The metastable behavior of the three-dimensional stochastic Ising model I*

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Abstract The metastable behavior of the stochastic Ising model in a finite three-dimensional torus is studied in the limit as the temperature goes to zero. All metastable states are characterized and a hierarchic structure is found. For a large class of initial states, the logarithmic asymptotics of the hitting time of the states are studied with all spins +1 or −1.

Keywords: **stochastic Ising model, metastable state, attractor, hierarchic structure, Hamiltonian.**

The problem of metastability has attracted much attention in the past decade[1,2]. In particular, the stochastic Ising model in a finite two-dimensional torus[3—7] has been extensively investigated. The three-dimensional case is more difficult and more important in physics, and remains open.

In this paper we consider the three-dimensional stochastic Ising model under a positive magnetic field. We characterize all metastable states, find out a hierarchic structure of these metastable states. For a large class of initial states, we classify them as supercritical or subcritical configuration, describe the typical evolution of the stochastic Ising model at very low temperature, calculate the logarithmic asymptotics of the hitting time of the configurations with all spins up or all spins down. These results provide a rigorous explanation of the phenomena observed in physics.

Our appproach is quite different from the previous studies[5—10]. We develop the large deviation theory of Freidlin-Wentzell for a family of exponentially perturbed Markov chains in a finite state space[11,12]. The main idea is to view the stochastic Ising model at very low temperature as a perturbation of it at zero temperature. As temperature vanishes, the asymptotic behavior is determined by the most possible path (the path with the highest order of probability) between metastable states (attractors). The investigation is thus reduced to the search for the most possible paths between any two metastable states. This approach has been also used in the study of the two-dimensional stochastic Ising model[3,4].

1 The metastable behavior

Let $\Lambda = \{1, 2, \cdots, N\}^3$ be the three-dimensional lattice torus with periodic boundary conditions. Points of Λ are denoted by u, v, etc. We say that u and v are adjacent if $\| u - v \| = 1$.

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Since Λ is a torus, points with coordinates $(1, y, z)$ and (N, y, z) are also adjacent.

Let $\xi(u)$ be the spin at site u, and spin up if $\xi(x) = +1$ and down if $\xi(x) = -1$. The collection $\xi = \{\xi(u) \mid u \in \Lambda\}$ is called a configuration. In particular, $+\mathbf{1}$ is a configuration with all spins up, $-\mathbf{1}$ is a configuration with all spins down, ξ^u is the configuration that differs from ξ only at u, i.e.

$$\xi^u(v) = \begin{cases} \xi(v), & \text{if } v \neq u, \\ -\xi(v), & \text{if } v = u. \end{cases} \tag{1.1}$$

The state space consists of all configurations, i.e. $S = \{-1, +1\}^\Lambda$. We shall freely use the one-to-one correspondence between $\xi(\in S)$ and the subset $\{u \in \Lambda \mid \xi(u) = +1\}$ of Λ. A connected component of $\{u \in \Lambda \mid \xi(u) = +1\}$ is called a cluster of ξ. In particular, we call ξ a cuboid if $\{u \in \Lambda \mid \xi(u) = +1\}$ is a cuboid $l_1 \times l_2 \times l_3$. By the symmetry of coordinates we may assume $l_1 \leqslant l_2 \leqslant l_3$.

For each configuration $\eta \in S$ assign the Hamiltonian:

$$\begin{aligned} H(\eta) &= -\frac{1}{2} \sum_{\substack{x, v \in \Lambda, \\ \| x - v \| = 1}} \eta(u)\eta(v) - \frac{h}{2}\sum_{u \in \Lambda}\eta(u) - \frac{h}{2}N^3 + \frac{3}{2}N^3 \\ &= \sum_{\substack{u, v \in \Lambda, \\ \| u - v \| = 1}} \frac{1}{2}(1 - \eta(u)\eta(v)) - h\sum_{u \in \Lambda}\frac{1}{2}(1 + \eta(u)), \end{aligned} \tag{1.2}$$

where the first sum runs over the pairs of adjacent sites of Λ (counting each pair only once), and is exactly the number of the pairs of adjacent sites with opposite spins. The second sum is the number of $+1$ spins. Note $H(-\mathbf{1}) = 0$.

The stochastic Ising model with nearest neighbor ferromagnetic interaction on Λ is defined as a Markov chain $\{\xi_n\}$ on S with transition probability:

$$p^\beta(\xi, \eta) = \begin{cases} N^{-3}[1 + \exp(-\beta(H(\xi) - H(\eta)))]^{-1}, & \text{if } \exists\, u \in \Lambda,\ \eta = \xi^u, \\ N^{-3}\sum_{u \in \Lambda}[1 + \exp(\beta(H(\xi) - H(\xi^u)))]^{-1}, & \text{if } \eta = \xi, \\ 0, & \text{otherwise}. \end{cases} \tag{1.3}$$

It is exclusively denoted by $\{\xi_n\}$. Constant h is the intensity of the external field. Parameter β is called the inverse temperature. We sometimes put β as a superscript to emphasize the dependence on β. We also put subscript ξ to indicate the initial state. Assume throughout this paper that

$$0 < h \ll 2,\ 4/h \ll N, \text{ and } 4/h \text{ is not an integer}. \tag{1.4}$$

This is the most interesting case. Introduce three related numbers:

$$L_2 = [2/h] + 1,\ L = [4/h] + 1,\ \Gamma_2 = 4L_2 - (L_2^2 - L_2 + 1)h,$$

where $[\cdot]$ means the integer part of a real number.

