Droplet growth for three-dimensional Kawasaki dynamics

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Abstract

The goal of this paper is to describe metastability and nucleation for a local version of the three-dimensional lattice gas with Kawasaki dynamics at low temperature and low density.

Let $\Lambda \subseteq \mathbb{Z}^3$ be a large finite box. Particles perform simple exclusion on Λ, but when they occupy neighboring sites they feel a binding energy $-U < 0$ that slows down their dissociation. Along each bond touching the boundary of Λ from the outside, particles are created with rate $\rho = e^{-\Delta\beta}$ and are annihilated with rate 1, where β is the inverse temperature and $\Delta > 0$ is an activity parameter. Thus, the boundary of Λ plays the role of an infinite gas reservoir with density ρ.

We consider the regime where $\Delta \in (U, 3U)$ and the initial configuration is such that Λ is empty. For large β, the system wants to fill Λ but is slow in doing so. We investigate how the transition from empty to full takes place under the dynamics. In particular, we identify the size and shape of the *critical droplet* and the time of its creation in the limit as $\beta \to \infty$.

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Contents

1 Introduction and main results

In this paper we study the metastable behavior of the three-dimensional lattice gas subject to Kawasaki dynamics. We consider the "local version" of the model, where particles live on a finite box and are created respectively annihilated at the boundary of this box in a way that reflects an infinite gas reservoir. Our main results generalize part of those obtained in den Hollander, Olivieri and Scoppola [5], [6], where the two-dimensional version of the same model was considered. In particular, we identify the size and shape of the critical droplet and the time of its creation in the limit of low temperature and low density.

Our results are comparable with those obtained by Ben Arous and Cerf [2] for the three-dimensional Ising model on a finite box with periodic boundary conditions subject to Glauber dynamics. However, Kawasaki dynamics has its own characteristics, which needs to be handled in the description of the nucleation. In particular, particle conservation on the interior of the box represents a serious obstacle in controlling the growing and the shrinking of droplets. Moreover, it turns out that particles can move along the border of a droplet more rapidly than they can arrive from the boundary. This leads to a shape of the critical droplet that is more complicated than the one for Ising spins under Glauber dynamics.

Obtaining a complete description of the typical nucleation path, as given in [2] for Glauber dynamics, turns out to be a rather difficult task for Kawasaki dynamics. In the present paper we do not obtain a complete description, but we do discuss in detail the geometry of the critical droplet representing the "gate" for the transition from the metastable state to the stable state. In this connection, a key role in our analysis is played by the discrete isoperimetric inequalities in Alonso and Cerf [1]. With the help of the latter we are able to show that there is a special set of values for the number of particles in the box, which we call magic numbers, such that all optimal paths realizing the minimax between any pair of consecutive magic numbers have a "focalization property", namely, they must visit the special set of configurations where the particles form a quasi-cube with a quasi-square attached to one of its faces. This focalization property allows us to identify the gate for the nucleation.

Our main results are Theorems 1.55 and 1.58 in Section 1.6. In Sections 1.1–1.2 we define the model, in Sections 1.3–1.4 we provide the heuristics behind the metastable behavior, while in Section 1.5 we list the definitions and notations that are necessary to formulate the theorems and that are used throughout the paper. In Section 1.7 we formulate some open problems. Section 2 contains the preparations and observations that form the background of the paper, while Section 3 provides the proof of the theorems. Section 4 looks at the motion of particles along the border of the droplet and contains some further reflections on the geometry of the critical droplet and on the typical nucleation path.

1.1 Hamiltonian and equilibrium

Let $\Lambda \subseteq \mathbb{Z}^3$ be a large finite box, let

$$\begin{aligned} \partial^-\Lambda &= \{x \in \Lambda \colon\ \exists y \notin \Lambda \colon\ |y-x| = 1\}, \\ \partial^+\Lambda &= \{x \notin \Lambda \colon\ \exists y \in \Lambda \colon\ |y-x| = 1\}, \end{aligned} \tag{1.1}$$

be the internal respectively the outer boundary of Λ, and let $\Lambda_- = \Lambda \setminus \partial^-\Lambda$ be the interior of Λ. 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 $\eta \in \mathcal{X} = \{0,1\}^\Lambda$. For $A \subseteq \Lambda$, let

$$N_A(\eta) = \sum_{x \in A} \eta(x) \tag{1.2}$$

be the number of particles in A. Each configuration $\eta \in \mathcal{X}$ has an energy given by the Hamiltonian

$$H(\eta) = -U \sum_{(x,y)\in\Lambda_-^*} \eta(x)\eta(y) + \Delta N_\Lambda(\eta), \tag{1.3}$$

where

$$\Lambda_-^* = \{(x,y)\colon\ x,y \in \Lambda_-\} \tag{1.4}$$

is the set of unoriented bonds in Λ_-. The interaction, which is acting only inside Λ_-, is a binding energy $-U < 0$ for each pair of nearest-neighbor particles. In addition, there is an activity energy $\Delta > 0$ for each particle in Λ. (Note that $H - \Delta N_{\partial^-\Lambda}$ is the Hamiltonian in Λ_- with 0 boundary conditions.)

The *grand-canonical Gibbs measure* associated with H is

$$\mu(\eta) = \frac{e^{-\beta H(\eta)}}{Z}, \qquad \eta \in \mathcal{X}, \tag{1.5}$$

with

$$Z = \sum_{\eta\in\mathcal{X}} e^{-\beta H(\eta)}. \tag{1.6}$$

1.2 Kawasaki and Glauber dynamics

We next define *Kawasaki dynamics* on Λ, with a boundary condition that mimicks the effect of an infinite gas reservoir outside Λ with density

$$\rho = e^{-\Delta\beta}. \tag{1.7}$$

Let $b = (x \to y)$ denote an oriented bond, i.e., an ordered pair of nearest-neighbor sites. Define

$$\begin{array}{rcl} \partial^*\Lambda^{out} &=& \{b = (x \to y)\colon\ x \in \partial^-\Lambda, y \in \partial^+\Lambda\},\\ \partial^*\Lambda^{in} &=& \{b = (x \to y)\colon\ x \in \partial^+\Lambda, y \in \partial^-\Lambda\},\\ \Lambda^{*,\,orie} &=& \{b = (x \to y)\colon\ x, y \in \Lambda\}, \end{array} \tag{1.8}$$

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

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

$$T_b\eta(z) = \begin{cases} \eta(z) & \text{if } z \neq x,y,\\ \eta(x) & \text{if } z = y,\\ \eta(y) & \text{if } z = x. \end{cases} \tag{1.9}$$

- $b = (x \to y) \in \partial^*\Lambda^{out}$:

$$T_b\eta(z) = \begin{cases} \eta(z) & \text{if } z \neq x,\\ 0 & \text{if } z = x. \end{cases} \tag{1.10}$$

- $b = (x \to y) \in \partial^*\Lambda^{in}$:

$$T_b\eta(z) = \begin{cases} \eta(z) & \text{if } z \neq y,\\ 1 & \text{if } z = y. \end{cases} \tag{1.11}$$

Note that, for $b \in \Lambda^{*,\,orie}$, $T_b\eta$ is invariant under a change of orientation of b, while for $b \in \partial^*\Lambda^{out}$ and $b \in \partial^*\Lambda^{in}$ it is not.

The Kawasaki dynamics is defined to be the discrete-time Markov chain $(\eta_t)_{t\in\mathbb{N}_0}$ on $\mathcal{X}$ given by the transition probabilities

$$P^K(\eta,\eta') = \begin{cases} \frac{1}{|\Lambda^{*,\,orie}|} e^{-\beta[H(\eta')-H(\eta)]_+} & \text{if } \eta \neq \eta', \eta \leftrightarrow^K \eta', \\ 0 & \text{if } \eta \neq \eta', \eta \not\leftrightarrow^K \eta', \end{cases} \tag{1.12}$$

and $P^K(\eta,\eta) = 1 - \sum_{\eta'\neq\eta} P^K(\eta,\eta')$, where $[a]_+ = a \vee 0$. This is a standard Metropolis dynamics with an open boundary: along each bond touching $\partial^-\Lambda$ from the outside, particles are created with rate ρ and are annihilated with rate 1, while inside Λ_- particles are conserved. Note that any change of particles inside $\partial^-\Lambda$ does not involve any change in energy because the interaction acts only inside Λ_- (see (1.3)).

Most of the present paper deals with Kawasaki dynamics. However, occasionally we will also need *Glauber dynamics*, which is defined to be the discrete-time Markov chain $(\eta_t)_{t\in\mathbb{N}_0}$ on $\mathcal{X}$ given by the transition probabilities

$$P^G(\eta,\eta') = \begin{cases} \frac{1}{|\Lambda|} e^{-\beta[H(\eta')-H(\eta)]_+} & \text{if } \eta \neq \eta', \eta \leftrightarrow^G \eta', \\ 0 & \text{if } \eta \neq \eta', \eta \not\leftrightarrow^G \eta', \end{cases} \tag{1.13}$$

and $P^G(\eta,\eta) = 1 - \sum_{\eta'\neq\eta} P^G(\eta,\eta')$, where now $\eta \neq \eta'$ are communicating states, written $\eta \leftrightarrow^G \eta'$, if there exists a site $x \in \Lambda$ such that $\eta' = T_x\eta$, where $T_x\eta$ is the configuration obtained from η as

$$T_x\eta(z) = \begin{cases} \eta(z) & \text{if } z \neq x, \\ 1-\eta(x) & \text{if } z = x. \end{cases} \tag{1.14}$$

On Λ_-, Kawasaki dynamics exchanges particles between nearest-neighbor sites, while Glauber dynamics creates or annihilates particles at single sites. Thus, on Λ_-, Kawasaki dynamics is *conservative*, while Glauber dynamics is *non-conservative*. It is easy to verify that both are reversible w.r.t. the grand-canonical Gibbs measure defined in (1.5).

1.3 Metastability: static heuristics

We will be interested in the regime

$$\Delta \in (U, 3U), \qquad \beta \to \infty. \tag{1.15}$$

To see why this regime is metastable, we argue as follows.

In the grand-canonical Gibbs measure the configuration can be represented in terms of spin variables. Indeed, after we make the substitution $\eta(x) = \frac{1+\sigma(x)}{2}$ in (1.3), where $\sigma(x) \in \{-1,+1\}$ is the spin variable, we can write

$$\begin{aligned} H(\sigma) &= -U \sum_{(x,y)\in\Lambda_-^*} \tfrac{1+\sigma(x)}{2}\tfrac{1+\sigma(y)}{2} + \Delta \sum_{x\in\Lambda} \tfrac{1+\sigma(x)}{2} \\ &= -\tfrac{U}{4} \sum_{(x,y)\in\Lambda_-^*} \sigma(x)\sigma(y) - \left(\tfrac{3U-\Delta}{2}\right) \sum_{x\in\Lambda} \sigma(x) + \text{ constant } + \text{ boundary terms.} \end{aligned} \tag{1.16}$$

This is a spin Hamiltonian with pair interaction $J = \frac{U}{4}$ and magnetic field $h = \frac{3U-\Delta}{2}$. The magnetic field vanishes when $\Delta = 3U$, which corresponds to the condensation point of the lattice gas. Indeed, at this condensation point the density of the liquid respectively the gas phase are

$$\rho_l(\beta) = \frac{1+m^*(\beta)}{2}, \qquad \rho_g(\beta) = \frac{1-m^*(\beta)}{2}, \tag{1.17}$$

where $m^*(\beta)$ is the spontaneous magnetization in the spin language. We have $m^*(\beta) = 1 - 2e^{-12J\beta}[1+o(1)]$ as $\beta \to \infty$, since when we flip the spin at the origin in the configuration $\sigma \equiv +1$ we reverse the sign of the interaction with the 6 nearest-neighbors of the origin. This shows that $e^{-3U\beta}[1+o(1)]$ is the density of the lattice gas at the condensation point, corresponding to $\rho = e^{-\Delta\beta}$ with $\Delta = 3U$.

Suppose next that we slightly increase the density (corresponding to $0 < 3U - \Delta \ll 1$), avoiding however the appearance of droplets in terms of a *restricted grand-canonical Gibbs measure* (see Lebowitz and Penrose [7], Capocaccia, Cassandro and Olivieri [4]). In other words, we consider the grand-canonical Gibbs measure restricted to a suitable subset of configurations, namely, those where all sufficiently large droplets of particles are suppressed. At low temperature this supersaturated gas will stay rarified, so that its metastable state can be described as an almost ideal gas phase with strong mixing properties. Let us denote by $\mu^*(m_1 \times m_2 \times m_3)$ the probability under the restricted measure to see an $m_1 \times m_2 \times m_3$ droplet centered at the origin. A rough calculation leads to

$$\mu^*(m_1 \times m_2 \times m_3) \approx \rho^{m_1 m_2 m_3} e^{\beta[3U m_1 m_2 m_3 - U(m_1 m_2 + m_2 m_3 + m_1 m_3)]}, \tag{1.18}$$

since ρ is the probability to find a particle at a given site and $-U$ is the binding energy between particles at nearest-neighbor sites. Substituting $\rho = e^{-\Delta\beta}$, we obtain

$$\mu^*(m_1 \times m_2 \times m_3) \approx e^{-\beta E(m_1, m_2, m_3)} \tag{1.19}$$

with

$$E(m_1, m_2, m_3) = -(3U - \Delta) m_1 m_2 m_3 + U(m_1 m_2 + m_2 m_3 + m_1 m_3). \tag{1.20}$$

The maximum of $E(m,m,m)$ occurs at $m = \frac{2U}{3U-\Delta}$. If this ratio is non-integer, then cubic droplets with side length $m < m_c$ have a probability decreasing in m, while cubic droplets with side length $m \geq m_c$ have a probability increasing in m, where

$$m_c = \left\lceil \frac{2U}{3U - \Delta} \right\rceil \tag{1.21}$$

plays the role of the *three-dimensional critical droplet size*. The regime $\Delta \in (U, 3U)$ corresponds to $m_c \in (1, \infty)$. In analogy with Glauber dynamics, studied by Ben Arous and Cerf [2], we expect metastable behavior when $h \in (0, 4J)$ with a critical droplet size $m_c = \lceil 4J/h \rceil$. This corresponds precisely to (1.15) and (1.21).

