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Metastable States in Homogeneous Ising Models

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Metastable states of homogeneous 2D and 3D Ising models are studied under free boundary conditions. The states are defined in terms of weak and strict local minima of the total interaction energy. The morphology of these minima is characterized locally and globally on square and cubic grids. Furthermore, in the 2D case, transition from any spin configuration that is not a strict minimum to a strict minimum is possible via non-energy-increasing single flips.

KEY WORDS: Homogeneous Ising model; metastable states; weak and strict interaction energy minima.

1. INTRODUCTION

In this paper we consider metastable states in homogeneous Ising models as local minima of an energy function that is defined as a sum of spin products $s_x \cdot s_u$ over pairs (x, u) of nearest neighbor points of a finite regular grid G, $G \subset R^d$. The local minima are described in terms of strict and weak minima.

In the case $d = 2$, the morphology of strict and weak minima is characterized in several theorems. Moreover, it is shown that a transition from an arbitrary spin configuration that is not a strict minimum to a strict minimum of lower energy can be achieved via a sequence of single flips. In the case $d \geqslant 3$, generalizations for some of the two-dimensional characterizations are made. Furthermore, the behavior of three-dimensional strict minima is studied on the surface of G. For the proofs, see Ref. 1.

Basic Definitions and Conventions. Let g, d be natural numbers with $g \geqslant 2$. We define a grid G, $G \subset R^d$, by

$$G := \{x \mid x = (x_1, x_2, \ldots, x_d) \in R^d,\ x_i \text{ natural},\ 1 \leqslant x_i \leqslant g\}$$

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Let $\Gamma_{d,g}$ be the set of all spin configurations C on G, $C=(s_x)$, where $s_x \in \{+1, -1\}$ for all $x \in G$. We use free boundary conditions. Consider the problem

$$E(C) := -\sum_{\text{n.n.}} s_x \cdot s_u = \text{local minimum}, \qquad C \in \Gamma_{d,g}$$

(n.n. denotes nearest neighbor). To specify the notion of local minimum of $E(C)$, we take the following steps: With arbitrary but fixed $C \in \Gamma_{d,g}$ and $x \in G$, let C_x be identical to C with the only exception at x, where the spin s_x in C is flipped to $-s_x$. Then

$$\Delta_x E(C) := E(C_x) - E(C) = 2 \sum_{\substack{\text{n.n.} \\ x \text{ fixed}}} s_x \cdot s_u$$

Definition 1. $E(C)$, $C \in \Gamma_{d,g}$, has a *local minimum* at C^* if

$$\Delta_x E(C^*) \geqslant 0 \qquad \text{for all} \quad x \in G \tag{1.1}$$

$E(C)$ has a *strict minimum* at C^* if

$$\Delta_x E(C^*) > 0 \qquad \text{for all} \quad x \in G \tag{1.2}$$

and $E(C)$ has a *weak minimum* at C^* if (1.1) holds and

$$\Delta_x E(C^*) = 0 \qquad \text{for at least one} \quad x \in G \tag{1.3}$$

Thus, a local minimum of $E(C)$ is either strict or weak.

2. ON THE CASE $d=2$

For $d=2$ the points (x, y) of a grid G consist of four *corner points*, $(g-2)^2$ *inner grid points*, and $4(g-2)$ *inner edge points*. We now characterize the strict minima of $E(C)$ locally in G.

Theorem 2.1. $E(C)$, $C \in \Gamma_{2,g}$, has a *strict minimum* at $C^* = (s^*_{x,y})$ iff

$$s^*_{x,y} \cdot s^*_{u,v} = 1 \tag{2.1}$$

holds for

(α) at least three nearest neighbors (u, v) of each inner grid point (x, y)
(β) and if (x, y) is a corner point, for the 2 n.n. (u, v)
(γ) and if (x, y) is an inner edge point, for at least 2 n.n. (u, v)

The conditions (α), (β), and (γ) are illustrated in Fig. 1.

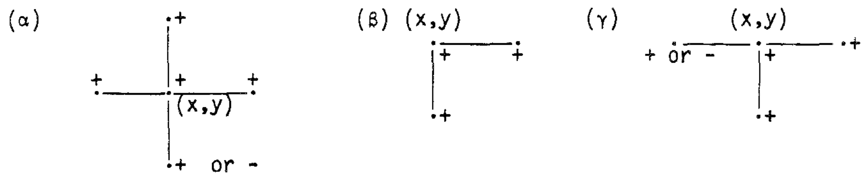

Fig. 1. Characterization of a strict minimum of $E(C)$, pointwise in G.

Next we characterize the strict minima of $E(C)$ globally on G.

