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The metastable behavior of the three-dimensional stochastic Ising model (Ⅱ)*

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Abstract The metastable behavior of the stochastic Ising model is studied in a finite three-dimensional torus, in the limit as the temperature goes to zero. The so-called critical droplet is determined, a clear view of the passage from the configuration that all spins are down $(-\mathbf{1})$ to the configuration that all spins are up $(+\mathbf{1})$ is given and the logarithmic asymptotics of the hitting time of $+\mathbf{1}$ starting at $-\mathbf{1}$ or *vice versa* is calculated. The proof uses large deviation estimates of a family of exponentially perturbed Markov chains.

Keywords: stochastic Ising model, metastable state, Hamiltonian, critical droplet.

1 Main result

This is a continuation of the study on the three-dimensional stochastic Ising model. In ref. [1] we have characterized all metastable states, found out a hierarchic structure of these metastable states. For a large class of initial states, we classify them as supercritical or subcritical ones, describe the typical evolution of the stochastic Ising model at very low temperature. In this paper we will use the notation and definitions introduced in ref. [1]. We will determine naturally the so-called critical droplet, give a clear view of the passage from the configuration that all spins are down $(-\mathbf{1})$ to the configuration that all spins are up $(+\mathbf{1})$, calculate the logarithmic asymptotics of the hitting time of $+\mathbf{1}$ starging at $-\mathbf{1}$, or *vice versa*. The key step is the following theorem.

Theorem 1. *Let* $\Gamma = 6L^2 - 4L - L^2(L-1)h + \Gamma_2$. *Then the minimum barrier from* $-\mathbf{1}$ *to* $+\mathbf{1}$ *is* Γ. *The minimum barrier from* $+\mathbf{1}$ *to* $-\mathbf{1}$ *is* $\Gamma + hN^3$.

The proof is very long; it is given in the next sections. The main results of this paper follows from this theorem.

Theorem 2. (i) $\lim_{\beta\to\infty}(1/\beta)\log E^{\beta}_{-1}\sigma(+\mathbf{1}) = \Gamma$;

$$\lim_{\beta\to\infty} P^{\beta}_{-1}(|(1/\beta)\log\sigma(+\mathbf{1}) - \Gamma| < \varepsilon) = 1 \quad \text{for any } \varepsilon > 0. \tag{1.1}$$

(ii) $\lim_{\beta\to\infty}(1/\beta)\log E^{\beta}_{+1}\sigma(-\mathbf{1}) = \Gamma + hN^3$;

$$\lim_{\beta\to\infty} P^{\beta}_{+1}(|(1/\beta)\log\sigma(-\mathbf{1}) - \Gamma - hN^3| < \varepsilon) = 1 \quad \text{for any } \varepsilon > 0.$$

Proof. By Proposition 3.3 of ref. [1], $-\mathbf{1}$ and $+\mathbf{1}$ are the only level $r+1$ attractors. Consequently, $S = B^{r+1}(+\mathbf{1}) \cup B^{r+1}(-\mathbf{1})$. By the same method as that used in Lemma 3.3 of

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ref. [2], one can show the following facts.

$$W(S \setminus \{+1, -1\}) = W(B^{(r+1)}(+1) \setminus (B^{(r+1)}(-1) \cup \{+1\})) + W(B^{(r+1)}(-1) \setminus \{-1\}). \quad (1.2)$$

$$W(S \setminus \{+1\}) = W(B^{(r+1)}(+1) \setminus (B^{(r+1)}(-1) \cup \{+1\})) + W(B^{(r+1)}(-1)). \quad (1.3)$$

$$W(S \setminus \{+1, -1\}) \leqslant W(S \setminus \{+1, \eta\}), \quad \forall \eta \in S. \quad (1.4)$$