Let $\sigma(\zeta) = \min\{n \mid \xi_n = \zeta\}$ be the first hitting time of configuration ζ by $\{\xi_n\}$.

Definition 1.1. We say configuration ξ is subcritical (supercritical) if

$$\lim_{\beta \to \infty} P_\xi^\beta(\sigma(-\mathbf{1}) < \sigma(+\mathbf{1})) = 1, (0 \text{ respectively}).$$

Theorem 1.1. *Suppose that the initial state ξ is a cuboid $l_1 \times l_2 \times l_3$, and $l_1 \leqslant l_2 \leqslant l_3 \leqslant N - 1$. ε is a positive number.*

(i) *If $l_1 < L_2$, then ξ is subcritical and*

$$\lim_{\beta\to\infty} P_{\xi}^{\beta}(\mid (1/\beta)\log\sigma(-\mathbf{1}) - (l_1 - 1)h \mid < \varepsilon) = 1.$$

(ii) *If* $L > l_1 \geqslant L_2, 2(l_1 + l_2) - hl_1 l_2 > 0$, *then* ξ *is subcritical and*

$$\lim_{\beta\to\infty} P_{\xi}^{\beta}(\mid (1/\beta)\log\sigma(-\mathbf{1}) - \Gamma_2 + 2(l_1 + l_2) - hl_1 l_2 \mid < \varepsilon) = 1.$$

(iii) *If* $l_1 \geqslant L$, *or* $L > l_1 \geqslant L_2$, $2(l_1 + l_2) - hl_1 l_2 < 0$, *then* ξ *is supercritical and*

$$\lim_{\beta\to\infty} P_{\xi}^{\beta}(\mid (1/\beta)\log\sigma(+\mathbf{1}) - \Gamma_2 \mid < \varepsilon) = 1.$$

Intuitively, a small cuboid tends to shrink and disappear, and a large cuboid tends to grow. Every cuboid is either subcritical or supercritical. Next, we extend this theorem to a larger class of initial states.

Definition 1.2. Configuration ξ is called a metastable state if $H(\xi) < H(\xi^u)$ for all $u \in \Lambda$. The collection of metastable states is denoted by $\mathscr{A}_1$

Definition 1.3. We say subset D of Λ is connected if for any $u, v \in D$ there is a sequence $\{w_0, w_1, \cdots, w_n\}$ such that $w_0 = u$, $w_n = v$, $w_i \in D$, w_i and w_{i+1} are adjacent. A connected component of $\{u \in \Lambda \mid \xi(u) = +1\}$ is called a cluster of ξ.

Definition 1.4. We say a configuration ξ is simple if $\{u \in \Lambda \mid \xi(u) = +1\}$ is connected and its intersection with any plane (parallel to a coordinate plane) or any line (perpendicular to a coordinate plane) is also connected. Let S^0 be the set of all simple configurations.

S^0 is large enough to contain most interesting configurations, such as $+\mathbf{1}$, $-\mathbf{1}$ and cuboids. A simple configuration is shown in figure 1.

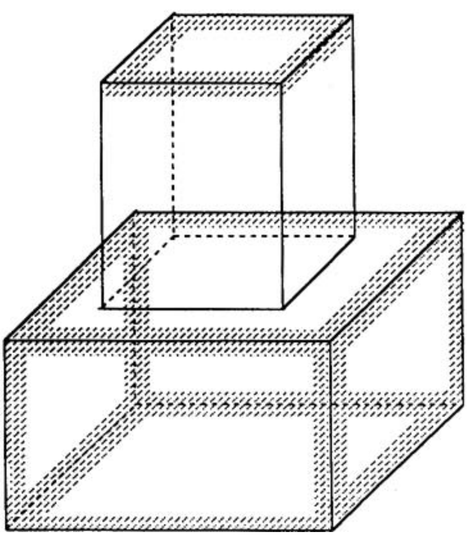

Fig. 1. A simple configuration and its exterior time (highlighted).

Definition 1.5. The boundary set of configuration ξ is defined as

$$\{u \in \Lambda \mid \xi(u) = +1, \ \exists\, v \in \Lambda, \ u, v \text{ are adjacent}, \ \xi(v) = -1\}.$$

The intersection of the boundary set with a plane (parallel to a coordinate plane) may have several connected components. Each connected component is called a face.

Suppose that $\xi \in S^0 \cap \mathscr{A}_1$. Remove one by one from ξ all the faces which can be contained in a $(L_1 - 1) \times (N - 1)$ rectangle. The resultant configuration is denoted by $\xi^{(-)}$. Note that $\xi^{(-)}$ is unique though there are different orders of removing faces. Let $\xi^{(+)}$ be the smallest cuboid containing $\xi^{(-)}$.

Theorem 1.2. *Suppose that* $\xi \in S^0 \cap \mathscr{A}_1$, *and* $\varepsilon > 0$.

(i) *If* $\xi^{(+)}$ *is subcritical, so is* ξ. *If* $\xi^{(+)}$ *is supercritical, so is* ξ.

(ii) $\lim_{\beta\to\infty}P_\xi^\beta((1/\beta)\log\sigma(\xi^{(+)})<2-h+\varepsilon)=1$.

(iii) $\lim_{\beta\to\infty}P_\xi^\beta(\sigma(\xi^{(-)})<\sigma(\xi^{(+)})<\sigma(+1))=1$.

