

## METASTABLE BEHAVIOR FOR CONSERVATIVE DYNAMICS ON A FINITE BOX WITH OPEN BOUNDARY

TAIZO CHIYONOBU AND YUSUKE TAKAGI

**ABSTRACT.** In this article will study the metastable behavior of the conservative lattice gas in two dimension subject to Kawasaki dynamics in the limit of low temperature and low density. We consider the model where particles live in a finite box and are created and annihilated respectively at the boundary of the box, with the boundary condition that reflects an infinite gas reservoir, and studied how the system nucleates, i.e., how the box is fully filled with particles starting from an empty box. Motivated by [2], we will study the metastable behavior for the modified model in two dimension. We consider the model where the rate of the creation and annihilation at the boundary is large, and investigate the asymptotic behavior for the average nucleation time.

### 1. Introduction.

In [2], Bovier et. al. studied the metastable behavior of the conservative lattice gas in two and three dimension subject to Kawasaki dynamics at low temperature and low density. They considered the local model where particles live in a finite box, hop between nearest-neighbor sites, have an attractive interaction when they are next to each other, and are created and annihilated respectively at the boundary of the box with the boundary condition that reflects an infinite gas reservoir. They studied how the system nucleates, i.e., how the box is fully filled with particles starting from an empty box. Their results are comparable with those by Bovier and Manzo [3] for the Ising model on a finite box subject to Glauber dynamics at low temperature.

Motivated by the work, in this article we will study the metastable behavior for the modified model in two dimension. We generalize the rate of the creation and annihilation at the boundary, namely we set the rate very large, and we investigate the asymptotic behavior for the average nucleation time, and show that the exponential rate for the time remains constant for values of the rate in a certain regime. For this purpose we perform the detailed analysis of the energy landscape for the dynamics and apply it to the potential theoretic argument developed by Bovier, Eckhoff, Gaynard and Klein [1]. For each value of the rate we identify the full geometry of the set of critical droplets for the nucleation, compute the

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average nucleation time up to  $1 + o(1)$ , express the proportionality constant for the average nucleation time in terms of certain capacities associated with simple random walk and compute the asymptotic behavior of the proportionality constant as the system size tends to infinity.

The analysis of the full asymptotics is important since it reflects the characteristic of each dynamics. Kawasaki dynamics differs from Glauber dynamics in that it is a conservative dynamics where particles are conserved in the interior of the box, and as is stressed in [2], in the metastable regime particles move along the border of a droplet more rapidly than they arrive from the boundary of the box. This leads to the fact that the set of the communication level set of Kawasaki dynamics is much more complicated, such as having plateaus, wells embedded in these plateaus and dead ends, than that of Glauber spin-flip dynamics, which is disconnected. This difference is casted in the difference of the full asymptotic behavior for the both dynamics([2], [3]). By taking the distinctive rates for the attractive interactions inside the box and the creation/annihilation of particles at the boundary, it is clearly seen how each of the rate affects the asymptotic behavior of the proportionality constant, and therefore affects the characteristic of the dynamics in contrast to spin-flip dynamics.

In the coming paper [4], we will discuss the same problem for the model where rate of the creation and annihilation at the boundary is large.

## 2. Description of the Model and Main Results

For  $M \in \mathbb{Z}$ , let

$$\Lambda = [-M, M]^2 \cap \mathbb{Z}^2 = \{-M, -(M-1), \dots, -1, 0, 1, \dots, M-1, M\}^2,$$

and

$$\partial^- \Lambda = \{x \in \Lambda; \exists y \notin \Lambda, |y - x| = 1\}, \quad \partial^+ \Lambda = \{x \notin \Lambda; \exists y \in \Lambda, |y - x| = 1\},$$

be the internal and external boundary of  $\Lambda$ , and put

$$\Lambda^- = \Lambda \setminus \partial^- \Lambda, \quad \Lambda^+ = \Lambda \cup \partial^+ \Lambda.$$

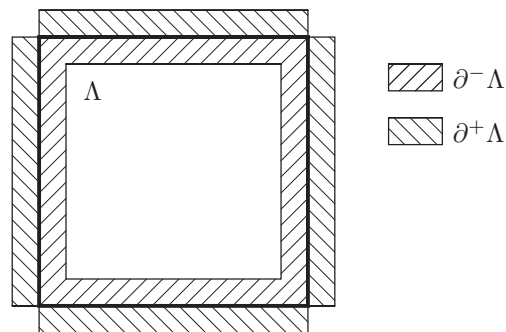


FIGURE 1. The internal and external boundary of  $\Lambda$

With each site  $x \in \Lambda$  we associate an occupation variable  $\eta(x)$ , assuming the values 0 or 1, indicating the absence or presence of a particle at  $x$ . A lattice configuration is denoted by  $\eta = (\eta(x); x \in \Lambda) \in \mathcal{X} = \{0, 1\}^\Lambda$ .

The energy for each configuration  $\eta \in \mathcal{X}$  is given by the Hamiltonian

$$H(\eta) = -U \sum_{(x,y) \in \Lambda^{*, -}} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda^-} \eta(x) + \Delta' \sum_{x \in \partial^- \Lambda} \eta(x), \quad \forall \eta \in \mathcal{X}, \quad (2.1)$$

where

$$\Lambda^{*, -} = \{(x, y); x, y \in \Lambda^-, |x - y| = 1\}$$

is the set of non-oriented bonds in  $\Lambda^-$ . The interaction consists of a binding energy  $-U < 0$  for each nearest-neighbor pair of particles in  $\Lambda^-$  and an activation energy  $\Delta > 0$  for particles in  $\Lambda$  and  $\Delta' > 0$  for particles in  $\partial \Lambda^-$ .

The Gibbs measure associated with  $H$  is

$$\mu_\beta(\eta) = \frac{e^{-\beta H(\eta)}}{Z_\beta}, \quad \eta \in \mathcal{X}, \quad (2.2)$$

with inverse temperature  $\beta > 0$  and partition sum

$$Z_\beta = \sum_{\eta \in \mathcal{X}} e^{-\beta H(\eta)}.$$

Next, we define Kawasaki dynamics on  $\Lambda$  with a boundary condition. An oriented bond, i.e., an ordered pair of nearest neighbor sites is denoted by  $b = (x \rightarrow y)$  and

$$\begin{aligned} \Lambda^{*, \text{orie}} &= \{b = (x \rightarrow y); x, y \in \Lambda\}, \\ \partial \Lambda^{*, \text{in}} &= \{b = (x \rightarrow y); x \in \partial^+ \Lambda, y \in \partial^- \Lambda\}, \\ \partial \Lambda^{*, \text{out}} &= \{b = (x \rightarrow y); x \in \partial^- \Lambda, y \in \partial^+ \Lambda\}, \\ \bar{\Lambda}^{*, \text{orie}} &= \Lambda^{*, \text{orie}} \cup \partial \Lambda^{*, \text{in}} \cup \partial \Lambda^{*, \text{out}}. \end{aligned}$$

Two configurations  $\eta, \eta' \in \mathcal{X}$  with  $\eta \neq \eta'$  are called communicating configurations, written  $\eta \leftrightarrow \eta'$ , if there exists a bond  $b \in \bar{\Lambda}^{*, \text{orie}}$ , orie such that  $\eta' = T_b \eta$ , where  $T_b \eta$  is the configuration obtained from  $\eta$  as follows:

- $b = (x \rightarrow y) \in \Lambda^{*, \text{orie}}$ :

$$(T_b \eta)(z) = \begin{cases} \eta(z), & \text{if } z \neq x, y, \\ \eta(x), & \text{if } z = y, \\ \eta(y), & \text{if } z = x. \end{cases}$$

- $b = (x \rightarrow y) \in \Lambda^{*, \text{in}}$ :

$$(T_b \eta)(z) = \begin{cases} \eta(z), & \text{if } z \neq y, \\ 1, & \text{if } z = y. \end{cases}$$

- $b = (x \rightarrow y) \in \Lambda^{*, \text{out}}$ :

$$(T_b \eta)(z) = \begin{cases} \eta(z), & \text{if } z \neq x, \\ 0, & \text{if } z = x. \end{cases}$$

These transitions correspond to particle motion in  $\Lambda$ , creation and annihilation in  $\partial^-\Lambda$ , respectively.