Note $\sigma(+1) = \tau(S \setminus \{+1\})$. Applying Lemma 2.1 of ref. [2] (with different notations) to $K = S \setminus \{+1\}$, we have

$$\begin{aligned}
&\lim_{\beta\to\infty} \frac{1}{\beta} \log E^{\beta}_{-1} \sigma(+1) \\
&= W(S \setminus \{+1\}) - W(S \setminus \{+1, -1\}) \wedge \min_{\eta\in S} W_{-1\eta}(S \setminus \{+1, \eta\}) \\
&= W(S \setminus \{+1\}) - W(S \setminus \{+1, -1\}) \quad \text{(by (1.4))} \\
&= W(B^{(r+1)}(-1) - W(B^{(r+1)}(-1) \setminus \{-1\}) \quad \text{(by (1.2),(1.3))} \\
&= V^{(r+1)}(-1) = \mathrm{MB}(-1, +1) \quad \text{(by Lemma 3.1 of ref. [1])} \\
&= \Gamma \quad \text{(by Theorem 1)}.
\end{aligned}$$

By the Chebyshev inequality we know immediately that for any $\varepsilon > 0$

$$\lim_{\beta\to\infty} P^{\beta}_{-1}\left(\frac{1}{\beta}\log\sigma(+1) - \Gamma < \varepsilon\right) = 1.$$

Notice that $\sigma(+1) \geqslant \tau(B^{r+1}(-1))$ if the initial state is -1. By Theorem 3.2 of ref. [2],

$$\lim_{\beta\to\infty} P^{\beta}_{-1}\left(\left|\frac{1}{\beta}\log\tau(B^{r+1}(-1)) - \Gamma\right| < \varepsilon\right) = 1.$$

Therefore (1.1) holds for any $\varepsilon > 0$. This finishes the proof of the first part. The rest is proved in the same way. Q.E.D.

2 Analysis of the Hamiltonian

We first show that $H(\cdot)$ is decreased by pushing all $+1$ spins in the x-axis direction towards $y-z$ plane as close as possible, keeping the number of $+1$ spins invariant. For $\xi \in S$, let $m(j,k) = \sum_{i=1}^{N} \frac{1}{2}(\xi(i,j,k) + 1)$ be the number of $+1$ spins along line $y=j$, $z=k$. Then we define "pushing" formally as the map $\phi: S \to S$ such that

$$\phi(\xi)(i,j,k) = \begin{cases} +1, & \text{if } 1 \leqslant i \leqslant m(j,k), \\ -1 & \text{if } i > m(j,k). \end{cases}$$

Lemma 2.1. $H(\phi(\xi)) \leqslant H(\xi)$.

Proof. Write $\eta = \phi(\xi)$ for simplicity. Then

$$\begin{aligned}
\sum_{u\in\Lambda} \eta(u) &= \sum_{j,k}\sum_{i} \eta(i,j,k) = \sum_{j,k}(2m(j,k) - N) \\
&= \sum_{j,k}\left(\sum_{i}[\xi(i,j,k) + 1] - N\right) = \sum_{j,k}\sum_{i}\xi(i,j,k) = \sum_{u\in\Lambda}\xi(u).
\end{aligned}$$

In the light of (1.2) of ref. [1], Lemma 2.1 is reduced to

$$\sum_{\|u-v\|=1} \xi(u)\xi(v) \leqslant \sum_{\|u-v\|=1} \eta(u)\eta(v).$$

It suffices to verify that

$$\sum_i \xi(i,j,k)\xi(i+1,j,k) \leqslant \sum_i \eta(i,j,k)\eta(i+1,j,k), \tag{2.1}$$

$$\sum_i \xi(i,j,k)\xi(i,j+1,k) \leqslant \sum_i \eta(i,j,k)\eta(i,j+1,k), \tag{2.2}$$

$$\sum_i \xi(i,j,k)\xi(i,j,k+1) \leqslant \sum_i \eta(i,j,k)\eta(i,j,k+1). \tag{2.3}$$