This theorem describes how the stochastic Ising model evolves starting at $\xi\in S^0\cap\mathscr{A}_1$. When β is very large, with nearly probability 1, $\{\xi_n\}$ evolves from ξ to $\xi^{(-1)}$ by removing the smallest face first, then the second smallest face, and so on; then from $\xi^{(-)}$ to $\xi^{(+)}$, by adding +1 spins. Because $\xi^{(+)}$ is a cuboid and $\{\xi_n\}$ is strong Markovian, after $\sigma(\xi^{(+)})$ the evolution is described by Theorem 1.1.

2 The idea of proof

The idea of proof is to use the large deviation estimates of a family of exponentially perturbed Markov chains[11]. By (1.3) define

$$p^\infty(\xi,\eta)=\begin{cases}N^{-3}, & \eta=\xi^u,\ H(\xi)>H(\xi^u),\\ 0, & \text{other } \eta\neq\xi,\end{cases}\tag{2.1}$$

and $p^\infty(\xi,\xi)$ appropriately. Then assumptions (0.1), (0.2) and (0.3) of ref. [11] are satisfied. With the convention that $\log 0=-\infty$, let

$$C(\xi,\eta)=\begin{cases}0, & \text{if } p^\infty(\xi,\eta)>0,\\ \lim_{\beta\to\infty}(-\log p^\beta(\xi,\eta))/\beta, & \text{if } p^\infty(\xi,\eta)=0,\end{cases}$$
$$=\begin{cases}0, & \text{if } \eta=\xi,\\ [H(\xi^u)-H(\xi)]^+, & \text{if } \exists\, u\in\Lambda,\ \eta=\xi^u,\\ \infty, & \text{otherwise.}\end{cases}\tag{2.2}$$

Definition 2.1 Let K be a proper subset of S. $G(K)$ is the set of maps $g:K\to S$ with the property that g maps no non-empty subset of K into itself. We say that $g\in G(K)$ leads $\xi\in K$ to $\eta\in S\setminus K$ if there is a sequence $\{\zeta_1,\cdots,\zeta_n\}$ of distinct elements in K such that

$$g(\xi)=\zeta_1,\ g(\zeta_n)=\eta,\ \text{and } g(\zeta_j)=\zeta_{j+1},\ 1\leqslant j\leqslant n-1.$$

Let $G_{\xi\eta}(K)=\{g\in G(K)\}$. *g leads* ξ *to* $\eta\}$.

Definition 2.2. Define

$$W(K)=\min_{g\in G(K)}\sum_{\zeta\in K}C(\zeta,g(\zeta)),\quad W_{\xi\eta}(K)=\min_{g\in G_{\xi\eta}(K)}\sum_{\zeta\in K}C(\zeta,g(\zeta)).$$

Definition 2.3. We say that sequence $\{\eta_k,k=0,1,\cdots,m\}$ leads ξ to η if $\xi=\eta_0$, $\eta=\eta_m$ and $\eta_{j+1}=\eta_j^{u_j}$ for some $u_j\in\Lambda$, $j=0,\cdots,m-1$. The quantity $\max_{0\leqslant j\leqslant m}H(\eta_j)-H(\eta)$ is called the barrier from ξ to η along sequence $\{\eta_j\}$ (if we interpret H of (1.1) as the potential energy). The minimum barrier from ξ to η is the minimum of barriers over all sequences leading ξ to η, and is denoted by $MB(\xi,\eta)$.

Definition 2.4. A recurrent calss of Markov chain $\{\xi_n^\infty\}$ is called a level 1 attractor. Level 1 attractors are denoted by $A_1^1,\cdots,A_s^1$. The corresponding attractive basin of A_i^1 is $B_i^1=\{\xi\mid MB(\xi\xi)=0$ for some $\zeta\in A_i^1$ is $0\}$. Let $V(1)=\min_i W(B_i^1)$.

We now define inductively higher level attractors and attractive basins. Suppose that we have already defined level k attractors and attractive basins, and $V(k)$.

Definition 2.5. We say $A_i^k \overset{(k)}{\Rightarrow} A_j^k$ if there exist $\zeta \in A_i^k$ and $\eta \in B_j^k \setminus B_i^k$ such that

$$W_{\zeta\eta}(B_i^k) - \min_{\zeta \in B_i^k} W(B_i^k \setminus \{\zeta\}) = V(B_i^k) = V(k).$$

We say $A_i^k \overset{(k)}{\rightarrow} A_j^k$ if there is a sequence $\{A_{n_0}^k, A_{n_1}^k, \cdots, A_{n_m}^k\}$ such that $A_i^k = A_{n_0}^k$, $A_{n_m}^k = A_j^k$ and $A_{n_l}^k \overset{(k)}{\Rightarrow} A_{n_{l+1}}^k$ for $l = 0, \cdots, m-1$.

We say $A_i^k \overset{(k)}{\leftrightarrow} A_j^k$ if $A_i^k \overset{(k)}{\rightarrow} A_j^k$ and $A_j^k \overset{(k)}{\rightarrow} A_i^k$. $\overset{(k)}{\leftrightarrow}$ defines an equivalent relation.

Definition 2.6. A level $(k+1)$ attractor A_i^{k+1} is a set of some level k attractors such that

(1) $\forall A_m^k, A_j^k \in A_i^{k+1}, A_m^k \overset{(k)}{\leftrightarrow} A_j^k$,

(2) if $A_m^k \in A_i^{k+1}$ and $A_m^k \overset{(k)}{\rightarrow} A_j^k$, then $A_j^k \in A_i^{k+1}$.