The Kawasaki dynamics is defined to be the continuous-time Markov chain  $(\eta_t)_{t \geq 0}$  on  $\mathcal{X}$  with transition rates

$$c_\beta(\eta, \eta') = 1_{\{\eta \leftrightarrow \eta'\}} e^{-\beta\{H(\eta') - H(\eta)\} \vee 0}, \quad \forall \eta, \eta' \in \mathcal{X}, \eta \neq \eta'. \quad (2.3)$$

This is a standard Metropolis dynamics with an open boundary: along each bond touching  $\partial^-\Lambda$  from the outside, particles are created with rate  $e^{-\Delta'\beta}$  and are annihilated with rate 1, while inside  $\Lambda^-$  particles are conserved and jump at a rate that depends on the change in energy associated with the jump, reflecting the binding energy. Note that a move of particles inside  $\partial^-\Lambda$  does not involve a change in energy because the interaction acts only inside  $\Lambda^-$ .

The measure  $\mu_\beta$  is the reversible equilibrium of the dynamics with transition rates  $c_\beta$ :

$$\mu_\beta(\eta)c_\beta(\eta, \eta') = \mu_\beta(\eta')c_\beta(\eta', \eta), \quad \forall \eta, \eta' \in \mathcal{X}, \eta \neq \eta'. \quad (2.4)$$

We will first assume that

$$\Delta \in (U, 2U), \quad (2.5)$$

Under the assumption, since  $e^{U\beta} \ll e^{\Delta\beta} \ll e^{2U\beta}$  as  $\beta \rightarrow \infty$ , single particles in  $\Lambda^-$  to one side of a droplet typically detach before the arrival of a next particle, while bars of two or more particles typically do not detach. Thus in this regime, droplets tend to grow slowly. We refer it to the *metastable regime*.

The energy  $E(\ell)$  of an  $\ell \times \ell$  droplet in  $\Lambda^-$  equals to

$$E(\ell) = -U(2\ell(\ell-1)) + \Delta\ell^2 = 2U\ell - (2U - \Delta)\ell^2 \quad (2.6)$$

which is maximal at  $\ell = \frac{U}{2U - \Delta}$  (see Fig. 2). Let

$$\ell_c = \left\lceil \frac{U}{2U - \Delta} \right\rceil \quad (2.7)$$

( $\lceil \cdot \rceil$  denotes the upper integer part), and we assume that

$$\frac{U}{2U - \Delta} \notin \mathbb{N}$$

in order to avoid ties. We call  $\ell_c$  the *critical droplet size*. We also assume that  $\ell_c \geq 3$ , thus along with (2.5) we assume that

$$\Delta \in \left(\frac{3}{2}U, 2U\right), \quad (2.8)$$

as in [2].

Let

$$\begin{aligned} \square &= \{\eta \in \mathcal{X}; \eta(x) = 0 \ \forall x \in \Lambda\}, \\ \blacksquare &= \{\eta \in \mathcal{X}; \eta(x) = 1 \ \forall x \in \Lambda^-, \eta(y) = 0 \ \forall y \in \partial^-\Lambda\}. \end{aligned} \quad (2.9)$$

We assume that  $\Lambda$  is so large that

$$H(\blacksquare) < H(\square) = 0.$$

In this case,  $\blacksquare$  is the global minimum of  $H$ .

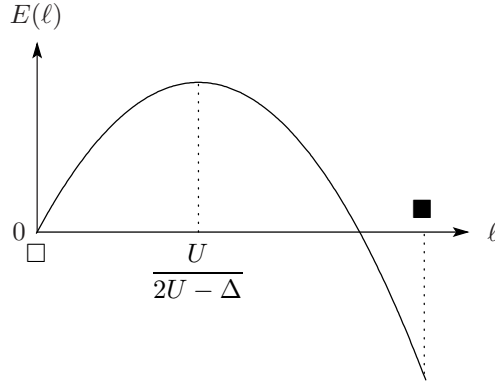


FIGURE 2.  $l \mapsto E(l)$

For  $\eta \in \mathcal{X}$ , write  $x \in \eta$  to indicate that  $\eta$  has a particle at  $x$ . Before we state our main results, we need to give some basic geometric definitions: A *path*  $\omega$  is a sequence  $\omega = (\omega_1, \dots, \omega_k), k \in \mathbb{N}$ , of communicating configurations, i.e.,  $\omega_i \in \mathcal{X}$  for  $i = 1, \dots, k$  and  $c_\beta(\omega_i, \omega_{i+1}) > 0$  for  $i = 1, \dots, k - 1$ . For  $\eta, \eta' \in \mathcal{X}$ , we write  $\omega : \eta \rightarrow \eta'$  to denote a path from  $\eta$  to  $\eta'$ . For  $\zeta \in \mathcal{X}$ , we write  $\zeta \in \omega$  when  $\omega$  visits  $\zeta$ . For  $\mathcal{A} \subseteq \mathcal{X}$ , we write  $\omega \subseteq \mathcal{A}$  when  $\omega$  stays inside  $\mathcal{A}$ . The *communication height* between  $\square$  and  $\blacksquare$  is defined by

$$\Gamma = \Phi(\square, \blacksquare) = \min_{\omega: \square \rightarrow \blacksquare} \max_{\zeta \in \omega} H(\zeta).$$

where the minimum runs over all admissible paths  $\omega$  connecting  $\square$  and  $\blacksquare$ , and the maximum runs over all configurations  $\zeta$  encountered along  $\omega$ . The *communication level set* between  $\square$  and  $\blacksquare$  is given by

$$\mathcal{S}(\square, \blacksquare) = \left\{ \zeta \in \mathcal{X}; \exists \omega : \square \rightarrow \blacksquare, \omega \ni \zeta : \max_{\xi \in \omega} H(\xi) = \Phi(\square, \blacksquare) \right\}.$$

Let, for  $\mathcal{A} \subset \mathcal{X}$ ,  $\tau_{\mathcal{A}}$  be the first hitting/return time of  $\mathcal{A}$  and for  $\eta \in \mathcal{X}$ ,  $\mathbb{P}_\eta$  be the law of  $(\eta_t)_{t \leq 0}$  starting from  $\eta_0 = \eta$ . We are interested in the asymptotic behaviour of the law of  $\tau_{\blacksquare}$  for the Markov chain starting from  $\square$ . We expect that the exponent of the transition time from the quasi-stable state  $\square$  to the globally stable state  $\blacksquare$  is  $\Gamma = \Phi(\square, \blacksquare)$ , and in the course of the transition the process passes through a configuration in  $\mathcal{S}$ . Namely, we expect that the formulas such as

$$\lim_{\beta \rightarrow \infty} P_\square \left( e^{(\Gamma-\delta)\beta} < \tau_{\blacksquare} < e^{(\Gamma+\delta)\beta} \right) = 1, \quad \forall \delta > 0 \tag{2.10}$$

and

$$\lim_{\beta \rightarrow \infty} P_\square (\tau_{\mathcal{S}} < \tau_{\blacksquare} | \tau_{\blacksquare} < \tau_\square) = 1 \tag{2.11}$$

hold. In this paper we will compute  $\Gamma$  in the case  $0 < \Delta' < \Delta - U$ , and we will derive the precise asymptotics for  $\mathbb{E}_\square(\tau_{\blacksquare})$ .

Let

$$\Gamma_0 = -U \left( (\ell_c - 1)^2 + \ell_c(\ell_c - 2) + 1 \right) + \Delta(\ell_c(\ell_c - 1) + 1),$$

which is the energy of the configurations having one cluster anywhere in  $\Lambda^-$  consisting of an  $(\ell_c - 1) \times \ell_c$  quasi-square with a 1-protuberance attached to one of its sides. See Figure 3.