Similarly, the probability to see an $l_1 \times l_2$ droplet on a face of a three-dimensional droplet is

$$\mu^*(l_1 \times l_2 | \text{face}) \approx \rho^{l_1 l_2} e^{\beta[3U l_1 l_2 - U(l_1 + l_2)]}, \tag{1.22}$$

so

$$\mu^*(l_1 \times l_2 | \text{face}) \approx e^{-\beta E(l_1, l_2)} \tag{1.23}$$

with

$$E(l_1, l_2) = -(3U - \Delta) l_1 l_2 + U(l_1 + l_2). \tag{1.24}$$

The maximum of $E(l,l)$ occurs at $l = \frac{U}{3U-\Delta}$. If this ratio is non-integer, then square droplets with side length $l < l_c$ have a probability decreasing in l, while square droplets with side length $l \geq l_c$ have a probability increasing in l, where

$$l_c = \left\lceil \frac{U}{3U - \Delta} \right\rceil \tag{1.25}$$

plays the role of the *two-dimensional critical droplet size on a face*. The regime $\Delta \in (2U, 3U)$ corresponds to $l_c \in (1, \infty)$, the regime $\Delta \in (U, 2U)$ to $l_c = 1$. Note that $m_c \in \{2l_c - 1, 2l_c\}$.

The above heuristics describes the metastable behavior from a *static* point of view. In physical terms, $\Delta \in (3U, \infty)$ represents the stable gas, $\Delta = 3U$ is the condensation point, $\Delta \in (U, 3U)$ represents the metastable gas, $\Delta = U$ is the spinodal point, and $\Delta \in (0, U)$ represents the unstable gas.

The most interesting part of the metastable regime is $0 < \epsilon \ll 1$ with

$$\epsilon = 3U - \Delta, \tag{1.26}$$

which corresponds to weak supersaturation with large l_c and m_c.

1.4 Metastability: dynamic heuristics

Let us next consider the metastable behavior from a *dynamic* point of view. We want to compare the probabilities of growing respectively shrinking for a cubic droplet of particles with a quadratic droplet attached to one of its faces. Again, the argument will be very rough.

The energy barriers for adding respectively removing a bar (= row or column) of length l from a two-dimensional droplet on the face of a three-dimensional droplet are given in terms of the minimal saddles of H (see Fig. 1):

$$\begin{array}{lcl} \text{adding bar} & = & 2\Delta - 2U = 4U - 2\epsilon, \\ \text{removing bar} & = & 3U + (3U - \Delta)(l-2) = 3U + \epsilon(l-2). \end{array} \tag{1.27}$$

The * in Fig. 1 indicates the minimal saddle. The two barriers in (1.27) balance at $l = \frac{U}{\epsilon}$, so

(1.25) again appears as the two-dimensional critical droplet size on a face.

FIG. 1. Adding or removing a bar of length l ($l = 4$).

Similarly, the energy barriers for adding respectively removing a face of side length m are (see Figs. 2 and 3):

$$
\begin{aligned}
& m < l_c : \\
& \\
& \text{adding face} \quad = \quad U(2m+3) - \epsilon(m^2 - m + 2), \\
& \text{removing face} \quad = \quad 3U + \epsilon(m-2), \\
& \\
& m \geq l_c : \\
& \\
& \text{adding face} \quad = \quad U(2l_c+3) - \epsilon(l_c^2 - l_c + 2), \\
& \text{removing face} \quad = \quad -U(2m - 2l_c - 3) + \epsilon(m^2 - l_c^2 + l_c - 2).
\end{aligned}
\tag{1.28}
$$

FIG. 2. Adding or removing a 2×2 droplet on a face.

FIG. 3. Adding or removing a face of side length m ($m = 6$, $l_c = 4$, $m_c = 8$).

The ** in Fig. 3 indicates the minimal saddle for adding or removing a 2×2 droplet (as in Fig. 2), the *'s in Fig. 3 indicate the minimal saddles for adding or removing successive bars (as in Fig. 1). The center of Fig. 3, consisting of a quasi-cube with a quasi-square plus protuberance attached to a face plus a free particle, is the minimal saddle for adding a face. The two barriers in (1.28) balance at $m = \frac{2U}{\epsilon}$, so (1.21) again appears as the three-dimensional critical droplet size.

1.5 Definitions and notations

In the sequel we use *italic* capital letters for subsets of Λ, *script* capital letters for subsets of $\mathcal{X}$, and *boldface* capital letters for events under the Kawasaki dynamics. We use this convention in order to keep the various notations apart.

In order to formulate our main results in Theorems 1.55 and 1.58, and to perform their proofs, we need some definitions. These are collected in items 1–10 below.

1. Suppose that the finite box $\Lambda \subseteq \mathbb{Z}^3$ is large enough to amply accomodate the critical droplet (say, it has side length $\geq 2m_c$).

(i) For $x \in \Lambda_-$, let $nn(x) = \{y \in \Lambda_-\colon |y - x| = 1\}$ be the set of nearest-neighbor sites of x in Λ_-.

(ii) A *free particle* in $\eta \in \mathcal{X}$ is a site $x \in \eta \cap \partial^-\Lambda$ or a site $x \in \eta \cap \Lambda_-$ such that $\sum_{y \in nn(x) \cap \Lambda_-} \eta(y) = 0$, i.e., a particle not in interaction with any other particle (remember from (1.3) that particles in the interior boundary $\partial^-\Lambda$ have no interaction with particles in the interior Λ_-).

(iii) A 1-*protuberance* in $\eta \in \mathcal{X}$ is a site $x \in \eta \cap \Lambda_-$ such that $\sum_{y \in nn(x) \cap \Lambda_-} \eta(y) = 1$.
A 2-*protuberance* in $\eta \in \mathcal{X}$ is a site $x \in \eta \cap \Lambda_-$ such that $\sum_{y \in nn(x) \cap \Lambda_-} \eta(y) = 2$.

For convenience we identify a configuration $\eta \in \mathcal{X}$ with its support $\mathrm{supp}(\eta) = \{x \in \Lambda\colon \eta(x) = 1\}$ and write $x \in \eta$ to indicate that η has a particle at x.

2. Given a configuration $\eta \in \mathcal{X}$, consider the set $C(\eta) \subseteq \mathbb{R}^3$ defined as the union of the closed unit cubes centered at the sites inside Λ_- where η has a particle. The maximal connected components $C_1, \ldots, C_m$, $m \in \mathbb{N}$, of $C(\eta)$ are called *droplets* of η. There is a one-to-one correspondence between configurations $\eta \subseteq \Lambda_-$ and sets $C(\eta)$. A configuration $\eta \subseteq \Lambda$ is characterized by a set $C(\eta)$, depending only on $\eta \cap \Lambda_-$, plus possibly a set of free particles in $\partial^-\Lambda$, namely, $\eta \cap \partial^-\Lambda$. Thus, we are actually identifying three different objects: a configuration $\eta \in \mathcal{X}$, its support $\mathrm{supp}(\eta) \subseteq \Lambda$, and the pair $(C(\eta), \eta \cap \partial^-\Lambda)$.

For $\eta \in \mathcal{X}$, let $|\eta|$ be the number of particles in η, $\gamma(\eta)$ the Euclidean boundary of $C(\eta)$, called the *contour* of η, and $|\gamma(\eta)|$ the area of $\gamma(\eta)$, i.e., the number of broken bonds in η. Then the energy associated with η is given by

$$H(\eta) = -(3U - \Delta)|\eta \cap \Lambda_-| + \frac{U}{2}|\gamma(\eta)| + \Delta N_{\partial^-\Lambda}(\eta). \tag{1.29}$$

3. A configuration whose single contour is a *parallelepiped* with side lengths m_1, m_2, m_3 is denoted by $P(m_1, m_2, m_3)$. Throughout the sequel we use the convention $m_1 \leq m_2 \leq m_3$ and *collect the parallelepipeds in an equivalence class modulo translations and rotations.* This equivalence class is denoted by $\mathcal{P}(m_1,m_2,m_3)$. A rectangle is a parallelepiped with side lengths $1,l_1,l_2$, a bar is a parallelepiped with side lengths $1,1,k$.

Given integers $m_1,m_2,m_3\geq 2$ and $l_1,l_2\geq 1$, with $m_1\leq m_2\leq m_3$, $l_1\leq l_2$, $m_3\geq l_2$ and $m_2\geq l_1$, define:

- $\mathcal{R}_{l_1,l_2}(m_1,m_2,m_3)$ is the set of configurations without free particles whose single contour in Λ_- is an $m_1\times m_2\times m_3$ parallelepiped plus an $l_1\times l_2$ rectangle attached to any face large enough to accomodate it.

A *quasi-cube* is a parallelepiped with side lengths $m,m+\delta,m+\theta$ with $m\geq 1$, $\delta,\theta\in\{0,1\}$, $\delta\leq\theta$. A cube is a quasi-cube with $\delta=\theta=0$. A *quasi-square* is a parallelepiped with side lengths $1,l,l+\alpha$ with $l\geq 1$, $\alpha\in\{0,1\}$. A square is a quasi-square with $\alpha=0$.

4. The configuration space $\mathcal{X}$ can be partitioned as

$$\mathcal{X}=\bigcup_{n=0}^{|\Lambda|}\mathcal{V}_n, \tag{1.30}$$

where

$$\mathcal{V}_n=\{\eta\in\{0,1\}\colon\ N_\Lambda(\eta)=n\} \tag{1.31}$$

is the set of configurations with n particles, called the *n-manifold.*

5. A *path* ω is a sequence $\omega=(\omega_1,\dots,\omega_k)$, $k\in\mathbb{N}$, $\omega_i\in\mathcal{X}$ for $i=1,\dots,k$, such that $P^K(\omega_i,\omega_{i+1})>0$ for $i=1,\dots,k-1$. We write $\omega\colon\ \eta\to\eta'$ to denote a path from η to η'. Given $\zeta\in\mathcal{X}$, we write $\zeta\in\omega$ when ω visits ζ. Given $\mathcal{A}\subseteq\mathcal{X}$, we write $\omega\cap\mathcal{A}$ to denote the set of sites in $\mathcal{A}$ visited by ω.

A set $\mathcal{A}\subseteq\mathcal{X}$ with $|\mathcal{A}|>1$ is *connected* if and only if for all $\eta,\eta'\in\mathcal{A}$ there exists a path $\omega\colon\ \eta\to\eta'$ such that $\omega_i\in\mathcal{A}$ for all i. Any singleton is connected. Given a non-empty set $\mathcal{A}\subseteq\mathcal{X}$, define its (external) *boundary* as

$$\partial\mathcal{A}=\{\zeta\notin\mathcal{A}\colon\ P^K(\zeta,\eta)>0\text{ for some }\eta\in\mathcal{A}\} \tag{1.32}$$

and the *first hitting time of* $\mathcal{A}$ as

$$\tau_\mathcal{A}=\min\{t\geq 0\colon\ \eta_t\in\mathcal{A}\}. \tag{1.33}$$

6. The *bottom* of a non-empty set $\mathcal{A}\subseteq\mathcal{X}$ is the set of *global minima* of the Hamiltonian H in $\mathcal{A}$, i.e.,

$$\mathcal{F}(\mathcal{A})=\Big\{\eta\in\mathcal{A}\colon\ H(\eta)=\min_{\zeta\in\mathcal{A}}H(\zeta)\Big\}. \tag{1.34}$$

The *communication height* between a pair $\eta,\eta'\in\mathcal{X}$ is

$$\Phi(\eta,\eta')=\min_{\omega\colon\ \eta\to\eta'}\max_{\zeta\in\omega}H(\zeta). \tag{1.35}$$

The set of configurations realizing the *minimal saddles* between $\eta,\eta'\in\mathcal{X}$ is

$$\mathcal{S}(\eta,\eta')=\Big\{\zeta\in\mathcal{X}\colon\ \exists\omega\colon\ \ \eta\to\eta',\,\omega\ni\zeta\colon\ \max_{\xi\in\omega}H(\xi)=H(\zeta)=\Phi(\eta,\eta')\Big\}. \tag{1.36}$$

Given a connected set $\mathcal{U}\subseteq\mathcal{X}$, the *communication height between* $\eta,\eta'\in\mathcal{U}$ *inside* $\mathcal{U}$ is

$$\Phi_\mathcal{U}(\eta,\eta')=\min_{\substack{\omega\colon\ \eta\to\eta'\\ \omega\subseteq\mathcal{U}}}\max_{\zeta\in\omega}H(\zeta), \tag{1.37}$$

where $\omega \subseteq \mathcal{U}$ means that $\omega_i \in \mathcal{U}$ for all i, and similarly for $\mathcal{S}_{\mathcal{U}}(\eta, \eta')$.

Given two non-empty sets $\mathcal{A}, \mathcal{B} \subseteq \mathcal{X}$, put

$$\Phi(\mathcal{A}, \mathcal{B}) = \min_{\eta \in \mathcal{A},\, \eta' \in \mathcal{B}} \Phi(\eta, \eta') \tag{1.38}$$

and

$$\mathcal{S}(\mathcal{A}, \mathcal{B}) = \bigcup_{\substack{\eta \in \mathcal{A},\, \eta' \in \mathcal{B}: \\ \Phi(\eta, \eta') = \Phi(\mathcal{A}, \mathcal{B})}} \mathcal{S}(\eta, \eta'). \tag{1.39}$$

Similarly for $\Phi_{\mathcal{U}}(\mathcal{A}, \mathcal{B})$ and $\mathcal{S}_{\mathcal{U}}(\mathcal{A}, \mathcal{B})$. Write

$$(\mathcal{A} \to \mathcal{B})_{opt} \tag{1.40}$$

to denote the *set of optimal paths* realizing the minimax in $\mathcal{X}$ between $\mathcal{A}$ and $\mathcal{B}$.