In particular, $\{A_i^k\}$ is a level $(k+1)$ attractor if $V(B_i^k) > V(k)$.

Definition 2.7. The attractive basin B_i^{k+1} of a level $(k+1)$ attractor A_i^{k+1} is defined as $B_i^{k+1} = \bigcup \{B_j^k \mid A_j^k \overset{(k)}{\rightarrow} A_m^k$ for some $A_m^k \in A_i^{k+1}\}$. Define $V(k+1) = \min_i V(B_i^{k+1})$.

3 The hierarchic structure of attractors

Proposition 3.1. *Every recurrent class of Markov chain* $\{\xi_n^\infty\}$ *with transition probability given by* (2.1) *consists of exactly one configuration. The following three statements are equivalent.*

(i) $\{\xi\}$ *is a recurrent class of Markov chain* $\{\xi_n^\infty\}$,

(ii) $\{\xi\}$ *is a metastable state,*

(iii) *at least three spins at the six adjacent sites of u are* $+1$ *if* $\xi(u) = +1$, *and at least four spins at the six adjacent sites of u are* -1 *if* $\xi(u) = -1$.

Proof. Suppose that $\xi_1, \xi_2, \cdots, \xi_n (n \geq 2)$ are in a recurrent class such that

$$\mathrm{p}^\infty(\xi_1, \xi_2) > 0,\ \mathrm{p}^\infty(\xi_2, \xi_3) > 0, \cdots,\ \mathrm{p}^\infty(\xi_{n-1}, \xi_n) > 0,\ \mathrm{p}^\infty(\xi_n, \xi_1) > 0.$$

Then it follows from (2.1) that $\xi_{j+1} = \xi_j^{u_j}$ for some $u_j \in \Lambda$ and that

$$H(\xi_1) > H(\xi_2) > H(\xi_3) > \cdots > H(\xi_n) > H(\xi_1).$$

The contradiction in the above inequalities shows that the first statement holds.

A single configuration $\{\xi\}$ is a recurrent class if and only if $\mathrm{p}^\infty(\xi, \eta) = 0$ for all $\eta \neq \xi$. Equivalently, $H(\xi) < H(\xi^u)$ for all $u \in \Lambda$. Notice that

$$H(\xi^u) - H(\xi) = \begin{cases} h + \sum_{\|v-u\|=1} \xi(v), & \text{if } \xi(u) = +1, \\ -\left[h + \sum_{\|v-u\|=1} \xi(v)\right], & \text{if } \xi(u) = -1. \end{cases} \tag{3.1}$$

The possible values of $\sum_{\|v-u\|=1} \xi(v)$ are ± 6, ± 4, ± 2 and 0, and $0 < h < 2$ by (1.4), hence the three statements are equivalent. Q.E.D.

It remains to identify attractors of higher levels. Thanks to the reversibility, the difficulty in computing $V(B_i^k)$ is greatly reduced.

Lemma 3.1. *Suppose that A_i^k is a level k attractor and $\zeta \in A_i^k$. Let B_i^k be the cooresponding attractive basin. Then*

$$V(B_i^k) = \min\{MB(\zeta, \zeta') \mid \zeta' \in A_j^k, \text{ for some } j \neq i\}. \tag{3.2}$$

Proof. The key observation here is by (2.2) that for any $\eta \in S$ and $u \in \Lambda$,

$$C(\eta^u, \eta) - C(\eta, \eta^u) = [H(\eta) - H(\eta^u)]^+ - [H(\eta^u) - H(\eta)]^+ = H(\eta) - H(\eta^u).$$

Take $\eta_1 \in B_i^k$ such that $\eta_0 = \eta_1^u \notin B_i^k$ for some u. By Lemma 3.1 of ref. [11] (with different notations), there is $g \in G_{\eta_1 \zeta}(B_i^k \setminus \{\zeta\})$ such that $\sum_{\eta \in B_i^k \setminus \{\zeta\}} C(\eta, g(\eta)) = W(B_i^k \setminus \{\zeta\})$. Let $\eta_{j+1} = g(\eta_j)$ for $j = 1, 2, \cdots$ until $\eta_{m+1} = \zeta$. In other words, sequence $\{\eta_0, \eta_1, \cdots, \eta_{m+1}\}$ leads η_0 to $\eta_{m+1} = \zeta$. Define

$$g'(\eta) = \begin{cases} \eta_{j-1} & \text{if } \eta = \eta_j, j = 1, 2, \cdots, m+1, \\ g(\eta), & \text{if } \eta \in B_i^k \setminus \{\eta_1, \cdots, \eta_{m+1}\}. \end{cases}$$

Then $g' \in G(B_i^k)$ and $W(B_i^k) \leqslant \sum_{\eta \in B_i^k} C(\eta, g'(\eta))$. We have

$$\begin{aligned} V(B_i^k) &= W(B_i^k) - W(B_i^k \setminus \{\zeta\}) \leqslant \sum_{\eta \in B_i^k} C(\eta, g'(\eta)) - \sum_{\eta \in B_i^k \setminus \{\zeta\}} C(\eta, g(\eta)) \\ &= \sum_{k=1}^{m+1} C(\eta_k, \eta_{k-1}) - \sum_{k=1}^{m} C(\eta_k, \eta_{k+1}) \\ &= C(\eta_1, \eta_0) + \sum_{k=1}^{m} [C(\eta_{k+1}, \eta_k) - C(\eta_k, \eta_{k+1})] \\ &= [H(\eta_0) - H(\eta_1)]^+ + \sum_{k=1}^{m} [H(\eta_k) - H(\eta_{k+1})] \\ &= [H(\eta_0) - H(\eta_1)]^+ + H(\eta_1) - H(\zeta). \end{aligned}$$