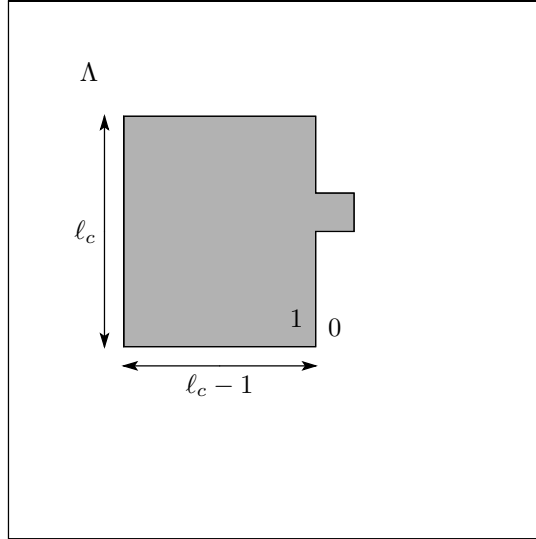


FIGURE 3

Now, we state our theorems.

**Theorem 2.1.** *We assume (2.8) and that  $0 < \Delta' < \Delta - U$ . Then the communication height between  $\square$ ,  $\blacksquare$  for  $H$  defined by (2.1) equals to*

$$\Phi(\square, \blacksquare) = \Gamma^{**} = \Gamma_0 + \Delta - U. \quad (2.12)$$

**Theorem 2.2.** *We assume (2.8) and that  $0 < \Delta' < \Delta - U$ . Then, there exists a constant  $K = K(\Lambda, \ell_c)$  such that*

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = Ke^{\Gamma^{**}\beta}[1 + o(1)], \quad \beta \rightarrow \infty. \quad (2.13)$$

Furthermore, as  $\Lambda \rightarrow \mathbb{Z}^2$ ,  $K(\Lambda, \ell_c)$  converges to a constant.

We will give some comments on our statements. In the case  $\Delta' \geq \Delta - U$ , in [4], we have showed that

$$\Phi(\square, \blacksquare) = \Gamma^{**} = \Gamma_0 + \Delta', \quad (2.14)$$

and thus along with Theorem 2.1, this result reveals how the annihilation/creation rate  $\Delta'$  affects the communication height between  $\square$  and  $\blacksquare$ . It shows that there is a transition in the behavior of  $\Gamma^{**}$  as a function of  $\Delta'$  at  $\Delta' = \Delta - U$ . See Figure 4.

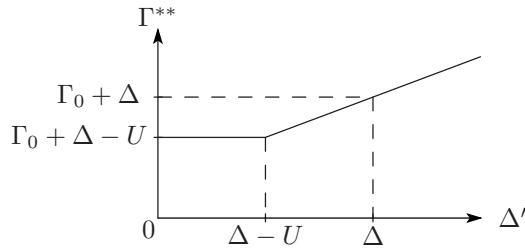


FIGURE 4. Graph of  $\Gamma^{**}$  as a function of  $\Delta'$

In [2], A. Bovier et. al. studied the Kawasaki dynamics on a finite box with open boundary that mimics the effect of an infinite gas reservoir outside  $\Lambda$  with density  $\rho_\beta = e^{-\Delta\beta}$ , i.e., the Metropolis dynamics with the Hamiltonian

$$H(\eta) = -U \sum_{(x,y) \in \Lambda^{*, -}} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x) \tag{2.15}$$

Notice that this is the case where  $\Delta' = \Delta$  in our Hamiltonian (2.1). They have showed in [2], Theorem 1.4.4. that the communication height between  $\square$  and  $\blacksquare$  for this  $H$  equals to

$$\Gamma^* = \Gamma_0 + \Delta,$$

and that there is a  $K = K(\Lambda, \ell_c)$  such that

$$\mathbb{E}_\square(\tau_\blacksquare) = K e^{\Gamma^* \beta} [1 + o(1)], \quad \beta \rightarrow \infty.$$

These results are evidently consistent with our results (2.12) and (2.13) in the case  $\Delta' = \Delta$ . Moreover, in [2], an asymptotic behavior for  $K = K(\Lambda, \ell_c)$  as  $\Lambda \rightarrow \mathbb{Z}^2$  is given

$$K(\Lambda, \ell_c) \sim \frac{1}{4\pi N(\ell_c)} \frac{\log |\Lambda|}{|\Lambda|} \tag{2.16}$$

with

$$N(\ell_c) = \frac{1}{3} (\ell_c - 1) \ell_c^2 (\ell_c + 1).$$

The detailed study of asymptotic behavior (2.16) for  $K$  is important in the sense that it gives further information on the dynamics. Let us compare (2.16) for the same type of asymptotics for Glauber dynamics. It is also the continuous-time Markov chain via Metropolis algorithm, but has the different mechanism of transition from Kawasaki dynamics. With the same lattice configuration space  $\Lambda$  and the same Hamiltonian given by (2.15), the rate of the dynamics is defined by

$$c_G(\eta, \eta') = \begin{cases} e^{-\beta \{H_G(\eta') - H_G(\eta)\} \vee 0}, & \text{for } \eta' = \eta^x \text{ for some } x \in \Lambda, \\ 0, & \text{otherwise,} \end{cases}$$

where  $\eta^x$  is the configuration obtained from  $\eta$  by flipping the spin at site  $x$ , i.e.,

$$\eta^x(z) = \begin{cases} \eta(z), & \text{if } z \neq x, \\ 1 - \eta(x), & \text{if } z = x. \end{cases}$$

It is showed in [3] that:

- This Glauber-type dynamics exhibits metastable behavior under the same assumption (2.5) on  $\Delta$  and  $U$ , and  $\blacksquare$  is the global minimum whereas  $\square$  is the local minimum.
- The critical droplets are the droplets given in the Figure 3, and

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = K e^{\Gamma_0} [1 + o(1)], \quad \beta \rightarrow \infty.$$

- As  $\Lambda \rightarrow \mathbb{Z}^2$ ,

$$K(\Lambda, \ell_c) \sim \frac{1}{4\pi N(\ell_c)} \frac{1}{|\Lambda|}$$

These results show that, the two dynamics having the same Hamiltonian has the same critical droplets, and the only difference is that Kawasaki dynamics has a free particle with the droplet as the critical configuration. On the other hand the constant  $K$  has different asymptotic behavior as  $\Lambda \rightarrow \mathbb{Z}^2$ . In this sense, the asymptotic behavior of  $K$  plays the indispensable role in characterizing the dynamics.

In the model treat in this paper, we have studied in [4] the asymptotic behavior of  $K(\Lambda, \ell_c)$  in the case  $\Delta' > \Delta - U$ . We set

$$\gamma_1 = \Delta - (2U - \Delta)(\ell_c - 2), \quad \gamma_2 = U + (2U - \Delta)(\ell_c - 2), \quad \gamma_3 = (2U - \Delta)(2\ell_c - 3). \quad (2.17)$$

Then we have the following.

- (I): In the case  $\Delta' > \Delta$ ,

$$K(\Lambda, \ell_c) \sim \frac{2}{|\Lambda| |\partial^+ \Lambda| N(\ell_c)}.$$

- (II): In the case  $\min\{\gamma_1, \gamma_2, \gamma_3\} \leq \Delta' < \Delta$ , there exist  $A(\ell_c)$  and  $B(\ell_c)$  such that

$$A(\ell_c) \leq |\partial^- \Lambda| N(\ell_c) \lim_{\Lambda \rightarrow \mathbb{Z}^2} K(\Lambda, \ell_c) \leq B(\ell_c).$$

- (III): In the case  $\Delta - U \leq \Delta' < \min\{\gamma_1, \gamma_2, \gamma_3\}$ , there exists a  $C(\ell_c)$  such that

$$K(\Lambda, \ell_c) \sim \frac{1}{4C(\ell_c)N(\ell_c)}.$$

The proof for the above result will be given in [4]. This result, along with 82.16), gives the asymptotics for  $K$  for all  $\Delta'$  greater than  $\Delta - U$ .