Notice that

$$\sum_i \xi(i,j,k)\xi(i+1,j,k)\begin{cases} = N, & \text{if } m(j,k) = N \text{ or } 0, \\ = N-4, & \text{if } m(j,k) = N-1 \text{ or } 1, \\ \leqslant N-4, & \text{if } 2 \leqslant m(j,k) \leqslant N-2, \end{cases}$$

and

$$\sum_i \eta(i,j,k)\eta(i+1,j,k) = \begin{cases} N, & \text{if } m(j,k) = N \text{ or } 0, \\ N-4, & \text{if } 1 \leqslant m(j,k) \leqslant N-1. \end{cases}$$

Combining them together, we get (2.1).

$$\sum_i I_{\{\xi(i,j,k)=+1,\,\xi(i,j+1,k)=-1\}} = \sum_i \left(I_{\{\xi(i,j,k)=+1\}} - I_{\{\xi(i,j,k)=+1,\,\xi(i,j+1,k)=+1\}}\right)$$
$$\geqslant (m(j,k) - m(j+1,k))^+$$

and

$$\begin{aligned} &\sum_i \xi(i,j,k)\xi(i,j+1,k) \\ &= N - 2\sum_i I_{\{\xi(i,j,k)=1,\,\xi(i,j+1,k)=-1\}} - 2\sum_i I_{\{\xi(i,j,k)=-1,\,\xi(i,j+1,k)=1\}} \\ &\leqslant N - 2(m(j,k) - m(j+1,k))^+ - 2(m(j+1,k) - m(j,k))^+ \\ &= N - 2\,|\,m(j,k) - m(j+1,k)\,|\,. \end{aligned}$$

Also

$$\sum_i \eta(i,j,k)\eta(i,j+1,k) = N - 2\,|\,m(j,k) - m(j+1,k)\,|\,.$$

Therefore (2.2) holds. Similarly, (2.3) holds. Q.E.D.

If $\eta = \phi(\xi)$, the intersection of $\{(i,j,k) \mid \eta(i,j,k) = +1\}$ and plane $x = i$ gets smaller as i increases, namely

$$\{(j,k) \mid \eta(i,j,k) = +1\} \supset \{(j,k) \mid \eta(i+1,j,k) = +1\}. \tag{2.4}$$

Next we try to make η more regular by rearranging $+1$ spins as square as possible in every plane $x = i$. This will further reduce $H(\cdot)$. Introduce the pseudo-square $S(m)$ of area m as

$$S(m) = \begin{cases} \{(j,k) \mid \max(j,k) \leqslant l \text{ or } j = l+1, k \leqslant m - l^2\}, \\ \qquad\qquad\qquad \text{if } l^2 < m \leqslant l^2 + l; \\ \{(j,k) \mid j \leqslant l+1, k \leqslant l \text{ or } k = l+1, j \leqslant m - l^2 - l\}, \\ \qquad\qquad\qquad \text{if } l^2 + l < m \leqslant (l+1)^2. \end{cases}$$

Let $m(i) = \sum_{j,k} \frac{1}{2}(\eta(i,j,k) + 1)$ be the number of $+1$ spins of η on plane $x = i$. Define the rearrangement as map $\psi_1 : S \to S$ such that

$$\psi_1(\eta)(i,j,k) = \begin{cases} +1, & \text{if } (j,k) \in S(m(i)), \\ -1, & \text{if } (j,k) \notin S(m(i)). \end{cases}$$

Lemma 2.2. *Let $\eta = \phi(\xi)$, $\zeta = \psi_1(\eta)$. Then $\zeta \in S^0$ and*

$$\{(j,k) \mid \zeta(i,j,k) = +1\} \supset \{(j,k) \mid \zeta(i+1,j,k) = +1\}, \tag{2.5a}$$

$$\{(i,j) \mid \zeta(i,j,k) = +1\} \supset \{(i,j) \mid \zeta(i,j,k+1) = +1\}, \tag{2.5b}$$
$$\{(i,k) \mid \zeta(i,j,k) = +1\} \supset \{(i,k) \mid \zeta(i,j+1,k) = +1\}. \tag{2.5c}$$

If $m(i) \leqslant N^2/4$ for all i, then $H(\psi_1(\eta)) \leqslant H(\eta)$.