If $H(\eta_0) > H(\eta_1)$, η_0 and η_1 would be in the same attractive basin of level 1. Consequently, η_0 and η_1 would be in the same attractive basin of higher levels. This contradicts the assumption that $\eta_0 \notin B_i^k$. Since η_1 is arbitrary,

$$V(B_i^k) \leqslant -H(\zeta) + \min\{H(\eta) \mid \eta \in B_i^k, \eta^u \notin B_i^k \text{ for some } u\}.$$

On the other hand, choose $f \in G(B_i^k)$ such that $\sum_{\eta \in B_i^k} C(\eta, f(\eta)) = W(B_i^k)$. Sequence $\{\eta_0 = \zeta, \eta_1, \eta_2, \cdots, \eta_{m+1}; \eta_{j+1} = f(\eta_j)\}$ leads ζ to $\eta_{m+1} \notin B_i^k$. Define

$$f'(\eta) = \begin{cases} \eta_{j-1}, & \text{if } \eta = \eta_j, j = 1, 2, \cdots, m, \\ f(\eta), & \text{if } \eta \in B_i^k \setminus \{\eta_1, \cdots, \eta_m\}. \end{cases}$$

Then $f' \in G(B_i^k \setminus \{\zeta\})$ and $W(B_i^k \setminus \{\zeta\}) \leqslant \sum_{\eta \in B_i^k \setminus \{\zeta\}} C(\eta, f'(\eta))$.

$$\begin{aligned} V(B_i^k) &= W(B_i^k) - W(B_i^k \setminus \{\zeta\}) \geqslant \sum_{\eta \in B_i^k} C(\eta, f(\eta)) - \sum_{\eta \in B_i^k \setminus \{\zeta\}} C(\eta, f'(\eta)) \\ &= \sum_{k=0}^{m} C(\eta_k, \eta_{k+1}) - \sum_{k=1}^{m} C(\eta_k, \eta_{k-1}) \end{aligned}$$

$$= C(\eta_m, \eta_{m+1}) + \sum_{k=1}^{m}[C(\eta_{k-1}, \eta_k) - C(\eta_k, \eta_{k-1})]$$

$$\geqslant \sum_{k=1}^{m}[H(\eta_k) - H(\eta_{k-1})] = H(\eta_m) - H(\zeta)$$

$$\geqslant - H(\zeta) + \min\{H(\eta) \mid \eta \in B_i^k, \eta^u \notin B_i^k \text{ for some } u\}.$$

We have proved that

$$V(B_i^k) = - H(\zeta) + \min\{H(\eta) \mid \eta \in B_i^k, \eta^u \notin B_i^k \text{ for some } u\}. \quad (3.3)$$

Suppose η is a configuration that reaches the minimum in (3.3) and η^u is in the attractive basin B_j^k of another level k attractor A_j^k, $j \neq i$. There is a sequence $\{\eta'_l\}$ leading η to $\zeta' \in A_j^k$ such that $H(\eta'_l) \leqslant H(\eta)$. Combine it with the sequence leading ζ to η to form a sequence leading ζ *to* ζ'. So (3.3) can be rewritten as (3.2). Q.E.D.

Definition 3.1. By exterior line we mean a line on the boundary set such that the two end sites have 3 adjacent -1 spins and every other site of the line has 2 adjacent -1 spins (figure 1).

Lemma 3.2. *The minimum barrier of adding an exterior line is* $2 - h$. *The minimum barrier of removing an exterior line of length* l *is* $(l-1)h$.

Proof. The proof for the two statements is the same and we shall only prove the latter. Flipping $+1$ spins along an exterior line one by one. Take u_1 as an end site of the exterior line. There are three adjacent -1 spins and three adjacent $+1$ spins. By (3.1), $H(\zeta^{u_1}) - H(\zeta) = \zeta(u_1)[h + \sum_{\|v-u_1\|=1}\zeta(v)] = h$. After that, take site u_2 of the exterior line next to site u_1. There are three adjacent $+1$ spins and three adjacent -1 spins (one at u_1 and the other two by definition). The (minimum) barrier of flipping the spin at u_2 is h again. By the same argument, the barrier of flipping the spin at u_i is h for $i = 2, 3, \cdots, l-1$. The barrier of flipping spin at the last site u_l is 0 because, having flipped $+1$ spin to -1 spin at site u_{l-1}, there are four adjacent -1 spins and two adjacent $+1$ spins. Let ζ' be the resulting configuration. Then the barrier from ζ to ζ' is $(l_1 - 1)h$. $\zeta' \in \mathscr{A}_1$ or there is a sequence leading ζ' to a metastable state with decreasing Hamiltonian. In the second case replace ζ' by the metastable state and denote the metastable state by ζ' (abusing notaion a little). Then the minimum barrier from ζ to ζ' is no greater than $(l-1)h$.

We shall thoroughly analyze the Hamiltonian in the sequel[1)] to finish the proof that the minimum barrier from ζ to ζ' is indeed $(l-1)h$. Q.E.D.