7. Given a pair $\eta, \eta' \in \mathcal{X}$, we say that $\mathcal{W}$ is a *gate* for the transition $\eta \to \eta'$ if $\mathcal{W} \subseteq \mathcal{S}(\eta, \eta')$ and $\omega \cap \mathcal{W} \neq \emptyset$ for all $\omega \in (\eta \to \eta')_{opt}$. We say that $\mathcal{W}$ is a *minimal gate* for the transition $\eta \to \eta'$ if it is a gate and for any $\mathcal{W}' \subsetneq \mathcal{W}$ there exists $\omega' \in (\eta \to \eta')_{opt}$ such that $\omega' \cap \mathcal{W}' = \emptyset$. In words, a minimal gate is a minimal (by inclusion) subset of $\mathcal{S}(\eta, \eta')$ that is visited by all optimal paths.

For a given transition $\eta \to \eta'$, a priori there may be several (not necessarily disjoint) minimal gates. We denote by $\mathcal{G}(\eta, \eta')$ the union of all the minimal gates:

$$\mathcal{G}(\eta, \eta') = \bigcup_{\mathcal{W}:\ \mathcal{W} \text{ minimal gate for } \eta \to \eta'} \mathcal{W}. \tag{1.41}$$

The configurations $\zeta \in \mathcal{S}(\eta, \eta') \setminus \mathcal{G}(\eta, \eta')$ (if any) are called *dead-ends*. Given any path $\omega \in (\eta \to \eta')_{opt}$ passing through a dead-end ζ, there exists another path $\omega' \in (\eta \to \eta')_{opt}$, not passing through ζ, that plays the role of a short-cut of ω.

Given two non-empty sets $\mathcal{A}, \mathcal{B}$, we define

$$\mathcal{G}(\mathcal{A}, \mathcal{B}) = \bigcup_{\eta \in \mathcal{A}, \eta' \in \mathcal{B}} \mathcal{G}(\eta, \eta'). \tag{1.42}$$

8. The upper index $(.)^{fp}$ is used to denote configurations obtained from configurations in $(\cdot)$ after addition of a free particle.

Given integers $m_1, m_2, m_3 \geq 3$ and $l_1, l_2 \geq 2$, with $m_1 \leq m_2 \leq m_3$, $l_1 \leq l_2$, $m_3 \geq l_2$ and $m_2 \geq l_1$, define:

- $\mathcal{R}^{fp}_{l_1,l_2}(m_1, m_2, m_3)$ is the set of configurations obtained from a configuration in $\mathcal{R}_{l_1,l_2}(m_1, m_2, m_3)$ by adding a free particle.
- $\mathcal{R}^{2pr}_{l_1,l_2}(m_1, m_2, m_3)$ is the set of configurations obtained from a configuration in $\mathcal{R}^{fp}_{l_1,l_2}(m_1, m_2, m_3)$ by attaching the free particle to one of the sides of the rectangle that is attached to one of the faces of the parallelepiped, so that it becomes a 2-protuberance.
- $\mathcal{D}^{2pr}_{l_1,l_2}(m_1, m_2, m_3)$ is the set of configurations given by

$$\begin{aligned} \mathcal{D}^{2pr}_{l_1,l_2}(m_1, m_2, m_3) \quad = \quad \Big\{ \eta' \in \mathcal{V}_n\colon\ \exists \eta \in \mathcal{R}^{2pr}_{l_1,l_2}(m_1, m_2, m_3)\colon \\ \Phi_{\mathcal{V}_n}(\eta, \eta') \leq H(\eta) + 2U,\ H(\eta) = H(\eta') \Big\} \end{aligned} \tag{1.43}$$

with $n = m_1 m_2 m_3 + l_1 l_2 + 1$. In words, $\mathcal{D}^{2pr}_{l_1,l_2}(m_1,m_2,m_3)$ is the set of configurations η' that can be reached from some $\eta \in \mathcal{R}^{2pr}_{l_1,l_2}(m_1,m_2,m_3)$ by a path $\omega = (\omega_1,\ldots,\omega_k)$, $k \in \mathbb{N}$, in $\mathcal{V}_n$ such that

$$\omega_1 = \eta, \quad \omega_k = \eta', \quad \max_{1 \le i < k} H(\omega_i) \le H(\eta) + 2U, \quad H(\eta) = H(\eta'). \tag{1.44}$$

In the subregime $\Delta \in (2U, 3U)$, going from $\mathcal{R}$ to $\mathcal{D}$ corresponds to moving particles along the border of the droplet. Indeed, $2U$ is the largest multiple of U below Δ, and so all moves with a maximal energy cost $2U$ must be taken into account, because these moves may occur before the arrival of the next free particle (see Section 4.1 for more details).

- $\mathcal{R}^{2pr,fp}_{l_1,l_2}(m_1,m_2,m_3)$ is the set of configurations obtained from a configuration in $\mathcal{R}^{2pr}_{l_1,l_2}$ (m_1,m_2,m_3) by adding a free particle. Similarly for $\mathcal{D}^{2pr,fp}_{l_1,l_2}(m_1,m_2,m_3)$ and $\mathcal{D}^{2pr}_{l_1,l_2}(m_1,$ $m_2,m_3)$.
- $\mathcal{R}^{spr}_{l_1,l_2}(m_1,m_2,m_3)$ is the set of configurations obtained from a configuration in $\mathcal{R}^{2pr,fp}_{l_1,l_2}$ (m_1,m_2,m_3) by attaching the free particle to an *external corner* of the contour in $\mathcal{R}^{2pr,fp}_{l_1,l_2}(m_1,m_2,m_3)$ (i.e., an empty site with three nearest-neighbor particles), giving rise to a "stable protuberance" of two nearest-neighbor particles attached to one of the sides of the rectangle that is attached to one of the faces of the parallelepiped.

9. A particularly important set of configurations, which play the role of "critical configurations" in the regime $\Delta \in (2U, 3U)$, is given by

$$\mathcal{C}^* = \mathcal{D}^{2pr,fp}_{l_c-1,l_c}(m_c - 1, m_c - \delta_c, m_c) \tag{1.45}$$

with l_c defined in (1.25), m_c defined in (1.21), and

$$\delta_c = \begin{cases} 1 & \text{if } \lceil \frac{2U}{\epsilon} \rceil - \frac{2U}{\epsilon} > \frac{1}{2} + \frac{1}{2}\left\{\sqrt{(\frac{2U}{\epsilon})^2 + 1} - \frac{2U}{\epsilon}\right\}, \\ 0 & \text{otherwise,} \end{cases} \tag{1.46}$$

where $\epsilon = 3U - \Delta$ as in (1.26). The δ_c comes from a fine tuning: depending on the round off error for m_c, either the oblate quasi-cube $P(m_c-1, m_c-1, m_c)$ or the prolate quasi-cube $P(m_c-1, m_c, m_c)$ has the lowest energy (recall (1.29)). By definition, $\mathcal{C}^* \subseteq \mathcal{V}_{n^*}$ with

$$n^* = m_c(m_c - \delta_c)(m_c - 1) + l_c(l_c - 1) + 2. \tag{1.47}$$

We denote by $\Gamma = \Gamma(U, \Delta)$ the energy of the critical configurations:

$$\begin{aligned} \Gamma = H(\mathcal{C}^*) \quad &= \quad -\epsilon[m_c(m_c - \delta_c)(m_c - 1) + l_c(l_c - 1) + 2] \\ &\quad + U[m_c(m_c - \delta_c) + m_c(m_c - 1) + (m_c - \delta_c)(m_c - 1) + 2l_c + 3] \end{aligned} \tag{1.48}$$

(recall (1.29) and see Fig. 4).

We will see in Proposition 2.13 that

$$\Gamma = \Phi(\square, \blacksquare), \tag{1.49}$$

where

$$\square = \{\eta \in \mathcal{X} \colon \eta(x) = 0 \ \forall x \in \Lambda\} \tag{1.50}$$

is the single configuration with Λ empty and

$$\blacksquare = \{\eta \in \mathcal{X}\colon\ \eta(x) = 1\ \forall x \in \Lambda_-\} \tag{1.51}$$

is the set of configurations with Λ_- full.

We note that $H(\square) = 0$ and that $\blacksquare \ni \mathcal{F}(\mathcal{X})$ (for Λ sufficiently large), where $\mathcal{F}(\mathcal{X})$ is the single configuration with Λ_- full and $\partial\Lambda_-$ empty (recall (1.34)). We further note that $\mathcal{S}(\square, \mathcal{F}(\mathcal{X})) = \mathcal{S}(\square, \blacksquare)$ (recall (1.39)) and that, for any $\eta' \in \blacksquare$, $\mathcal{W}$ is a gate (minimal gate) for $\square \to \eta'$ if and only if it is a gate (minimal gate) for $\square \to \mathcal{F}(\mathcal{X})$. Consequently, $\mathcal{G}(\square, \mathcal{F}(\mathcal{X})) = \mathcal{G}(\square, \blacksquare)$ (recall (1.42)).

Equations (1.48–1.49) imply that $\mathcal{C}^*$ is a set of minimal saddle configurations:

$$\mathcal{S}(\square, \blacksquare) \supseteq \mathcal{C}^*. \tag{1.52}$$

FIG. 4. A critical configuration with $m_c = 20$, $l_c = 10$ and $\delta_c = 0$.

10. In Proposition 2.86 we will see that $\mathcal{C}^*$ is a gate for the transition $\square \to \blacksquare$. We expect that

$$\mathcal{C}^* \supseteq \mathcal{G}(\square, \blacksquare), \tag{1.53}$$

but we are unable to prove this.

1.6 Main theorems: Theorems 1.55 and 1.58

For $\eta \in \mathcal{X}$, let $\mathbb{P}_\eta$ denote the law of $(\eta_t)_{t\in\mathbb{N}_0}$ given $\eta_0 = \eta$. Recall from (1.33) that $\tau_\square, \tau_\blacksquare$ are the first hitting times of $\square, \blacksquare$. Let

$$\begin{aligned} \theta_{\square,\blacksquare} &= \max\{0 \le t < \tau_\blacksquare\colon\ \eta_t \in \square\}, \\ \tau_{\square,\mathcal{C}^*,\blacksquare} &= \min\{t > \theta_{\square,\blacksquare}\colon\ \eta_t \in \mathcal{C}^*\}, \end{aligned} \tag{1.54}$$

be the last hitting time of $\square$ prior to the first hitting time of $\blacksquare$ respectively the first hitting time of $\mathcal{C}^*$ afterwards. Our main theorems read as follows.

Theorem 1.55 *Fix $\Delta \in (2U, 3U)$ such that $2U/(3U-\Delta)$ is not integer, and let Λ be sufficiently large.*
(a) Let Γ be the communication height between $\square$ and $\blacksquare$ defined in (1.48)*. Then*

$$\lim_{\beta\to\infty} \mathbb{P}_{\square}\Big(e^{(\Gamma-\delta)\beta} < \tau_{\blacksquare} < e^{(\Gamma+\delta)\beta}\Big) = 1 \qquad \forall \delta > 0. \tag{1.56}$$

(b) Let $\mathcal{C}^*$ be the set of critical configurations defined in (1.45)*. Then $\mathcal{C}^*$ is a gate for the transition $\square \to \blacksquare$, and*

$$\lim_{\beta\to\infty} \mathbb{P}_{\square}(\tau_{\square,\mathcal{C}^*,\blacksquare} < \tau_{\blacksquare}) = 1. \tag{1.57}$$

Theorem 1.58 *Fix $\Delta \in (2U, 3U)$ such that $2U/(3U-\Delta)$ is not integer, and let Λ be sufficiently large. Let $\mathcal{Q}$ be the set of configurations whose single contour is a quasi-cube. Then, for all $\eta \in \mathcal{Q}$,*

$$\begin{aligned} \eta \subseteq P(m_c-1, m_c-\delta_c, m_c) \quad &\Longrightarrow \quad \lim_{\beta\to\infty} \mathbb{P}_\eta(\tau_{\square} < \tau_{\blacksquare}) = 1, \\ \eta \supsetneq P(m_c-1, m_c-\delta_c, m_c) \quad &\Longrightarrow \quad \lim_{\beta\to\infty} \mathbb{P}_\eta(\tau_{\blacksquare} < \tau_{\square}) = 1. \end{aligned} \tag{1.59}$$

In words, Theorems 1.55 and 1.58 say the following:

- Theorem 1.55(a): The nucleation time from $\square$ to $\blacksquare$ is $e^{[\Gamma+o(1)]\beta}$.
- Theorem 1.55(b): The set $\mathcal{C}^*$ is a gate for the nucleation: all paths from the metastable state $\square$ to the stable state $\blacksquare$ pass through this set with a probability tending to 1 as $\beta \to \infty$.
- Theorem 1.58: Subcritical quasi-cubes shrink to $\square$, supercritical quasi-cubes grow to $\blacksquare$.

Incidentally, it follows from (1.48) that $\Gamma \sim 4U^3/\epsilon^2$ as $\epsilon \downarrow 0$, which identifies the nucleation time in the limit of weak supersaturation.

The subregime $\Delta \in (U, 2U)$, corresponding to $m_c = 2$ and $l_c = 1$, needs to be treated separately. Theorems 1.55 and 1.58 do carry over, but we must modify the definition of $\mathcal{C}^*$ in (1.45), namely,

$$\begin{aligned} \mathcal{C}^* = \Big\{\eta' \in \mathcal{V}_n\colon\ \exists \eta \in \mathcal{P}^{1pr}(1, 2-\delta_c, 2)\colon& \\ \Phi_{\mathcal{V}_n}(\eta,\eta') \le H(\eta) + U,\ H(\eta) = H(\eta')\Big\}^{fp}& \end{aligned} \tag{1.60}$$

with $n = 2(2-\delta_c)+1$. The analogue of Fig. 4 is a $2 \times (2-\delta_c)$ quasi-square with a particle attached to it anywhere plus a free particle. The difference with (1.45) is that now U is the largest multiple of U below Δ, so that only moves with a maximal energy cost U must be taken into account, because only these moves may occur before the arrival of the next free particle.