Proof. It is helpful to visualize the intervals of $+1$ spins as bars perpendicular to $y-z$ plane and index them by (y, z). Then ψ_1 acting on η is to rearrange these bars according to their lengths. As a result, $m(j,k)$ of $\psi_1(\eta)$ is decreasing in y and z. This gives (2.5b) and (2.5c). (2.4) is preserved as (2.5a). All these imply that $\zeta \in S^0$ (see Definition 2.4 in ref. [1]). To prove that $H(\psi_1(\eta)) \leqslant H(\eta)$, similar to the proof of Lemma 2.1, we only need to show that

$$\sum_{j,k} I_{\{\eta(i,j,k) = -\eta(i+1,j,k)\}} = \sum_{j,k} I_{\{\zeta(i,j,k) = -\zeta(i+1,j,k)\}} \tag{2.6}$$

and

$$\sum_{j,k} I_{\{\eta(i,j,k) = -\eta(i,j+1,k)\}} + \sum_{j,k} I_{\{\eta(i,j,k) = -\eta(i,j,k+1)\}}$$
$$\geqslant \sum_{j,k} I_{\{\zeta(i,j,k) = -\zeta(i,j+1,k)\}} + \sum_{j,k} I_{\{\zeta(i,j,k) = -\zeta(i,j,k+1)\}}. \tag{2.7}$$

Since η satisfies (2.4), the case of $\eta(i,j,k) = -1$, $\eta(i+1,j,k) = +1$ will never happen. Because the numbers of $+1$ spins of planes $x = i$ and $x = i+1$ are invariant under map ψ_1 and because ζ satisfies (2.5a) too,

$$\sum_{j,k} I_{\{\eta(i,j,k) = -\eta(i+1,j,k)\}} = m(i) - m(i+1) = \sum_{j,k} I_{\{\zeta(i,j,k) = -\zeta(i+1,j,k)\}}.$$

So (2.6) is true.

The statement of (2.7) is two-dimensional, and its proof is virtually by the isoperimetric inequality. Similar to Lemma 2.1, the LHS of (2.7) is reduced if the cluster of η is "pushed" first along y-axis, then "pushed" along z-axis. Suppose that the (two-dimensional) cluster after push circumscribes a rectangle $l_1 \times l_2$. Then $m(i) \leqslant l_1 l_2$ and

$$\sum_{j,k} I_{\{\eta(i,j,k) = -\eta(i,j+1,k)\}} + \sum_{j,k} I_{\{\eta(i,j,k) = -\eta(i,j,k+1)\}} = 2l_1 + 2l_2.$$

In all the squares with areas $m(i) \leqslant l_1 l_2$, the perimeter is minimized when l_1 and l_2 are as close as possible. If $l^2 < m(i) \leqslant l^2 + l$ we choose $l_1 = l$, $l_2 = l+1$ (or $l_1 = l+1$, $l_2 = l$). If $l^2 + l < m(i) \leqslant (l+1)^2$ we choose $l_1 = l_2 = l+1$. There are several ways to place $+1$ spins in rectangle $l \times (l+1)$ or square $(l+1) \times (l+1)$ with the minimum perimeter. One way is to put $+1$ spins in the pseudo-square of size $m(i)$. This gives the RHS of (2.7).

Since Λ is a torus, the perimeter of rectangle $l \times N$ is $2N$. When $m(i)$ is large it is better to place $+1$ spin in rectangle $l \times N$ instead of a pseudo-square. The assumption that $m(i) \leqslant N^2/4$ for all i is to exclude this possibility. Q.E.D.

Remark. Similarly we define ψ_2 as rearrangement on planes parallel to $x-z$ plane, and ψ_3 on planes parallel to $x-y$ plane. Then $H(\psi_2(\zeta)) \leqslant H(\zeta)$ and $H(\psi_3(\zeta)) \leqslant H(\zeta)$.