The plan of the paper is as follows. In the next section we identify the set of the critical configurations  $\mathcal{C}^{**}$ , or the subset of the communication level set between  $\square$  and  $\blacksquare$  such that the dynamics passes through on its way from  $\square$  to  $\blacksquare$  with a probability tending to 1 as  $\beta \rightarrow \infty$ , and we prove Theorem(2.1). In section 4, with the information given in the previous section, we perform the proo of the Theorem 2.2 with the potential theoretic argument adopted in [2].

### 3. Critical Droplets

In this section we prove Theorem(2.1). First we will give some notations. We denote by  $\mathcal{Q}$  the set of configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $(\ell_c - 1) \times \ell_c$  quasi-square with a 1-protuberance attached to its longest side. We denote by  $\mathcal{C}^{**}$  the set of configurations obtained from any configuration in  $\mathcal{Q}$  by adding an extra 1-protuberance to the side having a 1-protuberance (see Fig.5).



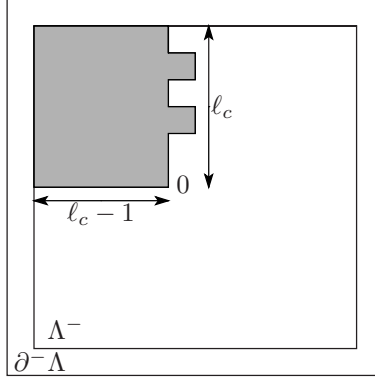


FIGURE 5. An element of  $\mathcal{C}^{**}$

**Proposition 3.1.** *We assume that  $0 < \Delta' < \Delta - U$ . Under the assumption, there exists a path  $\omega : \square \rightarrow \blacksquare$  such that  $\max_{\xi \in \omega} H(\xi) \leq \Gamma^{**}$  and pass through configurations in  $\mathcal{C}^{**}$ . Here  $\Gamma^{**}$  is the one given in (2.12).*

*Proof.* This proof is done in three steps. We set  $\alpha = \Delta' - \Delta$ .  
 (1) We first show that the configurations in  $\mathcal{Q}$  are connected to  $\square$  by a path that stays below  $\Gamma^{**}$ . Fix  $\eta^{1pr} \in \mathcal{Q}$ . Because the energy of configurations in  $\mathcal{C}^{**}$  is  $\Gamma^{**}$ ,  $H(\eta^{1pr}) = \Gamma^{**} - \Delta + U$ . We move the 1-protuberance to the outside of  $\Lambda$  by the process described in Figure 6. Until we get to the rightmost configuration of

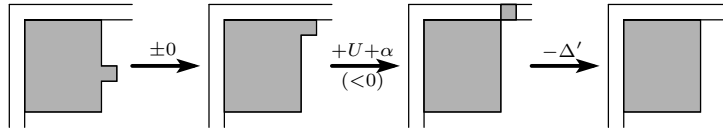


FIGURE 6

Figure 6 (the  $(\ell_c - 1) \times \ell_c$  quasi-square), the energy decreases and reaches

$$\Gamma^{**} - \Delta + U + U + \alpha - \Delta' = \Gamma^{**} - 2\Delta + 2U < \Gamma^{**}. \tag{3.1}$$

Next we slide the particles in the shortest side of the  $(\ell_c - 1) \times \ell_c$  square to get  $(\ell_c - 1) \times (\ell_c - 1)$  quasi-square as showed in Figure 7. Until we get to the configuration  $(*)_1$  in Figure 7 it cost us  $2U + \alpha - \Delta' = 2U - \Delta$  times  $\ell_c - 3$ , and so the energy reaches the highest at the configuration  $(*)_2$  in Figure 7 with the value

$$\Gamma^{**} - 2\Delta + 2U + (2U - \Delta)(\ell_c - 3) + U = \Gamma^{**} + (2U - \Delta)(\ell_c - 1) - U,$$

and by the definition of  $\ell_c$  in (2.7), the right-hand side is smaller than

$$\Gamma^{**} + (2U - \Delta) \left\{ \left( \frac{U}{2U - \Delta} + 1 \right) - 1 \right\} - U = \Gamma^{**}. \tag{3.2}$$

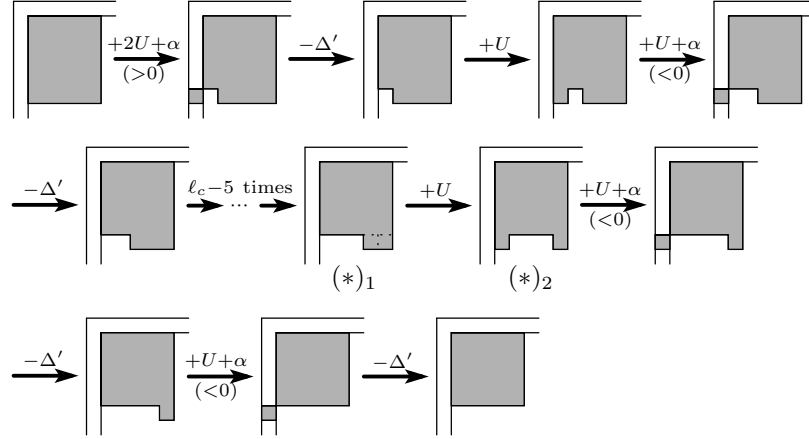


FIGURE 7

Hence the energy at the rightmost of the Figure 7 is

$$\Gamma^{**} + (2U - \Delta)(\ell_c - 1) - U + 2(U + \alpha) - 2\Delta' = \Gamma^{**} + (2U - \Delta)(\ell_c - 1) - 2\Delta + U$$

and by the definition of  $\ell_c$  in (2.7), this is smaller than

$$\Gamma^{**} - 2\Delta + 2U,$$

which is the energy of the  $(\ell_c - 1) \times \ell_c$  quasi-square as we have seen in (3.1). Thus the removal of a row of length  $\ell_c - 1$  from the  $(\ell_c - 1) \times \ell_c$  quasi-square in  $\eta^{1pr} \in \mathcal{Q}_{(f)}$  lowers the energy. We now have a square of side length  $\ell_c - 1$  which is next to  $\partial^- \Lambda$ . It is obvious that we can remove further rows without encountering new conditions, until we reach  $\square$ .

(2) Let  $\eta^{2pr}$  denote the set of configurations having one cluster consisting of an  $(\ell_c - 1) \times \ell_c$  quasi-square with a 2-protuberance attached to the corner of its longest side, which is not next to  $\partial^- \Lambda$  at one of corners of  $\Lambda^-$ . We next show that  $\eta^{2pr}$  is connected to  $\blacksquare$  by a path that stays below  $\Gamma^{**}$ . Fix  $\eta^{2pr}$ . Note that  $H(\eta^{2pr}) = \Gamma^{**} - U$ . First, we must construct an  $\ell_c \times \ell_c$  square, in order to go to  $\blacksquare$  from  $\eta^{2pr}$  without exceeding energy  $\Gamma^{**}$ . We create a particle in  $\partial^- \Lambda$ , which costs  $\Delta'$ , and attach it to the side having the 2-protuberance, which costs  $-U - \alpha (> 0)$ . This brings us to the energy

$$\Gamma^{**} - U + \Delta' - U - \alpha = \Gamma^{**} - 2U + \Delta < \Gamma^{**}.$$

We slide it next to the 2-protuberance, which pays  $U$ , thereby forming a bar of length 3. These operations pay  $2U - \Delta (> 0)$ . We can repeat these operations another  $\ell_c - 3$  times until the row is filled. By that time we have a square of side length  $\ell_c$  at a corner of  $\Lambda^-$  and energy

$$\Gamma^{**} - U - (2U - \Delta)(\ell_c - 2).$$

Second, we create another particle in  $\partial^- \Lambda$ , which costs  $\Delta'$ , and move it to  $\Lambda^-$  and attach it to the square to form a new 1-protuberance simultaneously, which costs

$-U - \alpha$ . This brings us to the energy

$$\Gamma^{**} - U - (2U - \Delta)(\ell_c - 2) + \Delta' - U - \alpha = \Gamma^{**} - (2U - \Delta)(\ell_c - 1) < \Gamma^{**},$$