1.7 Open problems

Theorems 1.55 and 1.58 give rise to a number of open problems:

1. Give a complete geometric description of the set $\mathcal{C}^*$. In Sections 4.1–4.2 we study the motion of particles along the border of the droplet starting from a configuration in $\mathcal{R}^{2pr}_{l_c-1,l_c}(m_c-1, m_c-\delta_c, m_c)$. This border motion shows that $\mathcal{C}^*$ is rather complex. We conjecture that (1.53) holds and that the inclusions in (1.52–1.53) are strict. In particular, we conjecture that all configurations where the quasi-square is attached to the "wrong" face of the quasi-cube (i.e., to the smallest face) are dead-ends in $\mathcal{C}^*$. In Proposition 4.3 we show that all configurations in $\mathcal{C}^*$ have the same circumscribing parallelepiped as the configurations in $\mathcal{R}^{2pr,fp}_{l_c-1,l_c}(m_c-1, m_c-\delta_c, m_c)$ when we ignore the free particle.

2. Identify which configurations return to $\square$ ("subcritical configurations") and which to $\blacksquare$ ("supercritical configurations"). Theorem 1.58 gives a partial answer, namely, for quasi-cubes. We will see in Proposition 2.47 that, starting from any configuration in $\mathcal{X}\setminus\{\square,\blacksquare\}$, the dynamics returns to $\{\square,\blacksquare\}$ in a time much shorter than the nucleation time (see also (3.18)).

3. Describe the typical nucleation path. Some discussion of the subcritical part is provided in Section 4.3. The description of the supercritical part remains open.

4. Give corrections to the asymptotics of the nucleation time for finite β. Bovier and Manzo [3] provide such a refinement for Glauber dynamics, leading to an estimate of the expected nucleation time up to and including order 1. This refinement depends on good control of the geometry of the critical droplet.

5. Show that the same results apply when the creation and annihilation of particles at the boundary of Λ occurs from an infinite gas reservoir surrounding Λ rather than from a boundary mimicking this reservoir. This issue was settled in den Hollander, Olivieri and Scoppola [5] for the two-dimensional version of the model (for the case where outside Λ particles do not interact). The proof relies on delicate coupling arguments, but probably carries over because it is largely independent of dimension.

2 Preparations

This section contains preparations for the proof of Theorems 1.55 and 1.58 in Section 3. The main ingredients that are needed are:

- Theorem 1.55(a): The proof requires

  (1) the construction of a particular path $\omega^K \in (\square \to \blacksquare)_{opt}$, called the reference path;

  (2) the evaluation of the communication height $\Phi(\square,\blacksquare)$, which is the maximal energy attained by ω^K ;

  (3) a recurrence property of Kawasaki dynamics to $\{\square,\blacksquare\}$ in a time exponentially shorter than $e^{\Gamma\beta}$.

  With these three items:

  (i) The upper bound on the nucleation time relies on the construction of a suitable nucleation event that exploits items (1) and (3) (see the proof of Proposition 3.1). Starting from any configuration, the dynamics quickly reaches the set $\{\square,\blacksquare\}$. From there, if not already in $\blacksquare$, it crosses $\mathcal{S}(\square,\blacksquare)\cap\omega^K$ in a time of order $e^{\Gamma\beta}$ and afterwards moves towards $\blacksquare$ without reaching again the energy $\Phi(\square,\blacksquare)$.

(ii) The lower bound on the nucleation time follows by using an argument based on reversibility that exploits item (2) (see the proof of Proposition 3.27). The probability of a path from $\square$ to any configuration in the global minimal saddle $\mathcal{S}(\square, \blacksquare)$ equals $e^{-\beta\Gamma}$ times the probability of the reversed path. The latter is of order 1.

Items (1), (2) and (3) are the subject of Sections 2.2, 2.3 and 2.4 respectively. Here, a key role is played by the isoperimetric inequalities obtained by Alonso and Cerf [1], which are summarized in Section 2.1.

- Theorem 1.58: The proof requires information on the local minimal saddles between quasi-squares and $\square$ or $\blacksquare$, which are obtained in Section 2.3 (see Proposition 2.19). For this purpose we use a very strong property of the reference path ω^K, namely, not only is it optimal for the transition $\square \to \blacksquare$, it is *self-minimax*. The latter means that any segment $(\omega_i^K, \omega_{i+1}^K, \ldots, \omega_{j-1}^K, \omega_j^K)$ with $i < j$ belongs to $(\omega_i^K \to \omega_j^K)_{opt}$, i.e., contains a minimal saddle between its extremes and never overshoots $\Phi(\omega_i^K, \omega_j^K)$ (see Proposition 2.8).
- Theorem 1.55(b): The proof is based on a focalization property (see the introduction) that is worked out in Section 2.5 (see Proposition 2.75).

2.1 Discrete isoperimetric inequalities

We recall some definitions and results from Alonso and Cerf [1].

Definition 2.1 (Alonso and Cerf [1], Section 3)
(a) A minimal polyomino is a configuration whose single contour has minimal surface among all those with the same volume.
(b) A principal polyomino is a configuration whose single contour is a quasi-cube with a quasi-square attached to one face of the quasi-cube and with a bar attached to one side of the quasi-square.
(c) A standard polyomino is a principal polyomino whose quasi-square is attached to one of the largest faces of the quasi-cube and whose bar is attached to one of the largest sides of the quasi-square.

Proposition 2.2 (Alonso and Cerf [1], Proposition 3.2)
For each $n \in \mathbb{N}$ there exists a unique 6-tuple $(m, l, k, \delta, \theta, \alpha)$ such that:
(i) $m, l, k \in \mathbb{N}_0$, $\delta, \theta, \alpha \in \{0, 1\}$,
(ii) if $m = 0$ then $\delta = \theta = 0$, if $l = 0$ then $\alpha = k = 0$,
(iii) $\delta \leq \theta$, $k < l + \alpha$, $l(l + \alpha) + k < (m + \delta)(m + \theta)$, and

$$n = m(m + \delta)(m + \theta) + l(l + \alpha) + k. \tag{2.3}$$

Because of Proposition 2.2, it is natural to associate with each $n \in \mathbb{N}$ a principal polyomino whose quasi-cube has side lengths $m, m + \delta, m + \theta$, whose quasi-square has side lengths $l, l + \alpha$, and whose bar has length k.

The following discrete isoperimetric inequality is a key ingredient in our analysis.

Theorem 2.4 (Alonso and Cerf [1], Theorems 3.1.and 3.6)
(a) All principal polyominoes are minimal polyominoes.
(b) The set of minimal polyominoes of volume n coincides with the set of principal polyminoes of volume n if and only if n is of the form "quasi-cube + quasi-square" or "quasi-cube -1".

Item (a) of Proposition 2.4 was in fact already proved by Neves [8]. In Alonso and Cerf [1], Conjectures 3.8 and 3.10, it is suggested what the minimal polyominoes should look like for other values of n.

Throughout the sequel, all polyominoes are collected in equivalence classes modulo trivial transformations, like translations and rotations of the full polyomino or, possibly, of suitable parts of it.

As will become clear in what follows, to determine the asymptotic behavior of the nucleation time (Theorem 1.55(a)) we will only need Theorem 2.4(a), whereas to obtain the gate for the nucleation (Theorem 1.55(b)) we will need both Theorem 2.4(a) and 2.4(b). The latter guarantees a suitable focalization property of optimal paths, based on the uniqueness (modulo translations and rotations) of the minimal polyominoes corresponding to particular values of the number of particles.

2.2 Reference path

We next construct a particular optimal nucleation path ω^K, i.e., an element of $(\square \to \blacksquare)_{opt}$. This path, which we call *reference path for the Kawasaki dynamics*, goes from $\square$ to $\blacksquare$ through a particular sequence of growing standard polyominoes.

To define ω^K, we first define the analogous *reference path for the Glauber dynamics*, which we denote by $\omega^G = \{\omega_n^G\}$ with $n = 0, \dots, |\Lambda_-|$, namely,

$$\omega_0^G = \square, \omega_1^G = \{x_0\}, \dots, \omega_{|\Lambda_-|}^G = \mathcal{F}(\mathcal{X}) \in \blacksquare, \tag{2.5}$$

where x_0 is any site in Λ_- and $\{\omega_n^G\}$ is a growing sequence of standard polyominoes, with $|\omega_n^G| = n$, such that $P^G(\omega_n^G, \omega_{n+1}^G) > 0$ and $\omega_n^G \subseteq \Lambda_-$ for all n. The parallelepiped circumscribing ω_n^G always is a quasi-cube, while the rectangle circumscribing the two-dimensional droplet attached to a face of the quasi-cube always is a quasi-square. The order of the directions of growth of the standard polyominoes may be picked arbitrarily and may depend on the starting point x_0, but it is fixed.

Given a choice for ω^G, we can construct the path $\omega^K = (\omega_{n,i}^K)$ as follows:

$$\omega_{n,0}^K = \omega_n^G, \quad n = 0, \dots, |\Lambda_-|, \tag{2.6}$$

and insert between each pair $(\omega_n^G, \omega_{n+1}^G)$, $n = 0, \dots, |\Lambda_-| - 1$, a sequence of configurations $\omega_{n,i}^K$, $i = 0, 1, \dots, i_n$, belonging to $(\omega_n^G)^{fp}$, that creates a particle at $\partial^-\Lambda$ and brings it to the droplet, i.e.,

$$\omega_{n,i}^K = \omega_n^G \cup x_i^{(n)} \tag{2.7}$$

with $x_1^{(n)}, \dots, x_{i_n}^{(n)}$ nearest-neighbor sites from $\partial^-\Lambda$ to $\omega_{n+1}^G \backslash \omega_n^G$. We obviously have $|\omega_{n,i}^K| = n + 1 - \delta_{i,0}$, where $\delta_{i,0}$ is the Kronecker symbol. For shortness, we replace the index n, i with a single index $s = s(n,i)$, i.e., $\omega_{n,i}^K = \omega_{s(n,i)}^K$.

Proposition 2.8 *$\omega^K \in (\square \to \blacksquare)_{opt}$. Moreover, ω^K self-minimax, i.e., for any $0 \le s_1 < s_2$,*

$$\Phi(\omega_{s_1}^K, \omega_{s_2}^K) = \max_{s \in [s_1, s_2]} H(\omega_s^K), \tag{2.9}$$

and realizes the minimal saddles between any pair of manifolds, i.e., for any $0 \le n_1 < n_2 \le |\Lambda_-|$,

$$\Phi(\mathcal{V}_{n_1}, \mathcal{V}_{n_2}) = \max_{s \in [s(n_1,0), s(n_2,0)]} H(\omega_s^K). \tag{2.10}$$

Proof. By definition, we have

$$\Phi(\square,\blacksquare) \le \max_s H(\omega_s^K) = H(\omega_{s_0}^K), \tag{2.11}$$

where $s_0 = \min\{s\colon H(\omega_s^K) \ge H(\omega_{s'}^K)\,\forall s'\}$. Since $\omega_{s_0}^K$ is either a standard polyomino or a standard polyomino plus a free particle, we have $H(\omega_{s_0}^K) = H(\omega_{s_0-1}^K) + \Delta$.

Let $n_0 = |\omega_{s_0}^K|$. Since any path $\omega\colon\square \to \blacksquare$ has to cross the n_0-manifold $\mathcal{V}_{n_0}$ for a first time, we have

$$\Phi(\square,\blacksquare) \ge \min_{\eta\in\mathcal{V}_{n_0-1}} H(\eta) + \Delta = H(\omega_{s_0-1}^K) + \Delta = H(\omega_{s_0}^K). \tag{2.12}$$

Indeed, the first equality follows from the fact that $\omega_{s_0-1}^K$ is a standard polyomino, so that, by Theorem 2.4(a), it is a configuration of minimal energy in $\mathcal{V}_{n_0-1}$. Combining (2.11–2.12), we get $\Phi(\square,\blacksquare) = H(\omega_{s_0}^K)$, proving that $\omega^K \in (\square \to \blacksquare)_{opt}$.

With the same argument we prove (2.9) and (2.10). ♡

2.3 Height of global minimal saddle and of local minimal saddles between quasi-cubes and empty or full configurations

According to Proposition 2.8, to evaluate the height of the global minimal saddle between $\square$ and $\blacksquare$ it suffices to determine the maximal energy reached by the reference path ω^K. By construction, this is the maximal energy of a standard polyomino plus Δ.

Proposition 2.13 $\Phi(\square,\blacksquare) = \Gamma$, *where* Γ *is given by (1.48).*

Proof. By an abuse of notation, we denote by $H(n)$ the energy of a standard polyomino of volume n. Let $n = m(m+\delta)(m+\theta)+l(l+\alpha)+k$ (recall from Proposition 2.2 that $m,l,k,\delta,\theta,\alpha$ are uniquely determined by n). We have

$$H(n) = H_3(m, m+\delta, m+\theta) + H_2(l, l+\alpha) + H_1(k), \tag{2.14}$$

where (recall (1.29))

$$\begin{aligned}
H_3(m,m+\delta,m+\theta) &= -\epsilon m(m+\delta)(m+\theta) \\
&\quad +U[m(m+\delta)+m(m+\theta)+(m+\delta)(m+\theta)], \\
H_2(l,l+\alpha) &= -\epsilon l(l+\alpha) + U(2l+\alpha), \\
H_1(k) &= \begin{cases} -\epsilon k + U & \text{if } k>0, \\ 0 & \text{if } k=0. \end{cases}
\end{aligned} \tag{2.15}$$

By Proposition 2.8, we have

$$\Phi(\square,\blacksquare) = \max_s H(\omega_s^K) = \max_{0\le n\le|\Lambda_-|} H(n) + \Delta. \tag{2.16}$$

Since

$$\max_{0\le n\le|\Lambda_-|} H(n) = \max_{m,\delta,\theta} H_3(m,m+\delta,m+\theta) + \max_{l,\alpha} H_2(l,l+\alpha) + \max_k H_1(k), \tag{2.17}$$

we have, by a direct computation based on (2.15),

$$\Phi(\square,\blacksquare) = H_3(m_c-1, m_c-\delta_c, m_c) + H_2(l_c-1,l_c) + H_1(1) + \Delta = \Gamma \tag{2.18}$$

with δ_c given in (1.46). ♡

Similarly, we can compare the local minimal saddles between quasi-cubes and $\square$ or $\blacksquare$.