Proposition 3.2. *Every level* k *attractor consists of one configuration if* $k \leqslant L_2 - 1$. *Let* $\mathscr{A}_k$ *be the set of level* k *attractors. If* $k \leqslant L_2 - 1$, *then*

$$\mathscr{A}_k = \{\zeta \in \mathscr{A}_1 \mid \zeta \textit{ has no exterior line of length} \leqslant k\},$$

$$V(k) = kh \text{ if } k < L_2 - 1; \quad V(L_2 - 1) = 2 - h. \quad (3.4)$$

ζ *is an attractor of level* L_2 *if and only if*

1) Chen, D., Feng, J., Qian, M. P., The metastable behavior of the three-dimensional stochastic Ising model Ⅱ, to appear in *Science in China*.

$\{u \in \Lambda \mid \zeta(u) = +1\}$ *consists of several cuboids, the side length of each cuboid is at least* L_2 *and the distance between two cuboids is at least* 3. (3.5)

Remark. For this reason we shall simply denote level k attractor by the configuration itself. $B^k(\zeta)$ is the corresponding attractive basin of level k attractor ζ and $V^k(\zeta)$ stands for $V(B^k(\zeta))$.

Proof. If $\zeta \in \mathscr{A}_1$, by Proposition 3.1 and (3.1) in particular, the possible values of minimum barrier $H(\zeta^u) - H(\zeta)$ are $h, 2 \pm h, 4 \pm h$ or $6 \pm h$. So h is the smallest minimum barrier. On the other hand, take $\eta_1 \in \mathscr{A}_1$ which has an exterior line of length 2. According to Lemma 3.1, $V^1(\zeta_1) \leqslant h$. So $V(1) = h$.

Suppose that $\eta \in \mathscr{A}_1$ has no exterior line of length 2. Suppose a sequence leading η to $\eta' \in \mathscr{A}_1$ satisfies (3.2). The difference between η and η' is at least an exterior line. The minimum barrier is at least $2h$ for deleting an exterior line of length $\geqslant 3$. On the other hand, the minimum barrier for adding one $+1$ spin is $2 - h$, exceeding $2h$ already (if h is very small). The minimum barrier for adding one exterior line will be no less than $2 - h$. In either case, $V^1(\eta) \geqslant 2h > V(1)$. Then $\eta \in \mathscr{A}_2$ by (the last line of) Definition 2.6.

If $\zeta \in \mathscr{A}_1$ and $V^1(\zeta) = h$, by the proof of Lemma 3.1, we can find $\zeta' \in \mathscr{A}_1$ and a sequence leading ζ to ζ' with minimum barrier h. Since $H(\zeta') \neq H(\zeta)$, $MB(\zeta', \zeta) > h$. So ζ cannot join ζ' to form a level 2 attractor. This shows that every level 2 attractor consists of one configuration. Therefore $\mathscr{A}_2 = \{\zeta \in \mathscr{A}_1 \mid \zeta$ has no exterior line of length 2$\}$.

For $\zeta \in \mathscr{A}_2$, $V^2(\zeta) \geqslant V^1(\zeta) \geqslant 2h$. On the other hand, there is $\eta \in \mathscr{A}_2$ such that $V^2_{(\eta)} = 2h$. For example, MB (cube $3 \times 3 \times 3$, $-\mathbf{1}) \leqslant 2h$, and hence $V^2(3 \times 3 \times 3) \leqslant 2h$. We have shown $V(2) = 2h$.

This argument is repeated inductively for levels $3, 4 \cdots, L_2 - 1$.

Suppose ζ is a level $(L_2 - 1)$ attractor. Then the length of its exterior line will be at least L_2 by the previous proof. The minimum barrier of removing one exterior line is at least $(L_2 - 1)h$ by Lemma 3.2. The minimum barrier of adding one $+1$ spin, hence one exterior line, is $2 - h$. Note that $(L_2 - 1)h > 2 - h$. The minimum barrier from one attractor of level $(L_2 - 1)$ to another is at least $2 - h$. On the other hand, it is easy to pick $\zeta \in \mathscr{A}_{L_2 - 1}$ such that $V^{L_2 - 1}(\zeta) = 2 - h$. So is $V(L_2 - 1)$.

Suppose that $\xi \in \mathscr{A}_{L_2 - 1}$ but does not satisfy (3.5). Flipping -1 spins to $+1$ spins in a certain way, we can construct a sequence leading ξ to $\xi' \in \mathscr{A}_{L_2 - 1}$. Here ξ' is obtained by expanding a cluster of ξ to a cuboid. Note that $MB(\xi, \xi') = 2 - h$ and $H(\xi') < H(\xi)$. This procedure can be repeated if ξ' does not satisfy (3.5). Thus $\xi \notin \mathscr{A}_{L_2}$, and cannot be equivalent to other $\xi' \in \mathscr{A}_{L_2 - 1}$ in the sense of Definition 2.5. So (3.5) is a necessary condition for $\xi \in \mathscr{A}_{L_2}$. On the other hand, if $\eta \in \mathscr{A}_{L_2 - 1}$ satisfies (3.5), then $V^{L_2 - 1}(\eta) > 2 - h$. Hence $\eta \in \mathscr{A}_2$ by (the last line of) Definition 2.6. Q.E.D.