We slide it to the corner of same side, which is not next to  $\partial^- \Lambda$ . We create another particle in  $\partial^- \Lambda$ , which costs  $\Delta'$ , and move it to  $\Lambda^-$  and attach it to the cluster simultaneously, which costs  $-U - \alpha$ . This brings us to the energy

$$\Gamma^{**} - (2U - \Delta)(\ell_c - 1) + \Delta' - U - \alpha = \Gamma^{**} - (2U - \Delta)\ell_c + U,$$

and by the definition of  $\ell_c$  in (2.7),

$$\Gamma^{**} - (2U - \Delta)\ell_c + U < \Gamma^{**} - U + U = \Gamma^{**}.$$

We slide it next to the 1-protuberance, which pays  $U$  (see Fig.8). This brings us

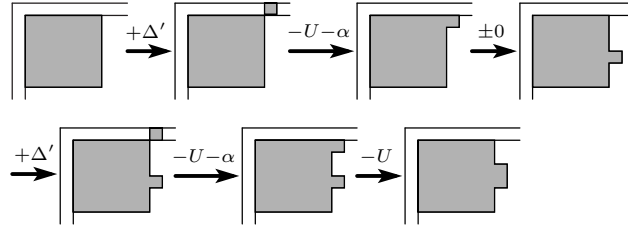


FIGURE 8

to the energy

$$\Gamma^{**} - (2U - \Delta)\ell_c < \Gamma^{**} - U,$$

which is below the energy of  $\eta^{2pr}$ . It is obvious that we can add further rows without encountering new conditions, until we reach  $\blacksquare$ .

(3) We can now conclude the proof of  $\Phi(\square, \blacksquare) \leq \Gamma^{**}$  by constructing a "bridge" between  $\eta^{1pr} \in \mathcal{Q}$  and  $\eta^{2pr}$  that does not exceed  $\Gamma^{**}$ . Namely, we create a particle in  $\partial^- \Lambda$ , which costs  $\Delta'$ , and attach it to the side having the 1-protuberance as new 1-protuberance, which costs  $-U - \alpha$  and raises energy to  $\Gamma^{**}$ . And we slide a 1-protuberance to the corner which is not next to  $\partial^- \Lambda$ , which costs 0, and slide another 1-protuberance next to it, which pays  $U$  (see Fig.9). The desired path

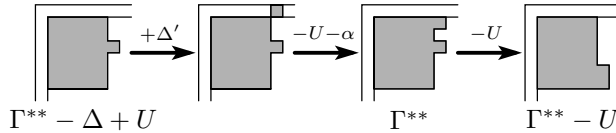


FIGURE 9. A bridge between  $\eta^{1pr}$  and  $\eta^{2pr}$

$\omega : \square \rightarrow \blacksquare$  is realized by tracing the path in (1) in the direction, back from  $\square$  to  $\eta^{1pr}$ , going over the bridge from  $\eta^{1pr}$  to  $\eta^{2pr}$ , and then following the path in (2) from  $\eta^{2pr}$  to  $\blacksquare$ . □

**Proposition 3.2.**  $\Phi(\square, \blacksquare) \geq \Gamma^{**}$ .

*Proof.* Any path  $\omega : \square \rightarrow \blacksquare$  must cross the set  $\nu_{\ell_c(\ell_c-1)}$ , which is the set of configurations with  $\ell_c(\ell_c - 1)$  particles, and in  $\nu_{\ell_c(\ell_c-1)}$  the unique configuration having minimal energy is the configuration having one cluster consisting of an  $(\ell_c - 1) \times \ell_c$  quasi-square. Such configuration has energy  $\Gamma^{**} - 2\Delta + 2U$ . We assume that the  $(\ell_c - 1) \times \ell_c$  quasi-square is at one of corners of  $\Lambda^-$ , because the necessary cost of a path that we move a particle created in  $\partial^- \Lambda$  to  $\Lambda^-$  and attach it to the cluster is lower than a path not using it. To increase the particle number starting from here, we must create a particle in  $\partial^- \Lambda$  at cost  $\Delta'$ . We do this operation, so we arrive at the energy  $\Gamma^{**} - 2\Delta + 2U + \Delta'$ . Next, we create another particle in  $\partial^- \Lambda$  at cost  $\Delta'$ , so we arrive at the energy

$$\Gamma^{**} - 2\Delta + 2U + 2\Delta' < \Gamma^{**} - 2\Delta + 2U + 2(\Delta - U) = \Gamma^{**}.$$

We move one of free particles to  $\Lambda^-$  and attach it to  $(\ell_c - 1) \times \ell_c$  quasi-square simultaneously at cost  $-U - \alpha$ , so we arrive at the energy

$$\Gamma^{**} - 2\Delta + U + 2\Delta' - \alpha = \Gamma^{**} - \Delta + U + \Delta' < \Gamma^{**}.$$

We slide a new 1-protuberance to the next. Next, we move another free particle to  $\Lambda^-$  and attach it next to the 1-protuberance simultaneously, which pays  $2U + \alpha$ , so we arrive at the energy

$$\Gamma^{**} - \Delta - U + \Delta' - \alpha = \Gamma^{**} - U.$$

A path from here to  $\blacksquare$  of which necessary cost is the lowest is a path passing through the set of configurations having one cluster consisting of an  $\ell_c \times \ell_c$  square at one of corners of  $\Lambda^-$  by repeating the operation that we move a particle created in  $\partial^- \Lambda$  to  $\Lambda^-$  and attach it to the side having the 2-protuberance. For this path, we must slide the 2-protuberance to the next by sliding particles of it one by one before we create a particle in  $\partial^- \Lambda$ . Since the energy raises during the process of the sliding, we reach at the energy  $\Gamma^{**}$ . Therefore,  $\Phi(\square, \blacksquare) \geq \Gamma^{**}$ .  $\square$

Combining Proposition 3.1 and Proposition 3.2, we prove  $\Phi(\square, \blacksquare) = \Gamma^{**}$  for all  $\Delta'$  with  $0 < \Delta' < \Delta - U$ .

#### 4. Average Nucleation Time: Proof of Theorem 2.2

First, let us view the configuration space  $\mathcal{X}$  as a graph whose vertices are configurations and whose edges connect communicating configurations.

- We denote by  $\mathcal{X}^*$  the subgraph of  $\mathcal{X}$  obtained by removing all vertices  $\eta$  with  $H(\eta) > \Gamma^{**}$  and all edges incident to these vertices,
- We denote by  $\mathcal{X}^{**}$  the subgraph of  $\mathcal{X}^*$  obtained by removing all vertices  $\eta$  with  $H(\eta) = \Gamma^{**}$  and all edges incident to these vertices,
- We denote by  $\mathcal{X}_{\square}$  and  $\mathcal{X}_{\blacksquare}$  the connected components of  $\mathcal{X}^{**}$  containing  $\square$  and  $\blacksquare$ , respectively.
- Each maximally connected component  $\mathcal{X}_i, i = 1, 2, \dots, I$  of  $\mathcal{X}^{**} \setminus (\mathcal{X}_{\square} \cup \mathcal{X}_{\blacksquare})$  is called a well, in other words, the configuration is in a well if its energy is  $< \Gamma^{**}$  but to move from it to either  $\square$  or  $\blacksquare$  the energy must reach  $\Gamma^{**}$ .

Notice that  $\mathcal{X}_{\square}$  and  $\mathcal{X}_{\blacksquare}$  are disconnected in  $\mathcal{X}^{**}$ .

**Proposition 4.1.** (1) *In the case  $\ell_c = 3$ , there is no well.*

(2) In the case  $\ell_c \geq 4$ , there are wells.

*Proof.* (1) In this case, the critical configurations are configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $2 \times 3$  quasi-square with two 1-protuberance attached to its longest side. Configurations communicating with the critical configurations without detaching a particle from the cluster are configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $2 \times 3$  quasi-square with 2-protuberance attached to its corner which is next to  $\partial^- \Lambda$  or is not next to  $\partial^- \Lambda$  of the longest side. The former configurations are in  $\mathcal{X}_{\square}$ , and the latter configurations are in  $\mathcal{X}_{\blacksquare}$ . Therefore, there is no well.

