Journal of Computational Physics **160,** 117–125 (2000)
doi:10.1006/jcph.2000.6437, available online at http://www.idealibrary.com on IDEAL®

Efficient Algorithm for Finding Ground-States in the Random Field Ising Model with an External Field

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Received July 6, 1999; revised December 27, 1999

We present an efficient algorithm that, combined with a max-flow, min-cut minimization algorithm, makes it possible to find the ground states of the Gaussian Random Field Ising model when the external applied field B is continuously varied from $-\infty$ to $+\infty$. The algorithm exactly finds all the possible ground states and their limiting range $(B_{\min}, B_{\max})$. Examples of the dependence of the magnetization and energy with B are shown for the 2d-RFIM. © 2000 Academic Press

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

1. INTRODUCTION

One of the recent trends in Statistical Mechanics has been the study of different model systems with quenched disorder. The goal of such studies is to become closer to the real physical phenomena. The complexity of such models is due not only to the disorder itself, but also to the competition with thermal fluctuations. Thus, a first step is to neglect such thermal fluctuations and focus on the study of the ground state ($T = 0$) properties of such models. In particular it is especially interesting to study the possiblity for $T = 0$ phase transitions which appear when the system is driven by an external field, or when certain parameters characterizing the quenched disorder are varied.

Among others, the Random Field Ising model (RFIM) is remarkably simple but, as occurred with the corresponding disorder-free model (Ising model) it includes the key ingredients for the study of phase transitions. Still many details of its phase diagram are not understood. The model is defined on a finite regular lattice with N sites. On each lattice site one defines a spin variable taking values $S_i = \pm 1$. The hamiltonian reads

$$\mathcal{H} = -J \sum_{i,j} S_i S_j - \sum_i h_i S_i - B \sum_i S_i, \tag{1}$$

0021-9991/00 $35.00

where the first sum (the standard Ising model) extends over nearest neighbor pairs, $J > 0$ is a ferromagnetic exchange coupling (we will take $J = 1$ as a unit of energy), B is the externally applied field, and h_i are quenched random fields, independent and distributed with a certain probability density $p(h)$. We shall concentrate, as an example, on the 2d square lattice with only nearest neighbor interactions, but the algorithm presented can be extended to regular lattices with other symmetries and exchange interactions of longer range, provided that no frustration appears. Without loss of generality we will assume that the random fields have zero mean (one can redefine the external field B to ensure this condition) and standard deviation σ:

$$\int_{-\infty}^{\infty} hp(h)\,\mathrm{d}h = 0, \qquad \int_{-\infty}^{\infty} h^2 p(h)\,\mathrm{d}h = \sigma^2. \tag{2}$$

For the present work it is of crucial importance that the distribution of random fields $p(h)$ is continuous. Then, one can ensure that two different configurations $\{S_i\}_1$ and $\{S_i\}_2$ have different energy $\mathcal{H}$, except for a set of values of the model parameters with zero measure. As an example we will focus on the case of gaussian random fields; i.e.,

$$p(h) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{h^2}{2\sigma^2}}. \tag{3}$$

In this case an exact theorem has proven that in the thermodynamic limit, for a fixed set of random fields h_i and B, the ground state is unique [1]. Note that this does not prevent the possibility of finding a phase transition when considering the full ensemble of copies of the system with different realizations of the random fields $\{h_i\}$ corresponding to a certain value of σ. The natural definition of an order parameter is:

$$m = \frac{\langle M \rangle}{N} = \frac{\left\langle \sum_{i=1}^{N} S_i \right\rangle}{N}, \tag{4}$$

where the symbol $\langle \ldots \rangle$ stands for the average over different realizations of the disorder corresponding to a certain value of σ. A first-order phase transition in the $\sigma - B$ phase diagram will be associated to a discontinuity of m.

Previous studies of the $T = 0$ properties of this model can be classified into two main groups:

- Equilibrium studies: they are rather scarce since the algorithms for searching the exact ground states require a computational effort that has been affordable only quite recently. Existing works have concentrated in the $B = 0$ case for both $d = 2$ [2, 3] and $d = 3$ [4, 5]. System sizes of 1000×1000 [2] and $80 \times 80 \times 80$ [5] have been studied. The complexity of the problem naively looks as if growing exponentially with system size as 2^N. Nevertheless it can be simplified into a polynomial growing (N^2) task by exploiting the mapping with the problem of computing the maximum flow through a network [6]. We are not going to discuss how such minimization algorithms work but rather assume that such a subroutine is available [7].
- Metastability studies: these are much more numerous and focus on the $T = 0$ hysteresis properties of the Random Field Ising models [8]. In this case, instead of looking for the exact ground states, the system is driven by sweeping the external field B from $-\infty$ to ∞

and backward, and the spins are flipped by using synchronous local relaxation dynamics based on a zero-temperature Glauber single-spin flip scheme. This makes the problem easy to simulate, and systems of size $30{,}000 \times 30{,}000$ can be reached [9]. The results suggest, indeed, the existence of a first-order phase transition line ending at a critical point at σ_c, with universal properties [10]. Nevertheless, the 2d case is still under discussion.

