut with capacity nearest the minimum can be written as

[2] We have fixed $\bar{w} \in (X^{min}, \bar{X}^{min})$, so $X^{min} \in S_{\bar{\omega}}^{\mathcal{N}}$.

ALGORITHM 1 (CUT WITH CAPACITY NEAREST THE MINIMUM OF $\mathcal{N}$).

1. **begin**
2. $C^{nm} := C(X^{min}) + \delta$
3. **for** $\bar{w} \in (X^{min}, \bar{X}^{min})$
4. $X_{\bar{w}} :=$ **min-cut**$(\mathcal{N}_{\bar{w}}^{\delta})$
5. **if** $C_{\bar{w}}^{\delta}(X_{\bar{w}}) < C^{nm}$ **then**
6. $C^{nm} := C_{\bar{w}}^{\delta}(X_{\bar{w}})$
7. $X^{nm} := X_{\bar{w}}$
8. **end if**
9. **end for**
10. **return** X^{nm}
11. **end**,

where **min-cut** is a function that, acting over a network, returns its min-cut. The algorithm starts by initializing C^{nm} to a large enough value. This can be achieved by choosing a large enough δ to satisfy Eq. (7). Then, for each $\mathcal{N}_{\bar{w}}^{\delta}$ (when $\bar{w}$ sweeps all the edges of X^{min}), the corresponding min-cut $(X_{\bar{w}})$ is found and its capacity in $\mathcal{N}_{\bar{w}}^{\delta}$ compared with C^{nm}. Conveniently, C^{nm} is updated to $C_{\bar{w}}^{\delta}(X_{\bar{w}})$ and X^{nm} is temporarily identified with $X_{\bar{w}}$. At the end of the algorithm X^{nm} is the cut with capacity nearest the minimum and C^{nm} its capacity.

4. PRELIMINARY RESULTS

To illustrate the kind of results that can be obtained and the efficiency of the algorithm presented above, we have studied the FES of the 2d RFIM (1) on a square lattice with periodic boundary conditions, $N = 32 \times 32$, and values of σ ranging from 0.25 to 2.0. For each value of σ we have analyzed 10^4 different realizations of the random fields $\{h_i\}$. For each realization we have constructed a network following the mapping of Section 2. For each network we found its min-cut and its cut with capacity nearest the minimum. Following Eq. (3), we found the ground state $\{S_i^0\}$ and the FES $\{S_i^1\}$.

To analyze the results we define the energy difference as

$$\Delta\mathcal{H} = \mathcal{H}\left(S_i^1\right) - \mathcal{H}\left(S_i^0\right) \tag{10}$$

and the overlap between the ground state and the FES as

$$q = \sum_{i=1}^{N} S_i^1 S_i^0. \tag{11}$$

Figure 1 shows the distribution of $\Delta\mathcal{H}$ for different values of σ. Each histogram is an approximation to the probability density $p(\Delta\mathcal{H})$ obtained by performing statistics over 10^4 different realizations of the random fields. As can be seen, for a certain value of $\sigma \simeq 1.0$ an energy gap between the ground state and the FES appears for most of the realizations of the random fields.

To investigate further the nature of these FES in Fig. 2 we show the diagram $\Delta\mathcal{H} - q$. Each circle on these plots corresponds to the pair $(q, \Delta\mathcal{H})$ found for one set $\{h_i\}$. For low values of disorder there is a small fraction of FES with values of the overlap corresponding