Theorem 2.2. $E(C)$, $C \in \Gamma_{2,g}$, has a *strict minimum* at $C^* = (s^*_{x,y})$ iff C^* falls under one of the following cases:

(α) $s^*_{x,y} = 1$ for all $(x, y) \in G$
(β) $s^*_{x,y} = -1$ for all $(x, y) \in G$
(γ) C^* consists of at least two either horizontal or vertical stripes, which alternate in spin sign and have a width of at least 2.

The case (γ) of Theorem 2.2 is illustrated on a 7×7 grid in Fig. 2.

In analogy to Theorem 2.1, we characterize the weak minima of $E(C)$.

Theorem 2.3. $E(C)$, $C \in \Gamma_{2,g}$, has a *weak minimum* at $C^* = (s^*_{x,y})$ iff (2.1) holds for

(α) at least one n.n. (u, v) of each corner point (x, y)
(β) at least two n.n. (u, v) of each noncorner point
(γ) $\Delta_{x,y} E(C^*) = 0$ for at least one $(x, y) \in G$.

As an illustration of Theorem 2.3, consider Fig. 3.

To characterize the weak minima of $E(C)$ globally on G, we introduce "quadrigas," "rings," "streets," and unions of these special subconfigurations.

There are only two types of *quadrigas*:

$$\begin{matrix} + & + \\ + & + \end{matrix} \quad \text{and} \quad \begin{matrix} - & - \\ - & - \end{matrix}$$

Figure 4 gives examples for unions of (+)-quadrigas.

	+	+	-	-	+	+	+		+	-	-	+	-	-	-	
	+	+	-	-	+	+	+		+	-	-	+	-	-	-	
strict	+	+	-	-	+	+	+		+	-	-	+	-	-	-	not a strict
minimum	+	+	-	-	+	+	+		+	-	-	+	-	-	-	minimum
	+	+	-	-	+	+	+		+	-	-	+	-	-	-	
	+	+	-	-	+	+	+		+	-	-	+	-	-	-	
	+	+	-	-	+	+	+		+	-	-	+	-	-	-	

Fig. 2. Example and counterexample for a strict minimum.

```
weak         + - - - - - +        - + - - - - +    not a weak
minimum      + - - - - - +        - + - + - - +    minimum
             + - + + + + +        - + - - - - +
             + - + + - - +        - + - - - + +
             + - - + - - +        - + - - - - -
             + - - + - - +        - + - - - - -
             + - - + + + +        - + - - - - -
```

Fig. 3. Example and counterexample for a weak minimum.

A *ring* ρ is a subconfiguration of at least eight points of the same spin σ such that every ring point has exactly two n.n. in ρ. It gives rise to a double point free, closed path P just connecting the points of ρ by straight lines, each line of length 1. All n.n. (u, v) of ring points, where the n.n. lie inside the region bounded by P, must have spin $-\sigma$. An example and counterexample of a ring are given in Fig. 5.

A *street* S is a subconfiguration of at least two points of the same spin σ such that every street point has at most two n.n. in S. It is not a subset of a ring and gives rise to a double point free, possibly closed path P, just connecting the points of S by straight lines, each line of length 1, such that

(S1) the endpoints (x, y) of P are either corner points with $s_{u,v} = s_{x,y}$ for exactly one n.n. (u, v) or otherwise $s_{u,v} = s_{x,y}$ for at least three n.n.

(S2) $s_{u,v} = -\sigma$ for all n.n. (u, v) of each $(x, y) \in S$ if $(u, v) \notin S$ and (x, y) is not an endpoint of P.

Examples and counterexamples for streets are given in Fig. 6.

With these definitions we can state the following result:

Theorem 2.4. $E(C)$, $C \in \Gamma_{2,g}$, has a *weak* minimum at $C^* = (s^*_{x,y})$ iff C^* is not a strict minimum and both subconfigurations of all plus-spins and all minus-spins are a union of quadrigas, rings, and streets of the same spin sign, respectively.