3 Minimum barrier

Let $S_k = \{\xi \in S;$ the number of $+1$ spins of ξ is $k\}$ and $H_k = \min\{H(\eta); \eta \in S_k\}$.

Lemma 3.1. *Assume $k \leqslant 64N^3/729$. Then*

$$H_k = \min\{H(\zeta) \mid \zeta = \psi_1 \circ \phi(\xi), \xi \in S_k\}. \tag{3.1}$$

Suppose $l^3 < k \leqslant (l+1)^3$. Let m be the integer part of $\sqrt{k - l^3}$. Then H_k is given in terms of l and m as follows.

H_k	k
$6l^2 + 4m + 2 - hk$	$l^3 + m^2 < k \leqslant l^3 + (m+1)m, 1 \leqslant m \leqslant l-1$
$6l^2 + 4m + 4 - hk$	$l^3 + (m+1)m < k \leqslant l^3 + (m+1)^2, 0 \leqslant m \leqslant l-1$
$6l^2 + 4l + 4m + 2 - hk$	$(l+1)l^2 + m^2 < k \leqslant (l+1)l^2 + (m+1)m, 1 \leqslant m \leqslant l$
$6l^2 + 4l + 4m + 4 - hk$	$(l+1)l^2 + (m+1)m < k \leqslant (l+1)l^2 + (m+1)^2, 0 \leqslant m \leqslant l-1$
$6l^2 + 8l + 4m + 4 - hk$	$l(l+1)^2 + m^2 < k \leqslant l(l+1)^2 + (m+1)m, 1 \leqslant m \leqslant l$
$6l^2 + 8l + 2 + 4m + 6 - hk$	$l(l+1)^2 + (m+1)m < k \leqslant l(l+1)^2 + (m+1)^2, 0 \leqslant m \leqslant l$

Proof. Notice first that all ϕ and ψ_i's map S_k into S_k. Lemmas 2.1 and 2.2 imply (3.1). To compute H_k we are to find a concrete $\eta \in S_k$ such that $H(\eta) = H_k$. Consequently, such η must satisfy the condition that for any $i, j, k \in \{1, 2, 3\}$:

$$H(\eta) = H(\psi_i(\eta)) = H(\psi_i \circ \psi_j(\eta)) = H(\psi_i \circ \psi_j \circ \psi_k(\eta)). \tag{3.2}$$

The following argument is by the isoperimetric inequality (used in the previous proof). The intersection of $\{u \in \Lambda \mid \eta(u) = +1\}$ with any plane is a square $l \times l$ or a rectangle $l \times (l+1)$, and the number of $+1$ spins in this intersection is at least $l(l-1) + 1$ or $l^2 + 1$. Otherwise, the Hamiltonian will strictly decrease after rearrangement. Let $l_1 = \max\{i; \eta(i,1,1) = +1\}$, $l_2 = \max\{j; \eta(1,j,1) = +1\}$, $l_3 = \max\{k; \eta(1,1,k) = +1\}$. Then l_1, l_2, l_3 can only differ by at most 1. Exchange x, y and z coordinates if necessary. The possible choices of (l_1, l_2, l_3) are $(l+1, l, l)$, $(l+1, l+1, l)$ and $(l+1, l+1, l+1)$.

The discussion of the three cases are parallel, so we shall only discuss the first case: $(l_1, l_2, l_3) = (l+1, l, l)$. When replacing η by $\psi_3(\eta)$, l_1, l_2, l_3 are invariant, and every intersection with plane $z = k$ is a pseudo-square. The intersection of the cluster with plane $z = 1$ is a pseudo-square $(l+1) \times l$, with a possible missing corner on line $x = l+1, z = 1$. So $(1, l, 1)$, $(l, l, 1)$, $(1, 1, 1)$ and $(l, 1, 1)$ are in the cluster. Now take the intersection with plane $x = 1$, since $(l, 1, 1)$, $(l, l, 1)$ are in the cluster, so is $(l, 1, l-1)$. Also on plane $y = l$, $(1, l, l-1)$ is in the cluster. Note that the intersection with $z = l-1$ is a pseudo-square containing $(l, 1, l-1)$, $(1, 1, l-1)$ and $(1, l, l-1)$. Hence the pseudo-square contains $l \times (l-1)$. By (2.5c) the cluster contains cuboid $l \times (l-1) \times (l-1)$. In other words, the cluster consists of cuboid $l \times (l-1) \times (l-1)$ with additional $+1$ spins placed on planes $z = l$, $y = l$ or $x = l+1$ (figure 1).