Proposition 2.19 *For any configuration η that is a quasi-cube, i.e., $\eta = P(m, m+\delta, m+\theta)$ for some m, δ, θ, the following inequalities hold:*
(a) If $\eta \subseteq P(m_c - 1, m_c - \delta_c, m_c)$, then η is subcritical, in the sense that

$$\Phi(\eta, \square) < \Phi(\eta, \blacksquare) = \Gamma. \tag{2.20}$$

(b) If $\eta \supsetneq P(m_c - 1, m_c - \delta_c, m_c)$, then η is supercritical, in the sense that

$$\Phi(\eta, \blacksquare) < \Phi(\eta, \square) = \Gamma. \tag{2.21}$$

Proof. By using the fact that ω^K is self-minimax (recall (2.9)), we immediately have

$$\Phi(\eta, \square) = \max_{s < s(\eta)} H(\omega_s^K), \qquad \Phi(\eta, \blacksquare) = \max_{s > s(\eta)} H(\omega_s^K), \tag{2.22}$$

where $s(\eta)$ is the time s at which $\omega_s^K = \eta$ (modulo translations and rotations). Let $s_0 = \min\{s \colon H(\omega_s^K) = \Gamma\}$ and note that ω_{s_0} has a free particle. If $\eta \subseteq P(m_c - 1, m_c - \delta_c, m_c)$, then $s(\eta) < s_0$, so that $\Phi(\eta, \blacksquare) = \Gamma$. Moreover, in this case

$$\Phi(\eta, \square) = \max_{s < s(\eta)} H(\omega_s^K) \leq H(\eta_-) + H_2(l_c - 1, l_c) + H_1(1) + \Delta < \Gamma, \tag{2.23}$$

where η_- is the maximal quasi-cube strictly contained in η. If, on the other hand, $\eta \supsetneq P(m_c - 1, m_c - \delta_c, m_c)$, then $s(\eta) > s_0$, so that $\Phi(\eta, \square) = \Gamma$. Moreover, in this case

$$\Phi(\eta, \blacksquare) = \max_{s > s(\eta)} H(\omega_s^K) \leq H(\eta) + H_2(l_c - 1, l_c) + H_1(1) + \Delta < \Gamma. \tag{2.24}$$

The strict inequalities in (2.23–2.24) are immediate from (2.18), because the first maximum in the right-hand side of (2.17) is uniquely attained at $H_3(m_c, m_c - \delta_c, m_c - 1)$. ♡

2.4 Reduction and recurrence

In Section 2.4.1 we introduce (maximal) cycles and paths along (maximal) cycles. In Section 2.4.2 we prove a recurrence result for general sets of configurations with a certain irreducibility property. In Section 2.4.3 we use this result to prove that recurrence to $\{\square, \blacksquare\}$ occurs in a time that is exponentially shorter than $e^{\Gamma\beta}$. The latter proof is somewhat involved, because it requires showing among others that Kawasaki dynamics does not want to create configurations with internal holes.

2.4.1 Cycles and cycle-paths

Definition 2.25 *A connected set $\mathcal{C}$ satisfying (recall (1.32))*

$$\max_{\eta \in \mathcal{C}} H(\eta) < \min_{\zeta \in \partial\mathcal{C}} H(\zeta) = H(\mathcal{F}(\partial\mathcal{C})) \tag{2.26}$$

is called a non-trivial cycle. Any set that is either a singleton $\{\eta\}$ or a non-trivial cycle is called a cycle.

1. It is easily seen that cycles are partially ordered by inclusion: given two cycles $\mathcal{C}_1, \mathcal{C}_2$ with $\mathcal{C}_1 \cap \mathcal{C}_2 \neq \emptyset$, either $\mathcal{C}_1 \subseteq \mathcal{C}_2$ or $\mathcal{C}_2 \subseteq \mathcal{C}_1$. The cycles containing a given $\eta \in \mathcal{X}$ are therefore totally ordered by inclusion. Note that a singleton $\{\eta\}$ can be a non-trivial cycle only when it is a local minimum of H.

2. For a non-trivial cycle $\mathcal{C}$, let

$$\bar{H}(\mathcal{C}) = H(\mathcal{F}(\partial\mathcal{C})), \qquad \Gamma(\mathcal{C}) = \bar{H}(\mathcal{C}) - H(\mathcal{F}(\mathcal{C})), \tag{2.27}$$

be the energy at the bottom of $\partial\mathcal{C}$ respectively the energy gap between the bottoms of $\partial\mathcal{C}$ and $\mathcal{C}$. For a trivial cycle $\{\eta\}$, put $\bar{H}(\{\eta\}) = H(\eta)$, $\Gamma(\{\eta\}) = 0$. For $\eta \in \mathcal{X}$, let

$$v(\eta) = \Phi(\eta, \mathcal{I}_\eta) - H(\eta) \quad \text{with} \quad \mathcal{I}_\eta = \{\zeta \in \mathcal{X}\colon H(\zeta) < H(\eta)\} \tag{2.28}$$

be the energy cost to move from η to a configuration with lower energy. It is easily seen that

$$v(\eta) = \Gamma(\mathcal{C}(\eta)), \tag{2.29}$$

where $\mathcal{C}(\eta)$ is the largest cycle containing η such that $\eta \in \mathcal{F}(\mathcal{C}(\eta))$. If η is not a local minimum of H, then $\mathcal{C}(\eta) = \eta$.

3. Given $V \geq 0$, define the set $\mathcal{X}_V$ of *V-irreducible configurations* as

$$\mathcal{X}_V = \{\eta \in \mathcal{X}\colon v(\eta) > V\}. \tag{2.30}$$

The complement $\mathcal{X} \setminus \mathcal{X}_V$ is the set of *V-reducible configurations.* A crucial step in what follows is the partition of $\mathcal{X} \setminus \mathcal{X}_V$ into maximal (by inclusion) cycles:

$$\mathcal{X} \setminus \mathcal{X}_V = \mathcal{C}_1 \cup \mathcal{C}_2 \cup \ldots \cup \mathcal{C}_n, \quad n \in \mathbb{N}. \tag{2.31}$$

It is obvious that

$$\Gamma(\mathcal{C}_i) \leq V \qquad \forall i = 1, \ldots, n. \tag{2.32}$$

Indeed, if $\Gamma(\mathcal{C}_i) > V$, then $v(\eta) > V$ for all $\eta \in \mathcal{F}(\mathcal{C}_i)$, contradicting $\eta \in \mathcal{X} \setminus \mathcal{X}_V$.

4. A *maximal-cycle-path* (mc-path) is a sequence $(\mathcal{C}'_1, \ldots \mathcal{C}'_k)$ with $\mathcal{C}'_j \in \{\mathcal{C}_1, \ldots, \mathcal{C}_n\}$ for $j = 1, \ldots, k$ and with $\mathcal{C}'_j$ connected to $\mathcal{C}'_{j+1}$ through a single transition for $j = 1, \ldots, k-1$. Note that, for Kawasaki dynamics, if a non-trivial cycle appears in an mc-path, then both the subsequent and the previous element in the mc-path must be a trivial cycle in its boundary. An mc-path $(\mathcal{C}'_1, \ldots \mathcal{C}'_k)$ is called *downhill* if $\bar{H}(\mathcal{C}'_{j+1}) \leq \bar{H}(\mathcal{C}'_j)$ for $j = 1, \ldots, k-1$. A collection of cycles is called *mc-connected* if for any pair of cycles in the collection there is an mc-path in the collection joining them.

For any $\hat{\mathcal{C}} \in \{\mathcal{C}_1, \ldots, \mathcal{C}_n\}$, we denote by $Q(\hat{\mathcal{C}})$ the maximal (by inclusion) mc-connected set of cycles $\{\mathcal{C}'_1, \ldots \mathcal{C}'_k\} \subseteq \{\mathcal{C}_1, \ldots, \mathcal{C}_n\}$ such that $\bar{H}(\mathcal{C}'_j) = \bar{H}(\hat{\mathcal{C}})$ for $j = 1, \ldots, k$. The reader should think of $Q(\hat{\mathcal{C}})$ as a maximal set of "communicating lakes": $Q(\hat{\mathcal{C}})$ is a disjoint union of maximal cycles $\mathcal{C}'_j$, connected through single transitions, that all have the same value of $\bar{H}(\mathcal{C}'_j)$.

2.4.2 General recurrence result

Let $T_V = e^{V\beta}$, and

$$\tau_{\mathcal{X}_V} = \min\{t \in \mathbb{N}_0\colon \eta_t \in \mathcal{X}_V\}. \tag{2.33}$$

Call $\beta \to f(\beta)$ superexponentially small (SES) if $\lim_{\beta\to\infty} \frac{1}{\beta} \log f(\beta) = -\infty$.

Proposition 2.34 ("$\mathcal{X}_V$-recurrence") *For every $\delta > 0$,*

$$\max_{\eta \in \mathcal{X} \setminus \mathcal{X}_V} P_\eta(\tau_{\mathcal{X}_V} > T_V e^{\delta\beta}) = \text{SES}. \tag{2.35}$$

Proof. The proof uses the partition in (2.31).

1. We will show that for all $\eta \in \mathcal{X} \setminus \mathcal{X}_V$ there is an event $\mathbf{E}_\eta^T \subseteq \mathcal{X}^{[0,T]\cap\mathbb{N}_0}$ with $T = T_V e^{\frac{\delta}{2}\beta}$ such that

$$\mathbf{E}_\eta^T \subseteq \{\eta_0 = \eta,\ \exists t \in [0,T] \cap \mathbb{N}_0 \colon \eta_t \in \mathcal{X}_V\} \tag{2.36}$$

and such that, for β sufficiently large,

$$\min_{\eta \in \mathcal{X}} P(\mathbf{E}_\eta^T) \geq e^{-\delta'\beta}, \qquad 0 < \delta' < \frac{\delta}{2}. \tag{2.37}$$

Proposition 2.34 follows from (2.36–2.37) because, by the Markov property,

$$\max_{\eta \in \mathcal{X} \setminus \mathcal{X}_V} P_\eta(\tau_{\mathcal{X}_V} > T_V e^{\delta\beta}) \leq (1 - e^{-\delta'\beta})^{e^{\frac{\delta}{2}\beta}} = \text{SES}. \tag{2.38}$$

2. To prove (2.36–2.37), fix $\eta \in \mathcal{X} \setminus \mathcal{X}_V$. Let $\tilde{\mathcal{C}} = \tilde{\mathcal{C}}(\eta)$ be the maximal cycle in (2.31) containing η, and set $H_0 = \bar{H}(\tilde{\mathcal{C}})$, $Q = Q(\tilde{\mathcal{C}})$. We will prove the following:

Claim 2.39 *Q is downhill connected (via a single transition) either to $\mathcal{X}_V$ or to some maximal cycle $\hat{\mathcal{C}}$ in* (2.31) *with $\bar{H}(\hat{\mathcal{C}}) < H_0$.*

Proof. The proof is by contradiction. Suppose that ∂Q neither contains configurations in $\mathcal{X}_V$ nor configurations in any $\hat{\mathcal{C}}$ in (2.31) with $\bar{H}(\hat{\mathcal{C}}) < H_0$. Now, there are no $\eta' \in \partial Q$ with $H(\eta') = H_0$, because of the maximality of Q. Moreover, ∂Q cannot be empty, otherwise the dynamics cannot escape from Q, which violates the ergodicity of the Markov chain because $Q \subseteq \mathcal{X} \backslash \mathcal{X}_V \subsetneq \mathcal{X}$. Thus, ∂Q is non-empty and only contains configurations η' with $H(\eta') > H_0$. Since $H(\eta') \leq H_0$ for all $\eta' \in Q$, we conclude that Q must be a cycle in $\mathcal{X} \backslash \mathcal{X}_V$ that strictly contains $\tilde{\mathcal{C}}$. But in this way we violate the maximality of $\tilde{\mathcal{C}}$ (a disjoint union of two or more cycles cannot be a cycle). We conclude that either Q is connected to $\mathcal{X}_V$ or to some $\hat{C}$ in (2.31) with $\bar{H}(\hat{\mathcal{C}}) < H_0$. ♡

3. We are now able to construct, for any maximal cycle $\tilde{\mathcal{C}}$ in (2.31), a downhill mc-path $(\mathcal{C}_1', \ldots, \mathcal{C}_k')$ beginning with $\mathcal{C}_1' = \tilde{\mathcal{C}}$ and ending in $\mathcal{X}_V$, in the sense that $\partial \mathcal{C}_k' \cap \mathcal{X}_V \neq \emptyset$. Indeed, by Claim 2.39, either we follow a suitable mc-path $(\mathcal{C}_1', \ldots, \mathcal{C}_k')$ in Q with constant height $\bar{H}(\mathcal{C}_i') = H_0$ and then step downhill and directly end in $\mathcal{X}_V$, or we have $\bar{H}(\mathcal{C}_k') < H_0$, in which case we can exploit the arbitrariness of the initial maximal cycle $\tilde{\mathcal{C}}$ to iterate the procedure. Since the energy is bounded from below, the iteration must eventually produce a downhill mc-path completed with a step downhill ending in $\mathcal{X}_V$.