The goal of the present paper is to present an efficient algorithm that, for a fixed set of $\{h_i\}$, makes it possible to find the sequence of ground states when scanning B from $-\infty$ to ∞, and study the $T = 0$ equilibrium behavior of the magnetization and other magnitudes. It should be mentioned that a recent paper [11] has also investigated the possibility for such scanning parameter algorithms in similar models, but the solutions proposed require that both the random fields and the hamiltonian parameters are integers.

2. ALGORITHM DETAILS

2.1. *Previous Considerations*

The idea behind the algorithm is to plot the energy of each state $\{S_i\}$ on a $\mathcal{H}$ vs B diagram. For each state, the energy behaves as a straight line with slope $-M$,

$$\mathcal{H}(\{S_i\}, B) = \mathcal{H}_0(\{S_i\}) - BM, \tag{5}$$

where $\mathcal{H}_0(\{S_i\}) = -\sum_{\langle i,j\rangle} S_i S_j - \sum_i h_i S_i$ is the energy axis intercept. Some of these lines are represented in Figs. 1 and 2. The different ground state corresponding to each value of B will be found by looking to the lines determining the lower bound in such a plot.

Let us consider a system of size $N = L^d$. Let $h_{\min}$ and $h_{\max}$ be the maximum and minimum values of the h_i fields for a certain realization of the disorder. Under such circumstances, since the system is finite, the ground state is unique, except for a set of values of B with zero measure. Note the following simple propositions:

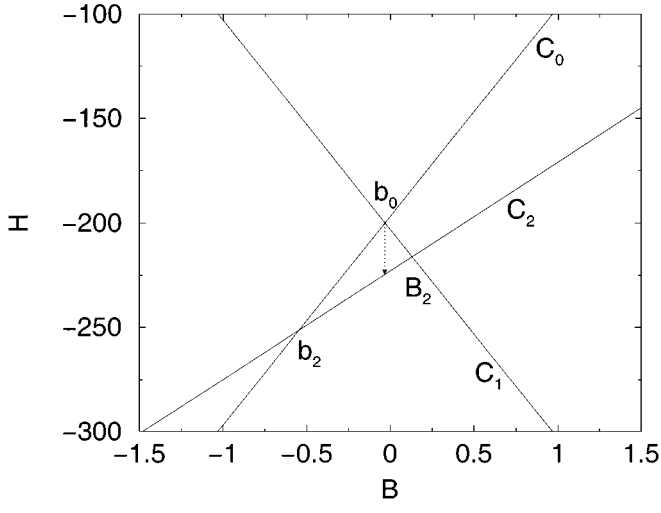

FIG. 1. First step in the search procedure in the $\mathcal{H}$–B diagram.

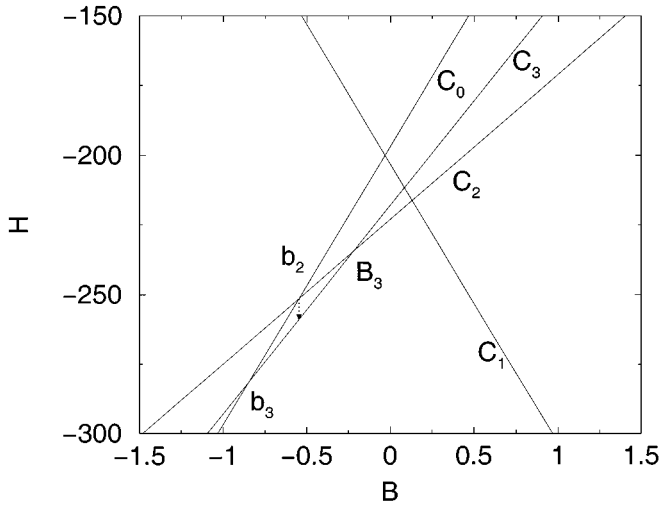

FIG. 2. Second step in the search procedure in the $\mathcal{H}$–B diagram.