Lemma 3.3. *Suppose that* $\zeta = l_1 \times l_2 \times l_3$ *and* $L_2 \leqslant l_1 \leqslant l_2 \leqslant l_3$. *Let* $\zeta' = l_1 \times l_2 \times (l_3$

$+1)$ *and* $\zeta'' = l_1 \times l_2 \times (l_3 - 1)$.

(i) *If* $l_1 \geqslant L$ *or* $L_2 \leqslant l_1 < L$, $2(l_1 + l_2) - hl_1 l_2 < 0$, *then* $H(\zeta') < H(\zeta) < H(\zeta'')$ *and* $MB(\zeta, \zeta') = \Gamma_2$.

(ii) *If* $L_2 \leqslant l_1 < L, 2(l_1 + l_2) - hl_1 l_2 > 0, l_3 < N$, *then* $H(\zeta'') < H(\zeta) < H(\zeta')$ *and* $MB(\zeta, \zeta'') = \Gamma_2 - 2(l_1 + l_2) + hl_1 l_2$.

Proof. Because of the symmetry, it suffices to show one part, say, i). If $l_1 \geqslant L$ or $L_2 \leqslant l_1 < L, 2(l_1 + l_2) - hl_1 l_2 < 0$, then we verify by direct computation: $H(\zeta') < H(\zeta) < H(\zeta'')$. Construct a sequence $\{\eta_j, j = 0, 1, \cdots, n\}$ leading ζ to ζ' by adding $+1$ spins adjacent to an $l_1 \times l_2$ face one by one to fill a 2×2 square first, and expand it to 2×3, to $3 \times 3, \cdots$, $L_2 \times (L_2 - 1)$, $L_2 \times L_2 \cdots, l_1 \times l_1$, $l_1 \times (l_1 + 1)$, $\cdots$, until $l_1 \times l_2$. Then $\max_j H(\eta_j) - H(\xi) = \Gamma_2$.

It remains to justify that the sequence constructed above indeed attains the minimum barrier. The difference of the numbers of $+1$ spins of ζ and ζ' is $l_1 l_2 \geqslant (L_2)^2$. Along any sequence leading ζ to ζ', there is a configuration ξ whose numbers of $+1$ spins is larger than tht of ξ by $(L_2)^2 - L_2 + 1$. Of all possible ways of placing $(L_2)^2 - L_2 + 1$ spins, the minimum Hamiltonian is reached by arranging them as a two-dimensional critical droplet. The full argument is deferred to the sequel of this paper.

Proposition 3.3. *There is an integer r such that* $-\mathbf{1}$ *and* $+\mathbf{1}$ *are the only two attractors of level* $(r+1)$.

(a) *If* $L \leqslant l_1 \leqslant l_2 \leqslant l_3$ *or* $l_1 \geqslant L_2, 2(l_1 + l_2) - hl_1 l_2 < 0$, *cuboid* $l_1 \times l_2 \times l_3$ *is a level r attractor, is in* $B^{r+1}(+\mathbf{1})$ *but not in* $B^{r+1}(-\mathbf{1})$. $MB(l_1 \times l_2 \times l_3, -\mathbf{1}) = \Gamma_2$.

(b) *If* $l_1 < L_2$ *or* $l_1 \geqslant L_2, 2(l_1 + l_2) - hl_1 l_2 > 0$, *cuboid* $l_1 \times l_2 \times l_3$ *is not a level r attractor, is in* $B^{r+1}(-\mathbf{1})$ *but not in* $B^{r+1}(+\mathbf{1})$, $MB(l_1 \times l_2 \times l_3, -\mathbf{1}) = \Gamma_2$.

Proof. For $\zeta \in S^0 \cap \mathscr{A}_k$, let $\zeta' \in \mathscr{A}_k$ and a sequence leading ζ to ζ' satisfy (3.2). If the sequence is not entirely in S^0, we may construct a new sequence in S^0 without increasing the minimum barrier. The details will be given in the sequel of this paper, Hence it suffices to compare $\zeta \in S^0 \cap \mathscr{A}_k$ with other $\zeta' \in S^0 \cap \mathscr{A}_k$ when applying Lemma 3.1 to determine if ζ is also an attractor of level $(k+1)$.

Suppose that cuboid $\zeta = l_1 \times l_2 \times l_3, L_2 \leqslant l_1 \leqslant l_2 \leqslant l_3$, and a sequence leads ζ to $\zeta' \in S^0 \cap \mathscr{A}_k$. The difference between ζ and ζ' is at least one face $l_1 \times l_2$. It is shown in the last part of the previous proof that $MB(\zeta, \zeta') \geqslant \Gamma_2$ or $\Gamma_2 - 2(l_1 + l_2) + hl_1 l_2$, respectively. That lower bound of minimum barrier is reached by adding or deleting a face.

Among six possibilities of adding or deleting a face, only three have lower Hamiltonian. Lemma 3.3 lists the minimum barriers from ζ to the three candidates. Take the smallest as $V^k(\zeta)$. Either $V^k(\zeta) > V(k)$, so $\zeta \in \mathscr{A}_{k+1}$, or there exists a cuboid ζ_1 satisfying (3.2). It is easy to see that $V^k(\zeta) = V^k(\zeta_1)$. We repeat the same procedure to find ζ_2, and so on, eventually stop at $+\mathbf{1}$ or $-\mathbf{1}$. If a cuboid of $\mathscr{A}_k \cap S^0$ is not a level $(k+1)$ attractor, then it is in $B^{k+1}(+\mathbf{1})$ or $B^{k+1}(-\mathbf{1})$, the attractive basin of $+\mathbf{1}$ or $-\mathbf{1}$ as level $(k+1)$ attractors.