4. Consider the completed downhill mc-path $(\tilde{\mathcal{C}}(\eta), \ldots, \mathcal{C}_k', \xi)$ with $\xi \in \partial \mathcal{C}_k' \cap \mathcal{X}_V$. We say that $(\eta_t)_{t\in\mathbb{N}_0}$ *follows* $(\mathcal{C}_1', \ldots, \mathcal{C}_k', \xi)$ *ϵ-regularly* if it visits these maximal cycles in the prescribed order, runs through all configurations in them, stays in each $\mathcal{C}_i'$ for a time at most $e^{[\Gamma(\mathcal{C}_i')+\epsilon]\beta}$, and ends up in ξ.

Claim 2.40 *For every $\delta, \epsilon > 0$ there exists $\beta_0 = \beta_0(\delta, \epsilon) > 0$ such that*

$$\min_{\eta \in \mathcal{X} \setminus \mathcal{X}_V} P_\eta\Big((\eta_t)_{t\in\mathbb{N}_0} \textit{ follows } (\tilde{\mathcal{C}}(\eta), \ldots, \mathcal{C}_k', \xi)\ \epsilon\textit{-regularly}\Big) \geq e^{-\delta\beta} \qquad \forall \beta > \beta_0. \tag{2.41}$$

Proof. This is an immediate consequence of the following result:

Proposition 2.42 (Olivieri and Scoppola [9], Proposition 3.7) *Let $\mathcal{C}$ be a non-trivial cycle.*
(a) For every $\delta > 0$ there exist $\kappa = \kappa(\delta) > 0$ and $\beta_0 = \beta_0(\delta) > 0$ such that

$$\min_{\eta \in \mathcal{C}} P_\eta\left(\tau_{\partial\mathcal{C}} < e^{\Gamma(\mathcal{C})\beta} e^{\delta\beta}\right) \geq 1 - e^{-\kappa\beta} \qquad \forall \beta > \beta_0. \tag{2.43}$$

(b) There exist $\delta_0 > 0$, $\kappa_0 > 0$ and $\beta_0 > 0$ such that

$$\min_{\eta,\eta' \in \mathcal{C}} P_\eta\left(\tau_{\eta'} < \tau_{\partial\mathcal{C}},\, \tau_{\eta'} < e^{\Gamma(\mathcal{C})\beta} e^{-\delta_0\beta}\right) \geq 1 - e^{-\kappa_0\beta} \qquad \forall \beta > \beta_0. \tag{2.44}$$

(c) For every $\delta > 0$ there exists $\beta_0 = \beta_0(\delta) > 0$ such that

$$\min_{\eta \in \mathcal{C}} P_\eta(\eta_{\tau_{\partial\mathcal{C}}} = \eta') \geq e^{-[H(\eta') - \bar{H}(\mathcal{C})]\beta} e^{-\delta\beta} \qquad \forall \eta' \in \partial\mathcal{C},\ \forall \beta > \beta_0. \tag{2.45}$$

Indeed, items (a) and (c) (for $\eta' \in \mathcal{F}(\partial\mathcal{C})$) guarantee that the dynamics starting from anywhere in $\mathcal{C}'_j$, $j = 1, \ldots, k$, reaches any configuration in $\partial\mathcal{C}'_j$ in a time of order $e^{[\Gamma(\mathcal{C}'_j)+\delta]\beta}$, while item (b) guarantees that all configurations in $\mathcal{C}'_j$ are hit beforehand with a probability $\geq e^{-\delta\beta}$. Pick $\epsilon < \delta$ to get (2.41). ♡

5. To prove (2.36), we pick $\eta \in \mathcal{X} \setminus \mathcal{X}_V$ and take for $\mathbf{E}^T_\eta$ the event where $(\eta_t)_{t\in\mathbb{N}_0}$ follows the downhill mc-path from $\tilde{\mathcal{C}}(\eta)$ to $\mathcal{X}_V$ $\frac{\delta}{4}$-regularly. Since the time needed to do so is at most

$$\sum_{j=1}^{k} e^{[\Gamma(\mathcal{C}'_j)+\frac{\delta}{4}]\beta} \leq |\mathcal{X} \setminus \mathcal{X}_V| e^{[V+\frac{\delta}{4}]\beta} \leq e^{[V+\frac{\delta}{2}]\beta} = T_V e^{\frac{\delta}{2}\beta} = T \qquad \forall \beta > \beta_0(\delta) \tag{2.46}$$

(recall 2.31–2.32)), (2.37) follows from Claim 2.40. ♡

2.4.3 Recurrence to empty or full configurations

The following proposition implies, with the help of Proposition 2.34, that from any configuration in $\mathcal{X}$ the Kawasaki dynamics hits $\square$ or $\blacksquare$ with an overwhelming probability in a time much less than the nucleation time.

Proposition 2.47 *There exists $\Gamma_0 < \Gamma$ such that $\mathcal{X}_{\Gamma_0} \subseteq \{\square, \blacksquare\}$.*

Proof. We will show that there exists $\Gamma_0 < \Gamma$ such that all $\eta \neq \square, \blacksquare$ are Γ_0-reducible (recall (2.30)), i.e.,

$$\forall \eta \neq \square, \blacksquare \;\; \exists \eta' \in \mathcal{X}: \quad H(\eta') < H(\eta),\ \Phi(\eta, \eta') \leq H(\eta) + \Gamma_0. \tag{2.48}$$

Suppose that $\eta \neq \square, \blacksquare$. Then

$$\exists\, x_0 \in \Lambda_-, y_0 \in \Lambda,\ |x_0 - y_0| = 1: \quad \eta(x_0) = 0, \eta(y_0) = 1. \tag{2.49}$$

If $y_0 \in \partial^-\Lambda$, then η is actually 0-reducible: it suffices to annihilate the particle at y_0 to decrease the energy. We may therefore assume that $y_0 \in \Lambda_-$ and $\Lambda_- \cap \eta = \emptyset$.

We will first give the proof pretending that the dynamics is Glauber, i.e., particles can be created and annihilated everywhere in Λ (see (1.13–1.14) for a precise definition). Afterwards we will show how the proof can be modified when the dynamics is Kawasaki.

I. Glauber:

1. Let ω^G be the reference path for the Glauber dynamics defined in Section 2.2. We have $|\omega_i^G| = i$ and, by Theorem 2.4(a),

$$\omega_i^G \in \mathcal{F}(\mathcal{V}_{|\omega_i^G|}) \qquad \forall i. \tag{2.50}$$

Define

$$\omega_i = \omega_i^G \cup \eta \quad \forall i, \qquad p = \inf\{i \geq 1\colon H(\omega_i^G) \leq 0\}. \tag{2.51}$$

We have $\omega_0^G = \square$, and without loss of generality we may pick $\omega_1^G = \{x_0\}$, with x_0 given by (2.49), and start growing from there.

2. For $1 \leq i \leq p$, write (recall (1.3))

$$H(\omega_i) - H(\eta) = \Big[H_{\Lambda_i}(\omega_i) + H_{\Lambda_i^c}(\omega_i) + W_{\Lambda_i,\Lambda_i^c}(\omega_i)\Big] - \Big[H_{\Lambda_i}(\eta) + H_{\Lambda_i^c}(\eta) + W_{\Lambda_i,\Lambda_i^c}(\eta)\Big], \tag{2.52}$$

where Λ_i is the support of ω_i^G, i.e., Λ_i =supp$\{x \in \Lambda\colon \omega_i^G(x) = 1\}$, $\Lambda_i^c = \Lambda \setminus \Lambda_i$, H_{Λ_i} is the Hamiltonian in (1.3) restricted to Λ_i, and

$$W_{\Lambda_i,\Lambda_i^c}(\eta) = -U \sum_{\substack{x\in\Lambda_i,\, y\in\Lambda_i^c \\ (x,y)\in\Lambda_-^*}} \eta(x)\eta(y) \tag{2.53}$$

is the interaction energy in η between Λ_i and Λ_i^c.

3. We have

$$\begin{aligned} &H_{\Lambda_i}(\omega_i) = H_{\Lambda_i}(\omega_i^G) = H(\omega_i^G),\\ &H_{\Lambda_i^c}(\omega_i) = H_{\Lambda_i^c}(\eta),\\ &W_{\Lambda_i,\Lambda_i^c}(\omega_i) \leq W_{\Lambda_i,\Lambda_i^c}(\eta), \end{aligned} \tag{2.54}$$

which hold, respectively, because ω_i and ω_i^G coincide on Λ_i, because ω_i and η coincide on Λ_i^c, because ω_i contains η. Substitution of (2.54) into (2.52) gives

$$H(\omega_i) - H(\eta) \leq H(\omega_i^G) - H_{\Lambda_i}(\eta). \tag{2.55}$$

Moreover,

$$H_{\Lambda_i}(\eta) > 0 \qquad \forall\, 1 \leq i \leq p. \tag{2.56}$$

Indeed, by (2.50) we have

$$H_{\Lambda_i}(\eta) \geq \min_{\xi\in\mathcal{V}_j} H_{\Lambda_i}(\xi) = H(\omega_j^G) \qquad \text{for } j = j(i) = |\Lambda_i \cap \eta|. \tag{2.57}$$

But $0 \leq j < p$ for $1 \leq i \leq p$, since in $\Lambda_i \cap \eta$ there is at least the empty site x_0. Since p is the smallest integer i with $H(\omega_i^G) \leq 0$, it follows that $H(\omega_j^G) > 0$. Thus, via (2.55) and (2.57),

$$H(\omega_i) - H(\eta) \leq H(\omega_i^G) - H(\omega_j^G) < H(\omega_i^G) \qquad \forall\, 1 \leq i \leq p. \tag{2.58}$$

Denoting by $\Phi^G(\eta,\eta')$ the communication height between η and η' for Glauber dynamics, we see that (2.58) in turn yields

$$\Phi^G(\eta,\omega_p) - H(\eta) \leq \max_{1\leq i\leq p} H(\omega_i) - H(\eta) < \max_{1\leq i\leq p} H(\omega_i^G) = \Gamma^G, \tag{2.59}$$

where Γ^G is the analogue of Γ for Glauber. Since $\omega_0 = \eta$ and $H(\omega_p^G) \le 0$, (2.58) gives

$$H(\omega_p) < H(\eta). \tag{2.60}$$

Equations (2.59–2.60) prove (2.48) with $\eta' = \omega_p$ and $\Gamma_0 < \Gamma^G$. ♡

II. Kawasaki:

We have to see how to modify the above argument when the dynamics is Kawasaki. The additional obstacle under Kawasaki is that, when we are growing the configuration by considering the union of η with the standard polyominoes Λ_i =supp(ω_i^G), as in (2.51), particles cannot be created arbitrarily but have to arrive from $\partial^-\Lambda$. We have to make sure that at any time the configuration is such that a particle coming from the boundary can be moved to where it is needed. This is achieved in Proposition 2.61 below.

To prove (2.48), we may restrict ourselves to $\eta \in \mathcal{X}_{3U}$. Otherwise, since $3U < \Gamma$ (see (1.48)), we can take $\Gamma_0 = 3U$ to get (2.48). Thus, we need to prove that any $\eta \in \mathcal{X}_{3U}$ has the property that when the union is taken with any monotone sequence of standard polyominoes, this union never contains closed off regions.

Proposition 2.61 *If $\eta \in \mathcal{X}_{3U}$, then, for any $0 \le i \le p$ (see (2.51)), every empty site x in the configuration $\omega_i = \omega_i^G \cup \eta$ is connected to $\partial^-\Lambda$ by a sequence $y_1(= x), \dots, y_n(\in \partial^-\Lambda)$ of nearest-neighbor empty sites.*

Proof. The proof is based on a number of technical lemmas. The key item is Claim 2.69 below.

1. We begin with some definitions (see Fig. 5):

(i) Given $x_0 \in \mathbb{R}^3$ and a lattice unit vector $e_1 \in \mathbb{R}^3$, let π_{e_1,x_0} be the plane orthogonal to e_1 and passing through x_0.

(ii) Given $x_0 \in \mathbb{Z}^3$ and a lattice unit vector $e_1 \in \mathbb{R}^3$, let P_{e_1,x_0} be the *slab of width 1* centered at π_{e_1,x_0}, i.e., the part of $\mathbb{R}^3$ lying between $\pi_{e_1,x_0-\frac{1}{2}e_1}$ and $\pi_{e_1,x_0+\frac{1}{2}e_1}$.

(iii) Given $x_0 \in \mathbb{Z}^3$ and two ordered mutually orthogonal lattice unit vectors $e_1, e_2 \in \mathbb{R}^3$, let L_{e_1,e_2,x_0} be the *pencil of width 1* centered at the line in the direction e_3 passing through x_0, i.e., the part of the slab P_{e_1,x_0} lying between $\pi_{e_2,x_0-\frac{1}{2}e_2}$ and $\pi_{e_2,x_0+\frac{1}{2}e_2}$.

(iv) Given $x_0 \in \mathbb{Z}^3$ and three ordered mutually orthogonal lattice unit vectors e_1, e_2, e_3, let $S_{e_1,x_0} \subseteq \mathbb{R}^3$ be that one of the two *halfspaces* $\mathbb{R}^3 \setminus P_{e_1,x_0}$ containing $x_0 + e_1$;
$S_{e_1,e_2,x_0} \subseteq P_{e_1,x_0}$ be that one of the two *halfslabs* $P_{e_1,x_0} \setminus \pi_{e_2,x_0+\frac{1}{2}e_2}$ containing $x_0 + e_2$;
$S_{e_1,e_2,e_3,x_0} \subseteq L_{e_1,e_2,x_0}$ be that one of the two *halfpencils* $L_{e_1,e_2,x_0} \setminus \pi_{e_3,x_0+\frac{1}{2}e_3}$ containing $x_0 + e_3$.