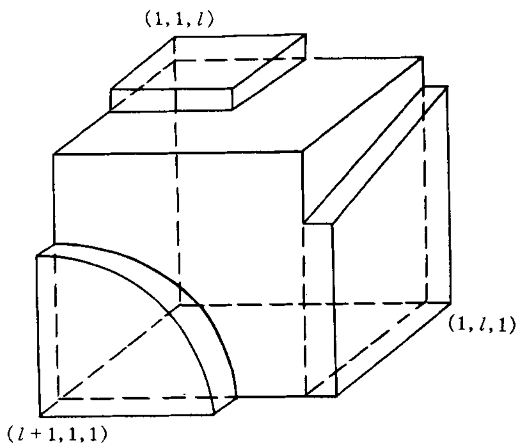

Fig. 1. A simple configuration.

The problem of how to find η satisfying (3.2) is reduced to the following problem: How to place these $+1$ spins on the three faces so that the total perimeter is the minimum. The Hamiltonian is not increased if spins on $x = l+1$ are transferred to fill planes $y = l$ and $z = l$ first. The minimum is reached by the configuration that contains a cube $l \times l \times l$ with remaining $+1$ spins placed in a pseudo-square in plane $x = l+1$ if $k > l^3$. Using (1.2) of ref. [1] to compute the Hamiltonian, we get k, the total number of $+1$ spins, so $-kh$ appears in the table. The surface area of the cube is $6l^2$. The pseudo-square on $x = l+1$ only contributes to its perimeter which is $4m+2$ or $4m+4$. These correspond to the first two rows of the table.

In the above proof we think of Λ as a subset of Z^3. A cube has the smallest surface with a fixed volume. But in a torus this is true only when the volume is not too large compared with the total volume of the torus. An elementary computation shows that the ratio cannot exceed 64/729.

Q.E.D.

Assumption (1.4) of ref. [1] guarantees that $L^3 \ll 64\ N^3/729$. For $k > 64\ N^3/729$, the RHS of (3.1) provides an upper bound. It is straightforward to conclude from Lemma 3.1 that

$$\max_k H_k = \Gamma = H_{k_c}, \tag{3.3}$$

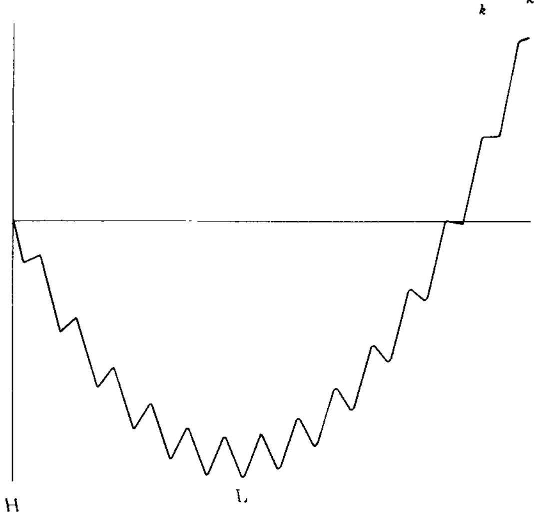

Figure 2.

where $k_c = L^3 - L^2 + L_2^2 - L_2 + 1$. H_k is far from being monotone in k, and there are many local maxima and minima. But roughly speaking, $H(k)$ increases as $0 \leqslant k \leqslant k_c$ and decreases as $k_c \leqslant k \leqslant N^3$ (see fig. 2). Depending on k, there are possibly several $\zeta \in S_k$ such that $H(\zeta) = H_k$ and these ζ's are not necessarily of the form $\psi_1 \circ \phi(\xi)$. However, if $k = l^3$ there is only one such configuration except translations.