PROPOSITION 2.1. *For $B < -h_{max}$ ($B > -h_{min}$) the ground state is $\{S_i = -1\}$ ($\{S_i = 1\}$).*

Proof. The proof is straightforward, since under such circumstances $\{S_i = -1\}$ ($\{S_i = 1\}$) minimizes not only the first term of the hamiltonian (1), but also the sum of the last two terms, $-\sum_i (h_i + B)S_i$. ■

PROPOSITION 2.2. *Let $C_1 = \{S_i\}_1$ be the ground state for $B = B_1$ and $C_2 = \{S_i\}_2$ ($C_2 \neq C_1$) be the ground state for $B = B_2 > B_1$. Let, also, M_1 and M_2 be the corresponding magnetizations. Then $M_2 > M_1$.*

Proof. Since the configurations C_1 and C_2 are the ground states at B_1 and B_2, respectively, we can write

$$\begin{aligned} \mathcal{H}_0(C_2) - B_2 M_2 &< \mathcal{H}_0(C_1) - B_2 M_1 \\ \mathcal{H}_0(C_1) - B_1 M_1 &< \mathcal{H}_0(C_2) - B_1 M_2. \end{aligned} \tag{6}$$

By adding both equations one inmediately arrives at

$$(B_2 - B_1)M_1 < (B_2 - B_1)M_2 \tag{7}$$

and since $B_2 > B_1$, then $M_2 > M_1$. ■

Thus the sequence of ground states when sweeping the external field from $B = -\infty$ to $B = \infty$ will exhibit strict increasing magnetization from $M = -N$ to $M = N$. This gives a maximum number of possible ground states N, since M grows from $-N$ to N in steps of 2 units. For low values of the disorder the number of ground states will be much lower.

COROLLARY 2.1. *In the $\mathcal{H}$–B diagram the slopes of the lines corresponding to the states C_1 and C_2 are different* (*so the lines intersect*) *and its intersection occurs at a field B_c such that $B_1 < B_c < B_2$.*

We will refer to this field as **crossing field between** C_1 **and** C_2 and represent it as $\mathcal{B}(C_1, C_2)$.

PROPOSITION 2.3. *Let $C_1 = \{S_i\}_1$ be the ground state for $B = B_1$, $C_2 = \{S_i\}_2$ the ground state for $B = B_2 > B_1$ and $B_c = \mathcal{B}(C_1, C_2)$. If there is no configuration C such that $\mathcal{H}(C, B_c) < \mathcal{H}(C_1, B_c) = \mathcal{H}(C_2, B_c)$ then:* **(i)** *C_1 is the ground state at least for the field range $B_1 < B < B_c$, and* **(ii)** *C_2 is the ground state at least for the field range $B_c < B \leq B_2$.*

Proof. **(i)** Let us suppose that there is a configuration $\tilde{C}$ such that for $B = \tilde{B}$ with $B_1 < \tilde{B} < B_c$ the relation $\mathcal{H}(\tilde{C}, \tilde{B}) < \mathcal{H}(C_1, \tilde{B})$ holds. Due to proposition 2.2 $\tilde{M} > M_1$. Thus, the energy of such a configuration at B_c would be

$$\begin{aligned} \mathcal{H}(\tilde{C}, B_c) &= \mathcal{H}(\tilde{C}, \tilde{B}) - (B_c - B)\tilde{M} \\ &< \mathcal{H}(C_1, \tilde{B}) - (B_c - B)\tilde{M} \\ &< \mathcal{H}(C_1, \tilde{B}) - (B_c - B)M_1 \quad \Rightarrow \\ \mathcal{H}(\tilde{C}, B_c) &< \mathcal{H}(B_1, B_c), \end{aligned} \tag{8}$$

in contradiction with the hypothesis of the proposition. The proof of **(ii)** is very similar. ■

The power of proposition 2.3 comes from the fact that it can be applied iteratively. Let us supose that we cannot apply proposition 2.3 at B_c. Then the ground state (C) at this point will satisfy $\mathcal{H}(C, B_c) < \mathcal{H}(C_1, B_c) = \mathcal{H}(C_2, B_c)$. By corollary 2.1 it will be $B_1 < \mathcal{B}(C_1, C) < B_c$ and $B_c < \mathcal{B}(C, C_2) < B_2$. We can try to apply proposition 2.3 for both $\mathcal{B}(C_1, C)$ and $\mathcal{B}(C, C_2)$. For each one of these fields that do not meet the hypothesis of proposition 2.3, we will find another ground state and two new fields to test the hypothesis. It must be noticed that each ground state found during the iteration procedure is the ground state for a certain range of fields between B_1 and B_2.