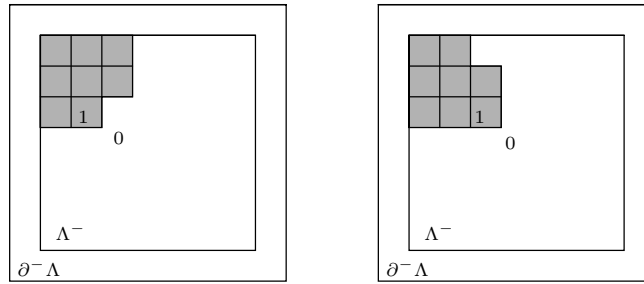


FIGURE 10. Configurations communicating with the critical configurations in the case  $\ell_c = 3$  without detaching a particle from the cluster

(2) In the case, we prove that configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $(\ell_c - 1) \times \ell_c$  rectangle with a 2-protuberance attached to the corner of its shortest side which is not next to  $\partial^- \Lambda$  (see Fig.11) are wells. The energy of these configurations is  $\Gamma^{**} - U$ . For the sake of simplicity, we express these configurations as  $W$ . In order to go to  $\square$  from  $W$ , we should slide 2-protuberance to the corner which is next to  $\partial^- \Lambda$  via the  $U$ -path. In the midst of using the  $U$ -path, the energy reach  $\Gamma^{**}$ . Next, we show that it is impossible to go to  $\blacksquare$  from  $W$  without exceeding the energy  $\Gamma^{**}$ . The path of the lowest communication height between  $W$  and  $\blacksquare$  is the following: We create a new particle in  $\partial^- \Lambda$ , which costs  $\Delta'$ , and move it to  $\Lambda^-$  and attach it to the cluster simultaneously, which costs  $-U - \alpha$ , thereby forming a new 1-protuberance. Then, the energy rises to

$$\Gamma^{**} - U + \Delta' - U - \alpha = \Gamma^{**} - 2U + \Delta < \Gamma^{**}.$$

We slide the 1-protuberance to 2-protuberance, which pays  $U$ , thereby forming a bar of length 3. We can repeat this operation another  $\ell_c - 4$  times until the row is filled. By that time we have an  $(\ell_c - 1) \times (\ell_c + 1)$  rectangle at one of corners of  $\Lambda^-$  and the energy

$$\Gamma^{**} - (2U - \Delta)(\ell_c - 3).$$

Then we attach a particle to the cluster and reach to an  $\ell_c \times \ell_c$  square via the  $U$ -path. In the midst of doing this operation, we must reach to the energy

$$\Gamma^{**} - (2U - \Delta)(\ell_c - 3) + \Delta' - U - \alpha + U = \Gamma^{**} - (2U - \Delta)(\ell_c - 3) + \Delta.$$

From  $\ell_c = \left\lceil \frac{U}{2U - \Delta} \right\rceil < \frac{U}{2U - \Delta} + 1$ , we see that

$$\begin{aligned} \Gamma^{**} - (2U - \Delta)(\ell_c - 3) + \Delta &> \Gamma^{**} - (2U - \Delta) \left( \frac{U}{2U - \Delta} + 1 - 3 \right) + \Delta \\ &= \Gamma^{**} + 3U - \Delta > \Gamma^{**} \end{aligned}$$

Hence, it is impossible to go to  $\blacksquare$  from W without exceeding the energy  $\Gamma^{**}$ . Therefore, configurations W are wells.  $\square$

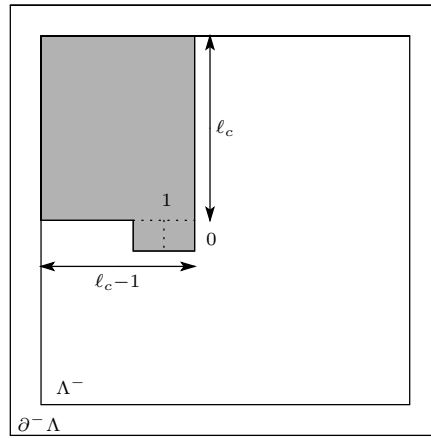


FIGURE 11. The example of wells in the case  $\ell_c \geq 4$

*Remark 4.2.* In the case  $\ell_c \geq 4$ , configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $(\ell_c - 1) \times \ell_c$  rectangle with 2-protuberance attached to the site of its shortest side which is not next to  $\partial^- \Lambda$  are also wells. In the case  $\ell_c \geq 5$ , configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $(\ell_c - 1) \times (\ell_c - 1)$  square with two bars of lengths  $k_1, k_2$  attached to its two corners which are next to  $\partial^- \Lambda$  satisfying

$$3 \leq k_1, k_2 \leq \ell_c - 2, \quad k_1 + k_2 = \ell_c + 1$$

(see (A) in Fig.12), and configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $(\ell_c - 2) \times \ell_c$  rectangle with two bars of lengths  $k_1, k_2$  attached to its two sides satisfying

$$3 \leq k_1, k_2 \leq \ell_c - 1, \quad k_1 + k_2 = \ell_c + 2$$

(see (B) in Fig.12) are also wells.

In order to prove Theorem 2.2, we introduce the capacity with respect to the dynamics.

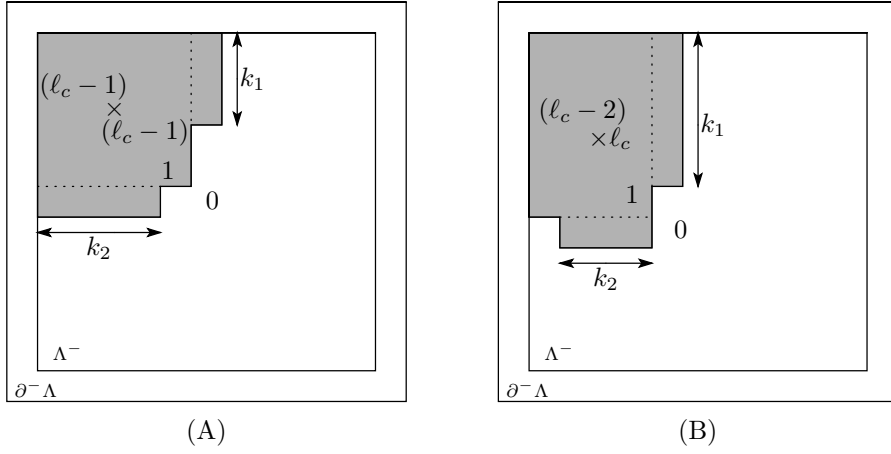


FIGURE 12. The example of wells in the case  $\ell_c \geq 5$

**Definition 4.3.** (i): For any function  $h : \mathcal{X} \rightarrow [0, 1]$ , the Dirichlet form is defined by

$$\varepsilon_\beta(h) = \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}} \mu_\beta(\eta) c_\beta(\eta, \eta') [h(\eta) - h(\eta')]^2, \quad (4.1)$$

where  $\mu_\beta$  is the Gibbs measure given by (2.2) and  $c_\beta$  are the transition rates of the Kawasaki dynamics given by (2.3).

(ii): For any two non-empty disjoint sets  $\mathcal{A}, \mathcal{B} \subseteq \mathcal{X}$ , the capacity of the pair  $\mathcal{A}, \mathcal{B}$  is defined by

$$\text{CAP}_\beta(\mathcal{A}, \mathcal{B}) = \min_{\substack{h: \mathcal{X} \rightarrow [0, 1] \\ h|_{\mathcal{A}} \equiv 1, h|_{\mathcal{B}} \equiv 0}} \varepsilon_\beta(h), \quad (4.2)$$

where  $h|_{\mathcal{A}} \equiv 1$  means that  $h(\eta) = 1$  for all  $\eta \in \mathcal{A}$  and  $h|_{\mathcal{B}} \equiv 0$  means that  $h(\eta) = 0$  for all  $\eta \in \mathcal{B}$ .