Proof of Theorem 1. Along any sequence $\{\xi_j\}$ leading $-\mathbf{1}$ to $+\mathbf{1}$, the number of $+1$ spins can only increase or decrease by one. There must exist $\xi_l \in S_{k_c}$,

$$\max_j H(\xi_j) - H(-\mathbf{1}) = \max_j H(\xi_j) \geqslant H(\xi_l) \geqslant H_{k_c} = \Gamma.$$

We now give a specific sequence $\{\xi_j\}$ to show that the lower bound can be reached. Successively flip -1 spins to $+1$ spins one by one so that $\xi_k \in S_k \cap S^0$ is a configuration that every intersection is a pseudo-square, namely the sequence goes successively through cube $l \times l \times l$, cuboid $(l+1) \times l \times l$, cuboid $(l+1) \times (l+1) \times l$, cube $(l+1) \times (l+1) \times (l+1)$, and so on, $l = 1, 2, 3, \cdots N$.

Q.E.D.

Definition 3.1. A configuration ζ is called a critical droplet if $\zeta \in S_{k_c}$ and $H(\zeta) = \Gamma$.

A critical droplet must be in the intersection of the level $(r+1)$ attractive basins of $+\mathbf{1}$ and $-\mathbf{1}$. This property distinguishes a critical droplet from other ζ's satisfying $H(\zeta) = \Gamma$. A critical droplet consists of a cuboid $(L-1) \times L \times L$, a rectangle $(L_2 - 1) \times L_2$ and a single $+1$ spin. The rectangle and the additional $+1$ spin are situated on an $L \times L$ face of the large cuboid. The single + 1 spin is next to the longer side of the rectangle (see fig. 3). Coincidentally the rectangle and the single + 1 spin constitute exactly a two-dimensional critical droplet. The critical droplet is unique up to translation, rotation and relocation of the attached two-dimensional critical droplet.

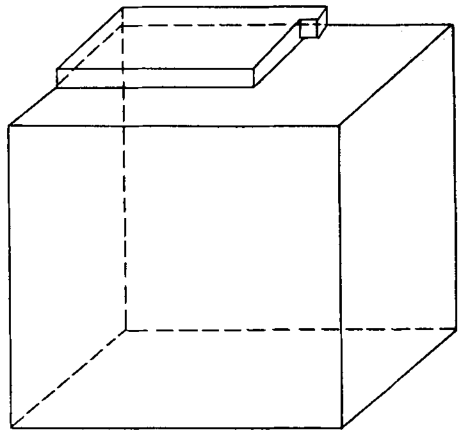

Fig. 3. A critical droplet.

Complement to the proof of Lemmas 3.2 *and* 3.3 *of ref.* [1]. By analzying the Hamiltonian of configurations in the neighborhood of a metastable state, one can establish a statement similar to Lemma 3.1. Then it is easy to show that the sequence constructed in the proof reaches the minimum barrier.

Complement to the proof of Proposition 3.3 *of ref.* [1]. 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) of ref. [1]. If the sequence is not entirely in S^0, we apply pushing, similar to map ϕ, to get a new sequence in S^0 without increasing the minimum barrier. If the end of the new sequence, namely the image of ζ' after pushing, is not a level k attractor, it lies in the attractive basin of a level k attractor. Extend the new sequence to that attractor to satisfy (3.2) of ref. [1]. If that attractor is not in S^0, repreat this procedure. Notice that the Hamiltonian strictly decreases in this procedure and is bounded below by $-hN^3$. After repeating finite times we will find a sequence which is entirely in S^0 and has the minimum barrier.

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