Fig. 5. Three pistons.

(v) The (external) *boundary* of a configuration η is

$$\partial^+\eta = \{x \notin \eta\colon nn(x) \cap \eta \neq \emptyset\}. \tag{2.62}$$

The subset of η^c that is connected to $\partial^-\Lambda$ by a sequence of empty nearest-neighbor sites $y_1, \dots, y_n$ is denoted by

$$(\eta^c)^{com} = \left\{x \in \eta^c\colon \exists\, y_1(=x), \dots, y_n(\in \partial^-\Lambda)\colon |y_j - y_{j+1}| = 1,\ y_j \in \eta^c\ \ \forall j\right\}, \tag{2.63}$$

and the subset η^c that cannot be connected to $\partial^-\Lambda$ by

$$(\eta^c)^{ncom} = \eta^c \setminus (\eta^c)^{com}. \tag{2.64}$$

For $B \subseteq \Lambda$, define:

(vi) $x \in B$ is a *B-corner* if at least 3 of its nearest-neighbor sites lie outside B, i.e., $|B^c \cap nn(x)| \geq 3$.

(vii) An *extremal corner of B* is a 4-tuple (e_1, e_2, e_3, x_0) with

1. x_0 is a B-corner;
2. e_1, e_2, e_3 are three ordered vectors such that

$$S_{e_1,x_0} \cap B = \emptyset, \qquad S_{e_1,e_2,x_0} \cap B = \emptyset, \qquad S_{e_1,e_2,e_3,x_0} \cap B = \emptyset. \tag{2.65}$$

(viii) $P(B)$ is the *parallelepiped circumscribing B*.

2. We next give some properties of the geometric objects defined above.

Lemma 2.66 *For all $B \subseteq \Lambda_-$, the number of extremal corners of B is 48.*

Proof. The extremal corners of B can be determined via any choice of the three ordered vectors e_1, e_2, e_3:

(1) Given e_1, we can find a sequence of slabs $P_{e_1,x_1}, \dots, P_{e_1,x_n}$, all orthogonal to e_1, by moving a piston from $\partial^-\Lambda$ in the direction opposite to e_1 one unit distance at a time, up to the first slab P_{e_1,x_n} such that $P_{e_1,x_n} \cap B \neq \emptyset$ (n depends on B and e_1).

(2) Given e_2 orthogonal to e_1, inside the slab P_{e_1,x_n} we can find a sequence of pencils $L_{e_1,e_2,\hat{x}_1}, \dots, L_{e_1,e_2,\hat{x}_{\hat{n}}}$, all orthogonal to e_2, by moving a piston from $\partial^-\Lambda$ in the direction opposite to e_2 one unit distance at a time, up to the first $L_{e_1,e_2,\hat{x}_{\hat{n}}}$ such that $L_{e_1,e_2,\hat{x}_n} \cap B \neq \emptyset$ ($\hat{n}$ depends on B and e_1, e_2).

(3) Given e_3 orthogonal to e_1 and e_2, inside the pencil $L_{e_1,e_2,\hat{x}_n}$ we can find a sequence of sites $\tilde{x}_1, \dots, \tilde{x}_{\tilde{n}}$ by moving a piston from $\partial^-\Lambda$ in the direction opposite to e_3 one unit distance at a time, up to the first site $\tilde{x}_{\tilde{n}}$ such that $\tilde{x}_{\tilde{n}} \in L_{e_1,e_2,\hat{x}_{\hat{n}}} \cap B$ ($\tilde{n}$ depends on B and e_1, e_2, e_3).

Put $x_0 = \tilde{x}_{\tilde{n}}$. In this way, given three ordered vectors e_1, e_2, e_3, we have a constructive method to find a unique extremal corner of B, (e_1, e_2, e_3, x_0). Thus, the number of extremal corners equals the number of choices for these vectors, namely, $6 \times 4 \times 2 = 48$. ♡

Lemma 2.67 *Divide Λ with a plane π (parallel to one of the sides of $\partial^-\Lambda$) and consider the two parts Λ' and Λ'' (with $\Lambda' \cup \Lambda'' = \Lambda$) obtained in this way. If $B \subseteq \Lambda$ is such that $B \cap \Lambda' \neq \emptyset$, then there are at least 8 extremal corners of B whose site is in Λ'.*

Proof. If $B \cap \Lambda' \neq \emptyset$, then we use the constructive method in the previous proof by moving a piston parallel to π in Λ'. In this way we determine a unique vector e_1, the one orthogonal to π in the direction of Λ'. We can repeat the argument to find the extremal corner for any possible choice of e_2, e_3, obtaining $4 \times 2 = 8$ extremal corners of B whose site is in Λ. ♡

3. In what follows we use Lemma 2.67 for a suitable choice of B contained either in η or in η^c, i.e., subsets of occupied or empty sites.

Lemma 2.68 *If $\eta \in \mathcal{X}_{3U}$, then there are no η^c-corners.*

Proof. If there exists an η^c-corner x, then $x \in \partial^+\eta$ and we can distinguish two cases:

(i) $x \in (\eta^c)^{com}$. In this case there exists a sequence of empty nearest-neighbor sites $y_1(= x), \dots, y_n(\in \partial^-\Lambda)$ such that $y_j \in \eta^c$ for $j = 1, \dots, n$. So, it is possible to reduce the configuration η by creating a particle in $y_n \in \partial^-\Lambda$, increasing the energy by Δ, and then bringing it to x by following the sequence $y_n, \dots, y_1$, decreasing the energy by $3U$ (when the particle is connected to the droplet). Since $\Delta < 3U$, in this way the configuration η is Δ-reduced, i.e., $\eta \in \mathcal{X} \backslash \mathcal{X}_\Delta$ (recall (2.30)), which contradicts the assumption that $\eta \in \mathcal{X}_{3U}$ because $\mathcal{X}_{3U} \subseteq \mathcal{X}_\Delta$.

(ii) $x \in (\eta^c)^{ncom}$. In this case $d((\eta^c)^{ncom}, \partial^-\Lambda) \geq 2$, because $d((\eta^c)^{ncom}, (\eta^c)^{com}) \geq 2$. Let (e_1, e_2, e_3, x_0) be an extremal corner of the connected component of $(\eta^c)^{ncom}$ containing x, and let S_{e_1,x_0} be the corresponding halfspace. We have $S_{e_1,x_0} \cap \eta \neq \emptyset$, since $x_0 \in (\eta^c)^{ncom}$ and $x_0 + e_1 \in \eta$. Let $\bar{\eta}$ be the connected component of η containing $x_0 + e_1$. Then Lemma 2.67 implies that $\bar{\eta}$ has at least 8 extremal corners whose site is in $S_{e_1,x_0} \cap \bar{\eta}$. We can move the particle at $x_0 + e_1$ to the empty site x_0, increasing the energy by $3U$. After that, at 0 energy cost, we can move the empty site in the direction e_1, always keeping it inside $S_{e_1,x_0} \cap \bar{\eta}$, up to the first instance when it arrives in $\partial\bar{\eta}$. After that, we can move it to an extremal corner of $\bar{\eta}$ whose site, say z, is in $\bar{\eta}$, decreasing the energy by $3U$ and obtaining a configuration, say $\tilde{\eta}$, with the same energy as η. Thus, the empty site originally at x_0 in η is moved to z in $\tilde{\eta}$. By iterating this argument we obtain a configuration $\hat{\eta}$ with $(\hat{\eta}^c)^{ncom} = \emptyset$. Now we proceed as in case (i).

♡

4. Let us finally prove that $(\omega_i^c)^{ncom} = \emptyset$, i.e., the statement of Proposition 2.61. We will argue by contradiction.

Claim 2.69 *Let $0 \leq i \leq p$ and $\omega_i = \omega_i^G \cup \eta$. If $(\omega_i^c)^{ncom} \neq \emptyset$, then there exists at least one extremal corner (e_1, e_2, e_3, x_0) of $(\omega_i^c)^{ncom}$ satisfying*

$$x_0 + e_1 \notin \Lambda_i, \quad x_0 + e_2 \notin \Lambda_i, \quad x_0 + e_3 \notin \Lambda_i. \tag{2.70}$$

Proof. Abbreviate $A = (\omega_i^c)^{ncom}$, and recall that $\Lambda_i = \mathrm{supp}(\omega_i^G)$ and $A \cap \partial^-\Lambda = \emptyset$. By Lemma 2.66, there exist extremal corners of $\Lambda_i \cup A$. We will prove that at least one of these is an extremal corner of A satisfying (2.70). We distinguish two cases:

(i) $P(\Lambda_i \cup A) \setminus P(\Lambda_i) \neq \emptyset$. In this case there is a direction e_1 such that, if we consider the sequence of slabs $P_{e_1,x_1}, \ldots, P_{e_1,x_n}$ obtained by moving a piston from $\partial^-\Lambda$ in the direction opposite to e_1, then this piston intersects $P(\Lambda_i \cup A)$ before $P(\Lambda_i)$. Any extremal corner of A with this direction e_1 satisfies (2.70).

(ii) $P(\Lambda_i \cup A) \setminus P(\Lambda_i) = \emptyset$. In this case Λ_i is not a quasi-cube and A is contained in the face F_i of the quasi-cube $P(\Lambda_i)$ where ω_i^G is growing at its i-th step. Let e_1 be the vector orthogonal to F_i in the direction external to Λ_i and let $P(\Lambda_i \cap F_i)$ be the rectangle circumscribing $\Lambda_i \cap F_i$. We have two cases.

(ii1) $A \not\subseteq P(\Lambda_i \cap F_i)$. In this case there is a direction e_2, orthogonal to e_1, such that, if we consider the sequence of pencils $L_{e_1,e_2,\hat{x}_1}, \ldots, L_{e_1,e_2,\hat{x}_{\hat{n}}}$ in the slab F_i obtained by moving a piston from $\partial^-\Lambda$ in the direction opposite to e_2, then it intersects A before $P(\Lambda_i \cap F_i)$. Any extremal corner of A with these e_1 and e_2 satisfies (2.70).

(ii2) $A \subseteq P(\Lambda_i \cap F_i)$. In this case A is contained in the pencil, say L_i, of $P(\Lambda_i \cap F_i)$ where ω_i^G is growing at step i. Let e_2 be the the vector orthogonal to L_i and to e_1 in the direction external to Λ_i. By the definition of Λ_i, it is immediate that there exists a vector e_3, orthogonal to e_1 and e_2, and a site $x_0 \in A$ such that (e_1, e_2, e_3, x_0) is an extremal corner of A satisfying (2.70).

♡

5. The proof of Proposition 2.61 follows from Claim 2.69 after we note that (2.70) implies that x_0 is an η^c-corner, because there exist 3 nearest-neighbors of x_0 in η,

$$x_0 + e_1 \in \eta, \quad x_0 + e_2 \in \eta, \quad x_0 + e_3 \in \eta, \tag{2.71}$$

which contradicts Lemma 2.68. Hence $(\omega_i^c)^{ncom} = \emptyset$. ♡

With Proposition 2.61 we have completed the proof of Proposition 2.47. It follows from Propositions 2.13 and 2.47 that

$$\mathcal{X}_{\Gamma_0} = \{\square, \mathcal{F}(\mathcal{X})\}, \tag{2.72}$$

because any configuration in $\blacksquare \setminus \mathcal{F}(\mathcal{X})$ is 0-reducible and therefore cannot be in $\mathcal{X}_{\Gamma_0}$.

2.5 Geometric description of minimal saddles and gates

In this section we develop the focalization property that was announced in the introduction and we identify a gate for the nucleation, i.e., a subset of those minimal saddle configurations the Kawasaki dynamics has to cross with high probability in its transition from the metastable state $\square$ to the stable state $\blacksquare$. Our main result is Proposition 2.86. In Section 2.5.1 we define magic numbers, in Section 2.5.2 we study focalization and gates, while in Section 2.5.3 we expand the argument slightly further.

2.5.1 Magic numbers

Let $d(n)\colon \mathbb{N} \to \mathbb{N}_0^3 \times \{0,1\}^3$ be the function that associates with n the unique 6-tuple $(m, l, k, \delta, \theta, \alpha)$ appearing in (2.3). Note that $d(n)$ is a bijection by Proposition 2.2.

A special role is played by the set $\bar{\mathbb{N}}$ of integers n such that $d(n) = (m, l, 0, \delta, \theta, \alpha)$. Borrowing terminology from nuclear physics [10], we call $\bar{\mathbb{N}}$ the set of *magic numbers*. For these numbers the principal polyominoes have the form "quasi-cube + quasi-square".