An example of a weak minimum is given in Fig. 3. Note that, if C^* is a weak minimum, then each ring in C^* contains at least one quadriga.

```
- - - - - -        + + - - + +    The union can be
- - + + - -        + + - - + +    partially disjoint
+ + + + + +        - - - - - -
+ + - + + +        - - + + - -
- - - - + +        + + + + + +
- - - - - -        + + + + + +
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Fig. 4. Unions of quadrigas.

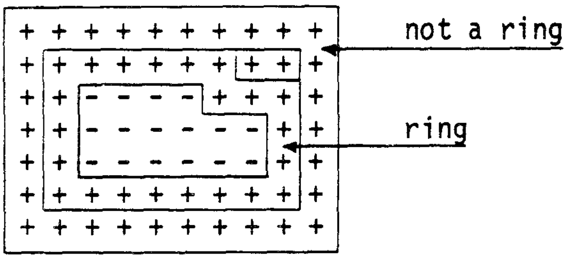

Fig. 5. Ring and ringlike subconfigurations.

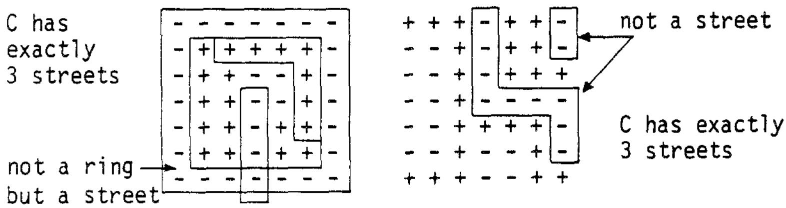

Fig. 6. Streets in 7 × 7-grid spin configurations.

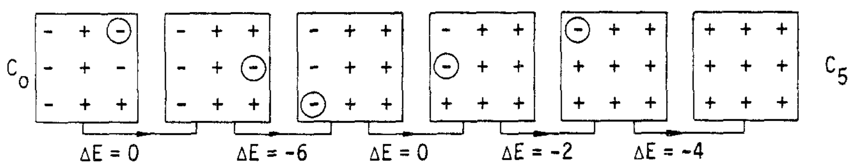

Fig. 7. A sequence of single flips not increasing the energy; the spins to be flipped are circled.

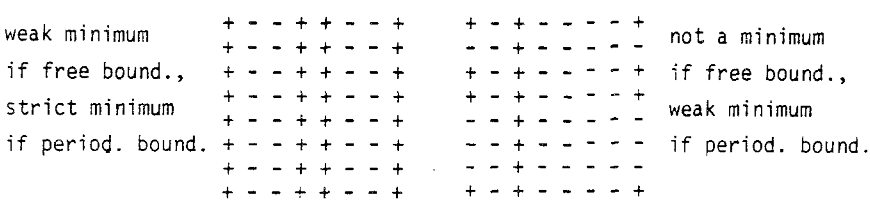

Fig. 8. The influence of periodic boundary conditions.

(Transition-) Theorem 2.5. Let C_0, $C_0 \in \Gamma_{2,g}$, be any configuration that is not a strict minimum of $E(C)$. Then there is a finite sequence $C_0, C_1, ..., C_{\omega_0}$, $C_i \in \Gamma_{2,g}$, and a strict minimum C_{ω_0} of $E(C)$ such that for $i = 0, 1, ..., \omega_0 - 1$, C_{i+1} is obtained from C_i by a single flip, where $E(C_{i+1}) \leqslant E(C_i)$ and $E(C_{\omega_0}) < E(C_0)$.

An illustration of Theorem 2.5 is given in Fig. 7.

A sequence of single flips can never reach a global minimum if C_0 has at least two stripes of width at least 2 and of opposite spin sign.

3. ON THE CASE $d \geqslant 3$

First we give the d-dimensional generalizations of Theorems 2.1 and 2.3.

Theorems 3.1 and 3.2. Let d be a natural number. With $x(k) = [(k+1)/2] - 1$ $\{\lambda(k) = [k/2]\}$, the energy $E(C)$, $C \in \Gamma_{d,g}$, has a strict (weak) minimum at C^* iff $s_x^* \cdot s_u^* = 1$ for at least $d - x(k)$ [at least $d - \lambda(k)$] n.n. u of each grid point x, which has exactly $2d - k$ n.n. u in G, $k = 0, 1, ..., d$ (and in the case of a weak minimum additionally (1.3) holds).

Here $[z]$ means the greatest integer less than or equal to z.

The next theorem describes the behavior of a three-dimensional strict minimum of $E(C)$ on the surface of G, $G \subset R^3$.

Theorem 3.3. If $E(C)$, $C \in \Gamma_{3,g}$, has a strict minimum at C^* and if $\bar{C}^*$ is the restriction of C^* to any of the six "faces" of G, then $\bar{C}^*$ is a local minimum of $E(C)$ on the face.

Finally we give a condition for a strict minimum $C^* \in \Gamma_{3,g}$ that is only sufficient.

Theorem 3.4. Let $C^* \in \Gamma_{3,g}$. If the restriction of C^* to each plane parallel to some face F of G yields the same configuration and if this configuration is a local minimum of $E(C)$, $C \in \Gamma_{2,g}$, then C^* is a strict minimum of $E(C)$, $C \in \Gamma_{3,g}$.

4. CONCLUDING REMARKS

The prospects of getting a three-dimensional analog to Theorem 2.2 and of extending Theorems 2.5 and 3.3 to higher dimensions are good.

Periodic boundary conditions lead, for instance, in the case $d = 2$ to simplified versions of Theorems 2.1 and 2.3. As for Theorems 2.2 and 2.4, there are some slight but essential changes to be made, as can be seen from Fig. 8.

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