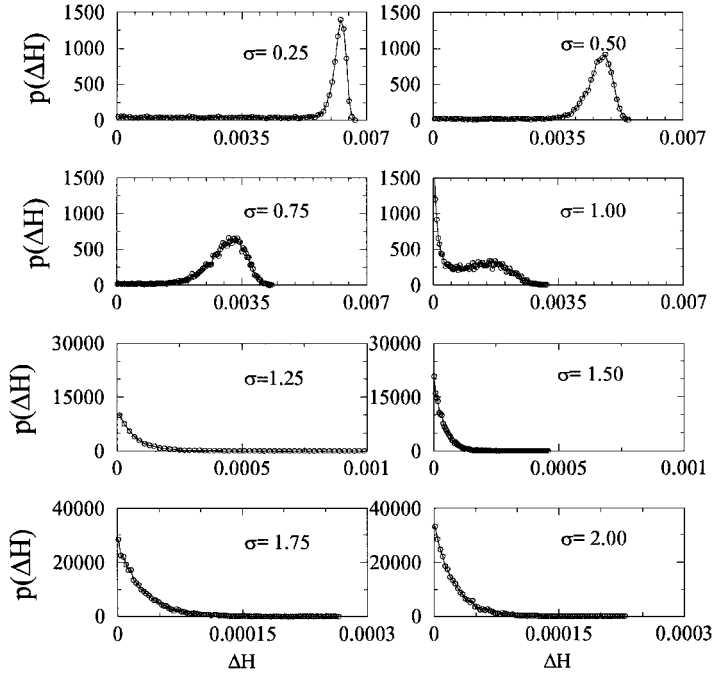

FIG. 1. Probability density $p(\Delta\mathcal{H})$ of the excess energy corresponding to the FES of the 2d RFIM for different values of σ. Results correspond to 10^4 realizations of an $N = 32 \times 32$ system.

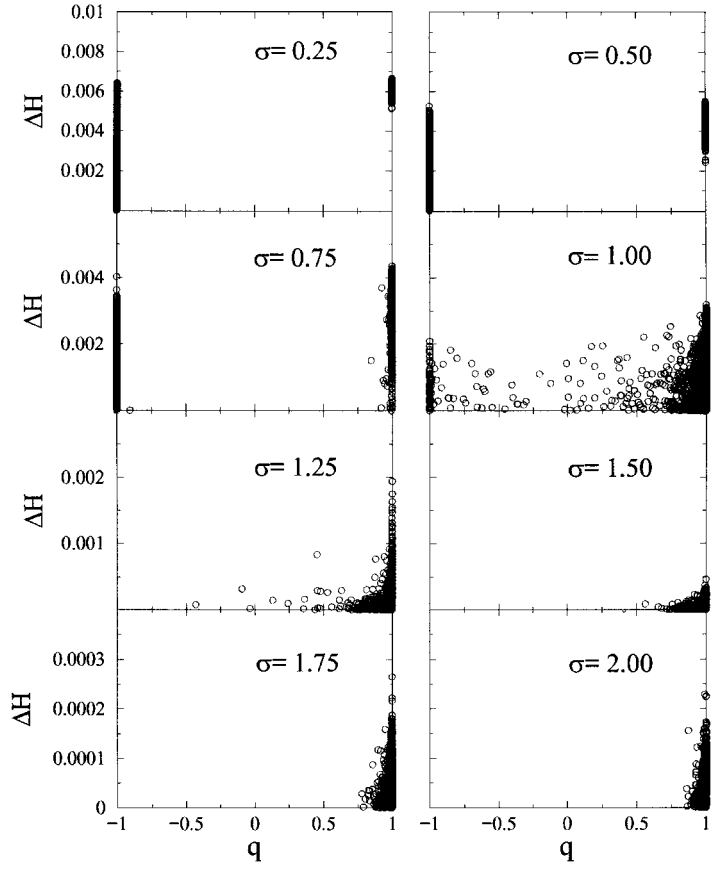

FIG. 2. $q-\Delta\mathcal{H}$ diagrams of a 2d RFIM with $N = 32 \times 32$. For each value of σ, 10^4 realizations of the disorder have been considered.