2.2. *Algorithm Formulation*

The algorithm constructs a list W of all the ground states, together with the values $B_{\min}$ and $B_{\max}$ that indicate the range of validity of each ground state. So, each element of the list W is formed by a state $\{S_i\}$ and two fields:

$$W_j = (C_j, b_j, B_j). \tag{9}$$

At the end of the algorithm each $C_j = \{S_i\}_j$ is the ground state for any external field $b_j < B < B_j$.

The starting point are the states $C_0 = \{S_i = -1\}$ (which is the ground state, at least, for any applied field $B < -h_{\max}$) and $C_1 = \{S_i = +1\}$ (which is the ground state, at least, for any applied field $B > -h_{\min}$). The algorithm then proceeds by analyzing its crossing point $\mathcal{B}(C_0, C_1)$.

The algorithm stores the successive crossing fields (B_i) to be checked in a queue q together with the indexes (k_i and l_i) of the states whose corresponding lines cross at that field [$q_i = (B_i, k_i, l_i)$, so that $B_i = \mathcal{B}(C_{k_i}, C_{l_i})$]. When one of those fields is checked it is erased. The algorithm finishes when q is empty. It is also possible to avoid a number of superfluous minimizations by arresting the procedure if, when analyzing the crossing field $\mathcal{B}(C_i, C_j)$, the magnetizations M_i and M_j are found to differ only by two units.

The next functions are supposed to exist:

- **minimize**: Given a configuration of random fields $\{h_i\}$ and an external field B, **minimize**($\{h_i\}$, B) returns the configuration that minimizes the energy.
- **pop**: This acts over a queue. It returns the zero-th element of the queue and erases it.

TABLE I
Initial State of the List W

Configuration	b	B
C_0	$-\infty$	b_0
C_1	b_0	∞

- **add**: Given a list or a queue and one or more elements this function adds the elements to the list or queue.
- **num**: Given a list it returns the number of elements on it.

ALGORITHM 1 (GROUND STATES($\{h_i\}$)).

```
1.  begin
2.     W = ∅
3.     q = ∅
4.     C_0 := {S_i = −1}
5.     C_1 := {S_i = +1}
6.     b_0 := B(C_0, C_1)
7.     add{W; (C_0, −∞, b_0), (C_1, b_0, ∞)}
8.     add{q; (b_0, 0, 1)}
9.     while q ≠ φ do
10.       (b, k, l) := pop(q)
11.       (C_k, b_k, B_k) := W_k
12.       (C_l, b_l, B_l) := W_l
13.       C := minimize({h_i}, b)
14.       if H(C, b) < H(C_k, b)(=H(C_l, b)) then
15.          B := B(C_k, C)
16.          b := B(C, C_l)
17.          W_k := (C_k, b_k, B)
18.          W_l := (C_l, b, B_l)
19.          add{q; (B, k,num(W)), {b, num(W), j)}
20.          add{W; (C, B, b)}
21.       end if
22.    end while
23. end.
```

where ∅ means either an empty list or queue.

Tables I, II, and III show the state of list W, at the beginning, after the first minimization (see Fig. 1), and after the second minimization (see Fig. 2), respectively.

TABLE II
State of the List W after the First Minimization Step

Configuration	b	B
C_0	$-\infty$	b_2
C_1	B_2	∞
C_2	b_2	B_2

TABLE III
State of the List *W* after the Second Minimization Step

Configuration	b	B
C_0	$-\infty$	b_3
C_1	B_2	∞
C_2	B_3	B_2
C_3	b_3	B_3

3. SOME RESULTS

Figure 3 shows an example of the minimization results for a system of size $L = 32$, periodic boundary conditions, and $\sigma = 1.5$. For comparison we also show the evolution of the system under the nonequilibrium dynamics described before, which has been used for the study of avalanche phenomena in this type of extended disordered systems [8].