The right-hand side of (4.2) has a unique minimizer  $h_{\mathcal{A}, \mathcal{B}}^*$ , called the equilibrium potential of the pair  $\mathcal{A}, \mathcal{B}$ , given by

$$h_{\mathcal{A}, \mathcal{B}}^*(h) = \mathbb{P}_\eta(\tau_{\mathcal{A}} < \tau_{\mathcal{B}}), \quad \eta \in \mathcal{X} \setminus (\mathcal{A} \cup \mathcal{B}).$$

This is the solution of the equation

$$\begin{aligned} (c_\beta h)(\eta) &= 0, & \eta \in \mathcal{X} \setminus (\mathcal{A} \cup \mathcal{B}), \\ h(\eta) &= 1, & \eta \in \mathcal{A}, \\ h(\eta) &= 0, & \eta \in \mathcal{B}, \end{aligned}$$

with  $(c_\beta h)(\eta) = \sum_{\eta' \in \mathcal{X}} c_\beta(\eta, \eta') h(\eta')$ . Moreover,

$$\text{CAP}_\beta(\mathcal{A}, \mathcal{B}) = \sum_{\eta \in \mathcal{A}} \mu_\beta(\eta) c_\beta(\eta, \mathcal{X} \setminus \eta) \mathbb{P}_\eta(\tau_{\mathcal{B}} < \tau_{\mathcal{A}}) \quad (4.3)$$

with  $c_\beta(\eta, \mathcal{X} \setminus \eta) = \sum_{\eta' \in \mathcal{X} \setminus \eta} c_\beta(\eta, \eta')$  the rate of moving out of  $\eta$ .

To obtain our sharp estimate of  $\mathbb{E}_\square(\tau_\blacksquare)$  (Theorem 2.2), we will use the following key relation (Proposition 3.2.3 in [2]):

**Proposition 4.4.** *As  $\beta \rightarrow \infty$ , we have*

$$\mathbb{E}_\square(\tau_\blacksquare) = \frac{1}{Z_\beta \text{CAP}_\beta(\square, \blacksquare)} [1 + o(1)], \quad \beta \rightarrow \infty.$$

Next, we reduce the full Dirichlet form to a Dirichlet form involving only the immediate vicinity of the communication level set. Recall that  $\mathcal{X}_i, i = 1, \dots, I$  are the wells. For all  $(C_1, \dots, C_I) \in [0, 1]^I$ , let

$$\mathcal{H}_{(C_1, \dots, C_I)} = \{h : \mathcal{X} \rightarrow [0, 1], h|_{\mathcal{X}_\square} \equiv 1, h|_{\mathcal{X}_\blacksquare} \equiv 0, h|_{\mathcal{X}_i} \equiv C_i (i = 0, \dots, I)\}.$$

**Proposition 4.5.** *There exists a  $\delta > 0$  such that for  $\beta \rightarrow \infty$ ,*

$$Z_\beta \text{CAP}_\beta(\square, \blacksquare) = [1 + O(e^{-\delta\beta})] \Theta e^{-\Gamma^{**}\beta},$$

where

$$\Theta = \min_{C_1, \dots, C_I} \min_{h \in \mathcal{H}_{(C_1, \dots, C_I)}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^*} 1_{\{\eta \leftrightarrow \eta'\}} [h(\eta) - h(\eta')]^2. \quad (4.4)$$

In the remainder of the paper, using the above proposition, we will give the proof of the Theorem(2.2) in the case  $0 < \Delta' < \Delta - U$  and  $\ell_c = 3$  and  $\ell_c = 4$ .

**Theorem 4.6.** *Assume that  $0 < \Delta' < \Delta - U$ . Then,  $K = K(\mathcal{D}, \ell_c)$  in Theorem(2.2) is a constant dependent only on  $\ell_c$ . In the case  $\ell_c = 3$ ,  $K = \frac{3}{8}$ , and in the case  $\ell_c = 4$ ,  $K = \frac{29}{248}$ .*

*Proof.* Under our assumption, the critical configurations are configurations having one cluster at one of corners of  $\Lambda^-$  consisting of an  $(\ell_c - 1) \times \ell_c$  quasi-square with two 1-protuberance attached to its longest side. So, the critical configurations depends only on  $\ell_c$ .

(i) First let  $\ell_c = 3$ . Since there is no well in this case, for  $\mathcal{H} = \{h : \mathcal{X} \rightarrow [0, 1], h|_{\mathcal{X}_\square} \equiv 1, h|_{\mathcal{X}_\blacksquare} \equiv 0\}$ , we have

$$\Theta = \min_{h \in \mathcal{H}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^*} 1_{\{\eta \leftrightarrow \eta'\}} [h(\eta) - h(\eta')]^2.$$

That the transitions that count on the calculation of  $\Theta$  are only the following three transitions:

- (a): Transitions between  $\mathcal{X}_\square$  and  $\mathcal{C}^{**}$ .
- (b): Transitions between  $\mathcal{X}_\blacksquare$  and  $\mathcal{C}^{**}$ .
- (c): Transitions in  $\mathcal{C}^{**}$ .

Thus

$$\Theta = \frac{1}{2} \sum_{\eta \in \mathcal{C}^{**}} \min_{h \in \mathcal{H}} \sum_{\eta' \in \mathcal{X}^{**}} 1_{\{\eta \leftrightarrow \eta'\}} [h(\eta) - h(\eta')]^2.$$

There are eight configurations in  $\mathcal{C}^{**}$  in this case, see Fig. 13. and for each  $\bar{\eta} \in \mathcal{C}^{**}$ , there are three communicating configurations in  $\mathcal{X}^{**}$ ,  $\eta_1, \eta_2$  and  $\eta_3$ , say. Fig. 14 shows them for upper-left  $\bar{\eta}$  in Fig. 13. Notice that  $\eta_1$  and  $\eta_2$  are in  $\mathcal{X}_\square$ ,



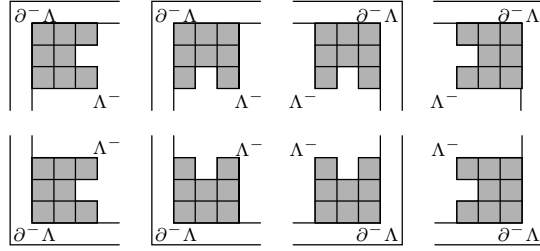


FIGURE 13. Critical configurations in the case  $\ell_c = 3$

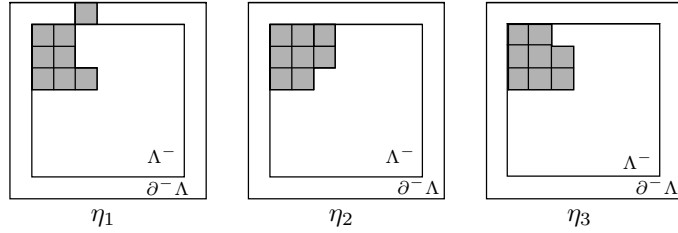


FIGURE 14. Configurations communicating with a critical configuration in  $\mathcal{X}^{**}$

$\eta_3$  is in  $\mathcal{X}_\blacksquare$ . Therefore,

$$\begin{aligned} & \min_{h \in \mathcal{H}} \sum_{\eta' \in \mathcal{X}^*} 1_{\{\bar{\eta} \leftrightarrow \eta'\}} [h(\bar{\eta}) - h(\eta')]^2 \\ &= \min_{h \in \mathcal{H}} \{ [h(\bar{\eta}) - h(\eta_1)]^2 + [h(\bar{\eta}) - h(\eta_2)]^2 + [h(\bar{\eta}) - h(\eta_3)]^2 \} \\ &= \min_{h: \mathcal{X}^* \rightarrow [0,1]} \{ [h(\bar{\eta}) - 1]^2 + [h(\bar{\eta}) - 1]^2 + h(\bar{\eta})^2 \} \\ &= \min_{h: \mathcal{X}^* \rightarrow [0,1]} \{ 3h(\bar{\eta})^2 - 4h(\bar{\eta}) + 2 \} = \frac{2}{3}, \end{aligned}$$

and thus we have  $\Theta = \frac{1}{2} \sum_{\eta \in \mathcal{C}^{**}} \frac{2}{3} = \frac{8}{3}$ . Hence by Proposition 4.4 and Proposition 4.5, we have  $K = \frac{3}{8}$  for this case.