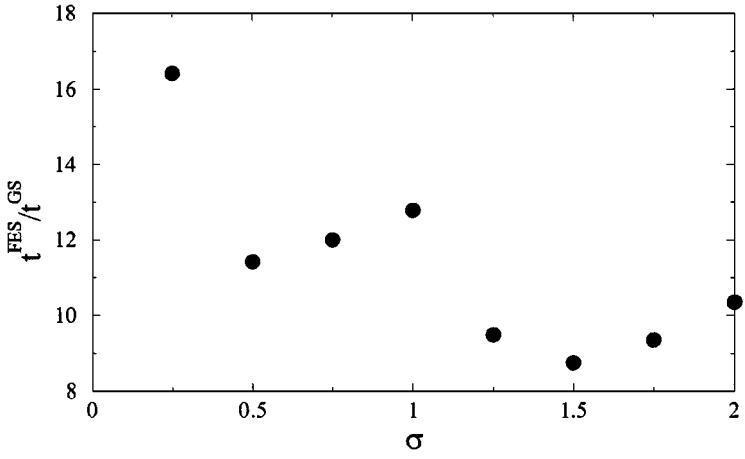

FIG. 3. Ratio between the average time t^{FES} needed to find the FES and the average time t^{GS} needed to find the ground state, for different values of σ. Data correspond to the study of a 2d RFIM with size $N = 32 \times 32$.

to the flip of all the spins in the system ($q = -1$), while the rest of the FES corresponds to the flip of a single spin ($q = 1 - 2/N$). This change of behavior found around $\sigma \simeq 1.0$ could be related to the disorder-induced phase transition discussed in Ref. [5]. Nevertheless, a clear answer can only be obtained after a finite-size scaling analysis of the results, which will be presented elsewhere.

Finally, to illustrate the speed of the proposed algorithm Fig. 3 shows the ratio between the average time t^{FES} needed to find the FES and the average time t^{GS} needed to find the ground state, for different values of σ. Note that the time needed for finding the FES is much smaller than the time one would need by using the trivial method of forcing the reversal of each individual spin of the system and finding the corresponding ground states. Such an algorithm would represent a ratio $t^{FES}/t^{GS} \simeq N$. It is known [11] that the time for finding the max-flow of $\mathcal{N}_w^{\delta}$ once the max-flow of $\mathcal{N}$ is determined behaves of $t \propto N$. Thus, $t^{FES}/t^{GS} \sim \mathcal{O}(1)$.

5. SUMMARY AND CONCLUSIONS

A deterministic and efficient algorithm for finding the first excited state of the random-field Ising model has been presented. The algorithm is based on the analysis of the ground state, which is found by means of any polynomial time minimization algorithm. The recursive study of the edges of the minimum cut makes it possible to find the cut with capacity nearest the minimum as has been proved in Section 3. If the min-cut algorithm used for the determination of the ground state has a polynomial efficiency $t \sim N^{\alpha} (\alpha \geq z)$, the present algorithm efficiency will also grow as $t \sim N^{\alpha}$. Moreover, it can be recursively used to find the sequence of the first, second, third, etc., excited states.

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REFERENCES

1. J. C. Picard and H. D. Radcliff, Minimum cut and related problems, *Networks* **5**, 357 (1974).
2. A. T. Ogielski, Integer optimization and zero-temperature fixed points in Ising random field systems, *Phys. Rev. Lett.* **57**, 1251 (1986).
3. H. Rieger, Frustrated systems: Ground state properties via combinatorial optimization, in *Advances in Computer Simulations*, edited by J. Kertesz and I. Kondor, Lecture Notes in Physics 501 (Springer-Verlag, Heidelberg, 1998).
4. E. T. Seppälä, V. Petäjä, and M. J. Alava, Disorder, order, and domain wall roughening in the two-dimensional random field Ising model, *Phys. Rev. E* **58**, R5217 (1998).
5. C. Frontera and E. Vives, Numerical signs for a transition in the two-dimensional random field Ising model at T = 0, *Phys. Rev. E* **59**, R1295 (1999).
6. J. C. Anglès d'Auriac and N. Sourlas, The 3-D random field Ising model at zero temperature, *Europhys. Lett.* **39**, 473 (1997).
7. S. Bastea and P. M. Duxbury, Active clusters in disordered systems, *Phys. Rev. E* **60**, 4941 (1999).
8. A. Schrijver, Theory of Linear and Integer Programming (John Wiley and Sons, Chichester, 1986).
9. G. Chartland, *Graphs and Digraphs* (Wadsworth, Belmont, CA, 1986).
10. R. E. Tarjan, *Data Structures and Network Algorithms* (Society for Industrial and Applied Mathematics, Philadelphia, 1983).
11. R. K. Ahuja, T. L. Magnati, and J. B. Orlin, *Network Flows* (Prentice Hall, Upper Saddle River, NJ, 1993).