Thus, every cuboid is led either to $+\mathbf{1}$ with minimum barrier Γ_2 or to $-\mathbf{1}$ with minimu barrier $< \Gamma_2$. Hence any configuration $\zeta \in S$ is led to $+\mathbf{1}$ or $-\mathbf{1}$ by a sequence with minimum barrier less than or equal to Γ_2. Consequently $\mathscr{A}_{r+1} = \{+\mathbf{1}, -\mathbf{1}\}$. Q.E.D.

4 Proof of theorems

Lemma A (Lemma 3.3 of ref. [11]). *Let* $U(K) = \min_{\zeta \in K} W(K \setminus \{\zeta\}) - \min_{\xi, \eta \in K} W(K \setminus \{\xi, \eta\})$. *Then*

$$U(B_i^k) \leqslant V(k-1) < V(k) \leqslant V(B_i^k).$$

Lemma B (Theorem 3.2 of ref. [11]). *Let* $\tau(\cdot)$ *be the first exit time of* $\{\xi_n\}$. *Namely* $\tau(K) = \min\{n;\ \xi_n \notin K\}$. *For any* $\xi \in B_i^k \setminus \bigcup_{j \neq i} B_j^k$ *and* γ *such that* $U(B_i^k) < \gamma < V(B_i^k)$,

$$\lim_{\beta \to \infty} \mathrm{P}_\xi^\beta (\sigma(\zeta) \leqslant \mathrm{e}^{\gamma\beta} \leqslant \tau(B_i^k)) = 1. \tag{4.1}$$

Proof of Theorem 1.1. Suppose $\xi = l_1 \times l_2 \times l_3$, $l_1 \geqslant L$ or $L > l_1 \geqslant L_2$, $2(l_1 + l_2) - hl_1 l_2 < 0$. By Proposition 3.3, ξ is a level r attractor, and is in $\mathrm{B}^{r+1}(+\mathbf{1})$ but not in $B^{r+1}(-\mathbf{1})$. By Lemma B, with very large probability $\{\xi_n\}$ will hit $-\mathbf{1}$ within $\exp((U^{r+1}(+\mathbf{1}) + \varepsilon)\beta)$. By Lemma A, $U^{r+1}(+\mathbf{1}) \leqslant V(r) = \Gamma_2$. Accordingly,

$$\lim_{\beta \to \infty} \mathrm{P}^\beta \left(\frac{1}{\beta} \log \sigma(+\mathbf{1}) < \Gamma_2 + \varepsilon \right) = 1.$$

On the other hand, $\sigma(+\mathbf{1}) \geqslant \tau(B^r(\xi))$, and $\xi \in B_i^k \setminus \bigcup_{j \neq i} B_j^k$. According to (4.1),

$$\lim_{\beta \to \infty} \mathrm{P}^\beta \left(\frac{1}{\beta} \log \tau(B^r(\xi)) > \Gamma_2 - \varepsilon \right) = 1.$$

With probability near 1, $\{\xi_n\}$ will hit $+\mathbf{1}$) before exiting $B^{\gamma+1}(+\mathbf{1})$ and hitting $-\mathbf{1}$. So ξ is supercritical. This proves (ⅲ). (ⅰ) and (ⅱ) can be proved in the same way. Q.E.D.

Proof of Theorem 1.2. By removing exterior lines, a configuration envolves from level 1 to level $(L_2 - 1)$ in the hierarchic structure of attractors. If ξ is simple, then ξ is in the level $(L_2 - 1)$ attractive basin of $\xi^{(-)}$ (introduced before Theorem 2). ξ cannot be in other level $(L_2 - 1)$ attractive basins (although it may be in several lower level attractive basins simultaneously). By Lemma B,

$$\lim_{\beta \to \infty} \mathrm{P}_\xi^\beta (\sigma(\xi^{(-)}) \leqslant \tau(B^{L_2 - 1}(\xi^{(-)}))) = 1. \tag{4.2}$$

Hamiltonian decreases along the sequence from ξ to $\xi^{(-)}$. From level $L_2 - 1$ upper, the minimum barrier of adding an exterior line is smaller than that of deleting an exterior line. Expanding the cluster of $\xi^{(-)}$ to $\xi^{(+)}$ corresponds to the envolution from level $L_2 - 1$ to level L_2 in the hierarchic structure. $\xi^{(-)}$ is in the attractive basin of level L_2 attractor $\xi^{(+)}$, but is not in other level L_2 attractive basins. Hence

$$\lim_{\beta \to \infty} \mathrm{P}_\xi^\beta (\sigma(\xi^{(+)}) \leqslant \tau(B^{L_2}(\xi^{(+)}))) = 1. \tag{4.3}$$

Again the Hamiltonian decreases. Part (ⅲ) is obtained by applying Lemma B to level $(L_2 - 1)$ attractor $\xi^{(-)}$ and level L_2 attractor $\xi^{(+)}$. By Lemma A and Proposition 3.2, $U^{L_2}(\xi^{(+)}) \leqslant V(L_2 - 1) = 2 - h$. Part (ⅱ) now follows from Lemma B. Because both $\sigma(+\mathbf{1})$ and $\sigma(-\mathbf{1})$ are larger than or equal to $\tau(B^{L_2}(\xi^{(+)}))$, (4.2) and (4.3) together with the strong Markovian property imply part (ⅰ). Q.E.D.

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