(ii) Next, let  $\ell_c = 4$ . In this case, unlike in the case  $\ell_c = 3$ , there are dead ends and a well. Since for any  $h \in \mathcal{H}_{(C_1, \dots, C_t)}$ ,  $[h(\eta) - h(\eta')]^2 = 0$  for all  $\eta, \eta' \in \mathcal{X}^*$  that are both in  $\mathcal{X}_\square$  or both in  $\mathcal{X}_\blacksquare$ , the transitions that count in the calculation of (4.4) are only the following transitions:

- (a): transitions between  $\mathcal{X}_\square$  and  $\mathcal{S}(\square, \blacksquare)$ ,
- (b): transitions between  $\mathcal{X}_\blacksquare$  and  $\mathcal{C}^{**} \subset \mathcal{S}(\square, \blacksquare)$ ,
- (c): transitions in  $\mathcal{S}(\square, \blacksquare)$ ,
- (d): transitions between set of wells and  $\mathcal{S}(\square, \blacksquare)$ ,

where  $\mathcal{S}(\square, \blacksquare) = \{\eta \in \mathcal{X}; H(\eta) = \Gamma^{**}\}$ . Notice also that there is only one well  $\eta_w$  in  $\mathcal{X}_{u.l.v.}$ . Thus we have

$$\Theta = 8 \cdot \min_C \min_{h \in \mathcal{H}_C} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}_{u.l.v.}} 1_{\{\eta \leftrightarrow \eta'\}} [h(\eta) - h(\eta')]^2. \tag{4.5}$$

where  $\mathcal{X}_{u.l.v.}$  be the set of configurations corner drawn in Fig. 15 and

$$\mathcal{H}_C = \{h : \mathcal{X}_{u.l.v.} \rightarrow [0, 1], h|_{\mathcal{X}_\square} \equiv 1, h|_{\mathcal{X}_\blacksquare} \equiv 0, h(\eta_w) = C\}.$$

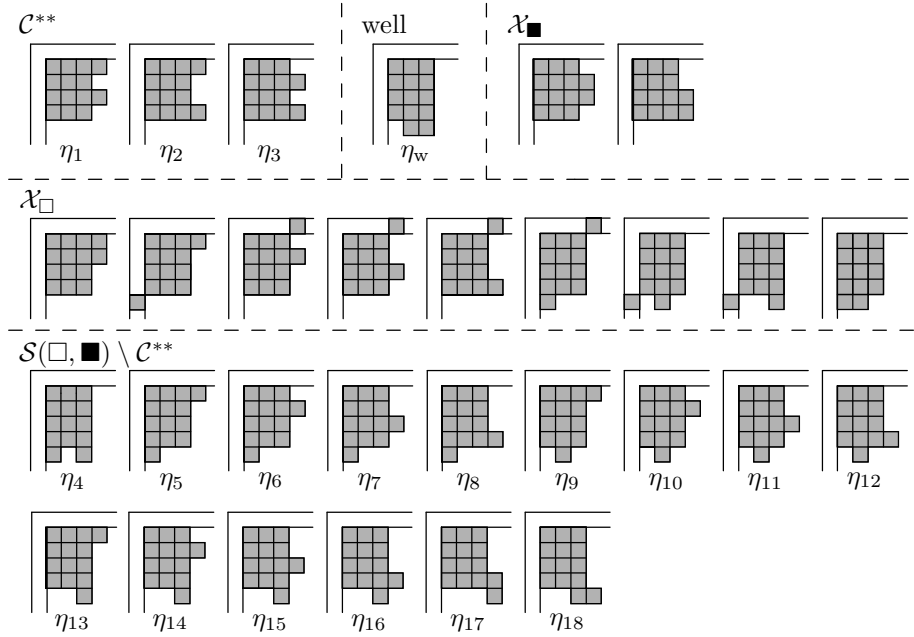


FIGURE 15. Configurations related to the calculation of  $\Theta$

Now, the transitions in  $\mathcal{X}_{u.l.v.}$  are the following:

$$\begin{array}{llllll} \eta_1 \longleftrightarrow \eta_2 & \eta_1 \longleftrightarrow \mathcal{X}_\square(\times 2) & \eta_1 \longleftrightarrow \mathcal{X}_\blacksquare & \eta_2 \longleftrightarrow \eta_3 & \eta_2 \longleftrightarrow \mathcal{X}_\square & \\ \eta_3 \longleftrightarrow \mathcal{X}_\blacksquare(\times 2) & \eta_4 \longleftrightarrow \eta_w & \eta_4 \longleftrightarrow \mathcal{X}_\square(\times 2) & \eta_5 \longleftrightarrow \eta_6 & \eta_5 \longleftrightarrow \eta_9 & \\ \eta_5 \longleftrightarrow \mathcal{X}_\square(\times 2) & \eta_6 \longleftrightarrow \eta_7 & \eta_6 \longleftrightarrow \eta_{10} & \eta_6 \longleftrightarrow \mathcal{X}_\square & \eta_7 \longleftrightarrow \eta_8 & \\ \eta_7 \longleftrightarrow \eta_{11} & \eta_7 \longleftrightarrow \mathcal{X}_\square & \eta_8 \longleftrightarrow \eta_{12} & \eta_8 \longleftrightarrow \mathcal{X}_\square & \eta_9 \longleftrightarrow \eta_{10} & \\ \eta_9 \longleftrightarrow \eta_{13} & \eta_9 \longleftrightarrow \mathcal{X}_\square & \eta_{10} \longleftrightarrow \eta_{11} & \eta_{10} \longleftrightarrow \eta_{14} & \eta_{11} \longleftrightarrow \eta_{12} & \\ \eta_{11} \longleftrightarrow \eta_{15} & \eta_{12} \longleftrightarrow \eta_{16} & \eta_{13} \longleftrightarrow \eta_{14} & \eta_{13} \longleftrightarrow \mathcal{X}_\square & \eta_{14} \longleftrightarrow \eta_{15} & \\ \eta_{15} \longleftrightarrow \eta_{16} & \eta_{16} \longleftrightarrow \eta_{17} & \eta_{16} \longleftrightarrow \eta_{18}, & & & \end{array}$$

Here  $(\times 2)$  denotes that there are two transitions. For example,  $\eta_1 \longleftrightarrow \mathcal{X}_\square(\times 2)$  denotes that there are two transitions  $\eta_1 \longleftrightarrow \eta_i$  and  $\eta_1 \longleftrightarrow \eta_j$  for  $\eta_i \neq \eta_j \in \mathcal{X}_\square$ . Hence we are able to compute the RHS of (4.5) and we obtain  $\Theta = 8 \times \frac{31}{29} = \frac{248}{29}$ .

(iii) As is clear from the argument above, in the case  $\ell_c \geq 5$ ,  $K = K(\mathcal{D}, \ell_c)$  is a constant dependent only on  $\ell_c$ , and the constant  $K$  is computable.  $\square$

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TAIZO CHIYONOBU: DEPARTMENT OF SCIENCE AND TECHNOLOGY, KWANSEI-GAKUIN UNIVERSITY, SANDA, HYOGO 6691337, JAPAN

*E-mail address:* [chiyo@kwansei.ac.jp](mailto:chiyo@kwansei.ac.jp)

YUSUKE TAKAGI: DEPARTMENT OF SCIENCE AND TECHNOLOGY, KWANSEI-GAKUIN UNIVERSITY, SANDA, HYOGO 6691337, JAPAN

*E-mail address:* [ehz76059@kwansei.ac.jp](mailto:ehz76059@kwansei.ac.jp)