We present the behavior of the different physical quantities of interest [12]: the internal energy $\mathcal{H}_0$ (a), the input energy $-BM$ (b), the total energy $\mathcal{H} = \mathcal{H}_0 - BM$ (c), and the magnetization M (d). A detailed comparison between the metastable and stable evolution will be presented elsewhere. Nevertheless, several interesting results can already be pointed out:

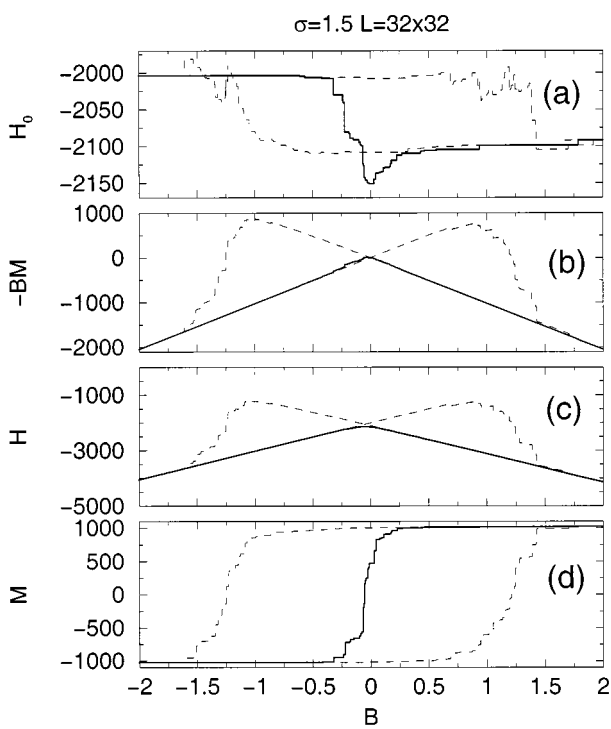

FIG. 3. Ground state evolution (continuous line) as a function of B for a system with $L = 32$ and $\sigma = 1.5$. The different figures show the evolution of (a) $\mathcal{H}_0$, (b) $-BM$, (c) $\mathcal{H} = \mathcal{H}_0 - BM$, and (d) M. Dashed lines show, for comparison, the metastable forward and backward metastable trajectory.

• The equilibrium trajectory is formed by the sequence of configurations which are absolute minimizers of the energy at each given field. Therefore, as expected from thermodynamic arguments, the equilibrium trajectory followed by the magnetization is the same independent of whether the field increases or decreases.

• The equilibrium trajectory exhibits avalanches of the magnetization very similar to the ones found in the metastable evolution. Contrary to the metastable evolution, however, there is no energy dissipation associated with equilibrium avalanches: the change of $\mathcal{H}_0$ is exactly compensated by the change in $-BM$ there. The equilibrium trajectory is anhysteretic.

• The dynamics of the equilibrium evolution corresponds to minimizing the energy when clusters of spins of any size, from a single spin to the whole system size, are allowed to flip simultaneously. On the other extreme, the metastable evolution provided by the synchronous relaxation dynamics corresponds to minimizing the energy when clusters of only one spin are allowed to flip at a time.

• The internal energy $\mathcal{H}_0$ exhibits a monotonously decreasing behavior for $B < 0$ and a monotonously increasing behavior for $B > 0$, going through a minimum at $B = 0$ (this is not the case for the metastable evolution, for which $\mathcal{H}_0$ displays oscillations). This result, that can be obtained directly from Eq. (5) and proposition 2.2 can also be understood in terms of standard equilibrium thermodynamics: the fundamental equation for such a simple magnetic system is $\mathrm{d}\mathcal{H}_0 = T\,\mathrm{d}S + B\,\mathrm{d}M$; therefore,

$$\left(\frac{\partial \mathcal{H}_0}{\partial B}\right)_T = T\left(\frac{\partial S}{\partial B}\right)_T + B\left(\frac{\partial M}{\partial B}\right)_T. \tag{10}$$

At $T = 0$ one gets:

$$\left(\frac{\partial \mathcal{H}_0}{\partial B}\right)_{T=0} = B\left(\frac{\partial M}{\partial B}\right)_{T=0}. \tag{11}$$

Note that the derivative in the second term is always positive due to stability conditions, and thus the variation of the internal energy $\mathcal{H}_0$ with B must have the sign of B.

• The efficient computation of the M–B equilibrium line opens new possibilities for the study of criticality in Random Field Ising models. In particular, it may allow the direct determination of the critical exponent δ which characterizes the dependence of the magnetization on the external field at $\sigma = \sigma_c$: $B \sim |M|^\delta \operatorname{sgn} M$.

Finally, we point out a possible improvement of the present algorithm, on the basis of the following conjecture: when the field is swept from $-\infty$ to ∞ no reverse spin flips occur in the equilibrium trajectory. This allows an easy simplification, since the spins $S_i = +1$ for a certain value of B can be removed from the ground state analysis for all higher values of the external field.

ACKNOWLEDGMENTS

The authors thank Antoni Planes for fruitful discussions. This work has received financial support from the CICyT (Spain), Projects MAT97-0699, MAT98-0315, and PB97-0906.

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