If $\bar{n} \in \bar{\mathbb{N}}$, then by Theorem 2.4(b) the associated (equivalence class of) principal polyominoes $\mathcal{R}_{\bar{l},\bar{l}+\bar{\alpha}}(\bar{m}, \bar{m}+\bar{\delta}, \bar{m}+\bar{\theta})$ (defined in Section 1.5 item 3) satisfies

$$\mathcal{R}_{\bar{l},\bar{l}+\bar{\alpha}}(\bar{m}, \bar{m}+\bar{\delta}, \bar{m}+\bar{\theta}) = \Big\{\eta \in \mathcal{V}_{\bar{n}}\colon\, H(\eta) = \min_{\eta' \in \mathcal{V}_{\bar{n}}} H(\eta')\Big\}. \tag{2.73}$$

We order $\bar{\mathbb{N}}$: $\bar{\mathbb{N}} = \{\bar{n}_1, \bar{n}_2, \ldots\}$ with $\bar{n}_1 < \bar{n}_2 < \ldots$ Given $\bar{n}_i \in \bar{\mathbb{N}}$ with $d(\bar{n}_i) = (\bar{m}_i, \bar{l}_i, 0, \bar{\delta}_i, \bar{\theta}_i, \bar{\alpha}_i)$, we have

$$\bar{n}_{i+1} = \bar{n}_i + 1 \;\text{ if } \bar{l}_i = 0, \qquad \bar{n}_{i+1} = \bar{n}_i + \bar{l}_i + \bar{\alpha}_i \;\text{ if } \bar{l}_i \geq 1. \tag{2.74}$$

2.5.2 Focalization and gates

The main result in this section is Proposition 2.86. Its proof relies on the following (recall Section 1.5 items 3 and 8):

Proposition 2.75 *Fix i and let $d(\bar{n}_i) = (\bar{m}_i, \bar{l}_i, 0, \bar{\delta}_i, \bar{\theta}_i, \bar{\alpha}_i)$.*
(a) Let $\bar{n}_i$ be such that $\bar{l}_i + \bar{\alpha}_i > 1$. Then $\mathcal{D}^{2pr,fp}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i, \bar{m}_i+\bar{\delta}_i, \bar{m}_i+\bar{\theta}_i) \subseteq \mathcal{V}_{\bar{n}_i+2}$ is a gate for $\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}}$.
(b) Let $\bar{n}_i$ be such that $\bar{l}_i + \bar{\alpha}_i \leq 1$. Then $\mathcal{R}^{fp}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i, \bar{m}_i+\bar{\delta}_i, \bar{m}_i+\bar{\theta}_i) \subseteq \mathcal{V}_{\bar{n}_i+1}$ is a gate for $\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}}$.

Proof. The proof comes in steps.

1. We begin with the elementary observation that, for all $n \in \mathbb{N}$ and $\eta, \eta' \in \mathcal{V}_n$,

$$H(\eta) - H(\eta') = kU \text{ for some } k \in \mathbb{Z}, \tag{2.76}$$

which is immediate from (1.3) and (1.31) since $N_\Lambda(\eta) = N_\Lambda(\eta')$.

2. Next, we consider two consecutive magic manifolds.

Lemma 2.77 *Fix i and let $d(\bar{n}_i) = (\bar{m}_i, \bar{l}_i, 0, \bar{\delta}_i, \bar{\theta}_i, \bar{\alpha}_i)$. Then all paths in $(\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$ pass through $\mathcal{R}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i, \bar{m}_i+\bar{\delta}_i, \bar{m}_i+\bar{\theta}_i) \subseteq \mathcal{V}_{\bar{n}_i}$ during the transition from $\mathcal{V}_{\bar{n}_i}$ to $\mathcal{V}_{\bar{n}_i+1}$.*

Proof. Abbreviate $\mathcal{R}_i = \mathcal{R}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i, \bar{m}_i+\bar{\delta}_i, \bar{m}_i+\bar{\theta}_i)$. Let $\omega^K(\bar{n}_i, \bar{n}_{i+1})$ be the part of the reference path ω^K between the standard polyomino of volume $\bar{n}_i$ and that of volume $\bar{n}_{i+1}$.

If $\bar{n}_i$ is such that $\bar{l}_i + \bar{\alpha}_i > 1$, which means that the corresponding polyomino is neither a quasi-cube nor a quasi-cube plus a 1-protuberance, then by (2.74) we have $\bar{n}_{i+1} \geq \bar{n}_i + 2$, and so

$$\Phi(\mathcal{V}_{\bar{n}_i}, \mathcal{V}_{\bar{n}_{i+1}}) \leq \max_{\eta \in \omega^K(\bar{n}_i, \bar{n}_{i+1})} H(\eta) \leq H(\mathcal{R}_i) + 2\Delta - 2U, \tag{2.78}$$

because 2Δ is the cost to create the $(\bar{n}_i+1)$-st and the $(\bar{n}_i+2)$-nd particle, while $-2U$ is the binding energy when the $(\bar{n}_i+1)$-st particle is attached to the droplet. Suppose that there exists $\omega \in (\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$ not passing through $\mathcal{R}_i$. We will show that, for any such ω,

$$\max_{\eta \in \omega} H(\eta) \geq H(\mathcal{R}_i) + \Delta + U. \tag{2.79}$$

Equations (2.78–2.79) give a contradiction because $\Delta + U > 2\Delta - 2U$. To prove (2.79), use that $\mathcal{R}_i = \mathcal{F}(\mathcal{V}_{\bar{n}_i})$ by Theorem 2.4(b). By (2.76), if ω does not pass through $\mathcal{R}_i$, then the configurations $\eta \in \omega \cap \mathcal{V}_{\bar{n}_i}$ have energy $H(\eta) \geq H(\mathcal{R}_i) + U$. Since the transition from $\mathcal{V}_{\bar{n}_i}$ to

$\mathcal{V}_{\bar{n}_i+1}$ comes with a further increase in energy by Δ due to the next incoming free particle, it is clear that ω satisfies (2.79).

If $\bar{n}_i$ is such that $\bar{l}_i + \bar{\alpha}_i \leq 1$, then by (2.74) we have $\bar{n}_{i+1} = \bar{n}_i + 1$, and so

$$\Phi(\mathcal{V}_{\bar{n}_i}, \mathcal{V}_{\bar{n}_{i+1}}) \leq \max_{\eta \in \omega^K(\bar{n}_i, \bar{n}_{i+1})} H(\eta) = H(\mathcal{R}_i) + \Delta. \tag{2.80}$$

We can now repeat the previous argument via contradiction, because $\Delta + U > \Delta$. ♡

3. We return to the proof of Proposition 2.75(a,b):

(a) We know from Lemma 2.77 that any $\omega \in (\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$ passes through $\mathcal{R}_i \subseteq \mathcal{V}_{\bar{n}_i}$ and hence crosses $\mathcal{V}_{\bar{n}_i+1}$ in $\mathcal{R}_i^{fp}$. The first non-trivial subsequent move can only consist in attaching the free particle in $\mathcal{R}_i^{fp}$ to the droplet in $\mathcal{R}_i^{fp}$. Indeed, annihilation of the free particle would mean to return to $\mathcal{V}_{\bar{n}_i}$, while without annihilation the following restrictions are in force:

(i) No other free particle can arrive before the free particle is attached, because otherwise we would have

$$\max_{\eta \in \omega} H(\eta) = H(\mathcal{R}_i) + 2\Delta > H(\mathcal{R}_i) + 2\Delta - 2U \geq \Phi(\mathcal{V}_{\bar{n}_i}, \mathcal{V}_{\bar{n}_{i+1}}), \tag{2.81}$$

where the last inequality uses (2.78).

(ii) It is not possible to separate a particle from one of the corners of the droplet before attaching the free particle, since this would increase the energy by at least U (namely, when the free particle is next to the site the particle from the corner moves to, the energy increases by $2U - U = U$), and so we would have

$$\max_{\eta \in \omega} H(\eta) \geq H(\mathcal{R}_i) + \Delta + U > H(\mathcal{R}_i) + 2\Delta - 2U \geq \Phi(\mathcal{V}_{\bar{n}_i}, \mathcal{V}_{\bar{n}_{i+1}}). \tag{2.82}$$

After attaching the free particle we enter the set $\mathcal{R}_i^{2pr}$, and so we are in the set

$$\mathcal{C}_\eta^{2U}(\mathcal{R}_i^{2pr}) = \left\{\eta' \in \mathcal{V}_{\bar{n}_i+1} \colon \Phi_{\mathcal{V}_{\bar{n}_i+1}}(\eta, \eta') \leq H(\eta) + 2U\right\} \tag{2.83}$$

for some $\eta \in \mathcal{R}_i^{2pr}$.

Now, ω^K visits $\mathcal{V}_{\bar{n}_i+1}$ for the last time in $\mathcal{F}(\mathcal{V}_{\bar{n}_i+1})$. Therefore, by comparison with ω^K and using (2.78), we deduce that any path in $(\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$ has to perform the passage from $\mathcal{V}_{\bar{n}_i+1}$ to $\mathcal{V}_{\bar{n}_i+2}$ as a single transition $\eta \to \sigma$ (with $\eta \in \mathcal{V}_{\bar{n}_i+1}$, $\sigma \in \mathcal{V}_{\bar{n}_i+2}$), where $\eta \in \mathcal{F}(\mathcal{V}_{\bar{n}_i+1})$ and σ is obtained from η by creating a particle in $\partial^-\Lambda$, so that $H(\sigma) = H(\eta) + \Delta$. Moreover, it is clear that any path in $(\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$ cannot visit any configuration in $\mathcal{V}_{\bar{n}_i+1}$ with energy strictly larger than $H(\mathcal{F}(\mathcal{V}_{\bar{n}_i+1})) + 2U$ since, by (2.76), this would imply a value of the energy larger than or equal to $H(\mathcal{F}(\mathcal{V}_{\bar{n}_i+1})) + 3U$, which is strictly larger than the maximal energy in ω^K. So, we cannot leave $\mathcal{V}_{\bar{n}_i+1}$ unless we return to $\mathcal{V}_{\bar{n}_i}$. This implies that the transition to $\mathcal{V}_{\bar{n}_i+2}$ has to be performed through the set (recall (1.43))

$$\left(\bigcup_{\eta \in \mathcal{R}_i^{2pr}} \mathcal{F}(\mathcal{C}_\eta^{2U}(\mathcal{R}_i^{2pr}))\right)^{fr} = \mathcal{D}^{2pr,fp}_{\bar{l}_i, \bar{l}_i + \bar{\alpha}_i}(\bar{m}_i, \bar{m}_i + \bar{\delta}_i, \bar{m}_i + \bar{\theta}_i). \tag{2.84}$$

To complete the proof, we note that $\mathcal{D}^{2pr,fp}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i,\bar{m}_i+\bar{\delta}_i,\bar{m}_i+\bar{\theta}_i) \subseteq \mathcal{S}(\mathcal{V}_{\bar{n}_i},\mathcal{V}_{\bar{n}_{i+1}})$ since, by (2.10),

$$\Phi(\mathcal{V}_{\bar{n}_i},\mathcal{V}_{\bar{n}_{i+1}}) = \max_s H(\omega^K(\bar{n}_i,\bar{n}_{i+1})) = H\left(\mathcal{D}^{2pr,fp}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i,\bar{m}_i+\bar{\delta}_i,\bar{m}_i+\bar{\theta}_i)\right). \tag{2.85}$$

(b) The proof is immediate via Lemma 2.77 and the same reasoning as prior to (2.83). ♡

We may now conclude with the main result of this section:

Proposition 2.86 *$\mathcal{C}^*$ is a gate for $\square \to \blacksquare$.*

Proof. This is immediate from Proposition 2.13 and Proposition 2.75(a). ♡

2.5.3 Further properties of optimal paths between successive magic manifolds

In this section we prove the following extension of Lemma 2.77.

Lemma 2.87 *Fix i and let $d(\bar{n}_i) = (\bar{m}_i,\bar{l}_i,0,\bar{\delta}_i,\bar{\theta}_i,\bar{\alpha}_i)$ with $\bar{l}_i \neq 0$. Then all paths in $(\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$ pass through the set obtained from $\mathcal{R}^{fp}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i,\,\bar{m}_i+\bar{\delta}_i,\bar{m}_i+\bar{\theta}_i)$ by attaching the free particle to the face of the quasi-cube containing the quasi-square.*

Proof. Again we abbreviate $\mathcal{R}_i = \mathcal{R}_{\bar{l}_i,\bar{l}_i+\bar{\alpha}_i}(\bar{m}_i,\bar{m}_i+\bar{\delta}_i,\bar{m}_i+\bar{\theta}_i)$.

If $\omega \in (\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$, then, by Lemma 2.77, ω passes through $\mathcal{R}^{fp}_i \subseteq \mathcal{V}_{\bar{n}_i+1}$. We know from (a) and (b) in the proof of Proposition 2.75 that the creation of another free particle or the separation of a particle from the droplet are not possible in ω before the free particle is attached. We want now to prove that if ω passes from $\mathcal{R}^{fp}_i$ to a configuration in which the free particle in $\mathcal{R}^{fp}_i$ is attached to a wrong face of the droplet (i.e., a face that does not contain the quasi-square) or to the top of the quasi-square, then ω returns to $\mathcal{R}^{fp}_i$ before reaching $\mathcal{V}_{\bar{n}_{i+1}}$. This goes as follows.

Let $\mathcal{R}^{wpr}_i$ be the set of configurations that are obtained from a configuration in $\mathcal{R}^{fp}_i$ by attaching the free particle to a wrong face or to the top of the quasi-square (leading to a "wrong protuberance"). We claim that any configuration $\eta' \notin \mathcal{R}^{wpr}_i$ that can be obtained from $\eta \in \mathcal{R}^{wpr}_i$ without again separating the attached particle from the droplet has an energy $H(\eta') \geq H(\eta) + 2U$, which is strictly larger than $\Phi(\mathcal{V}_{\bar{n}_i},\mathcal{V}_{\bar{n}_{i+1}})$. To see why this claim is true, note that in η all the particles, with the exception of the attached one, have at least 3 nearest-neighbors in the cluster. To move a particle of the quasi-square while keeping it on the same face has energy cost $\geq 2U$, because the attached particle cannot be a nearest-neighbor of the site this particle moves to. To move a particle of the quasi-square away from the face also has energy cost $\geq 2U$ (possibly with the help of the attached particle when it is on top of the quasi-square). To move a particle of another face again has energy cost $\geq 2U$ (possibly with the help of the attached particle when it is on that same face). Thus, we would have

$$\max_{\eta\in\omega} H(\eta) = H(\mathcal{R}_i) + \Delta - U + 2U > \Phi(\mathcal{V}_{\bar{n}_i},\mathcal{V}_{\bar{n}_{i+1}}), \tag{2.88}$$

where the inequality uses (2.78) and (2.80). This contradicts $\omega \in (\mathcal{V}_{\bar{n}_i} \to \mathcal{V}_{\bar{n}_{i+1}})_{opt}$. ♡

Lemma 2.87 is only a first step towards describing in more detail what the optimal paths look like. The problem is to extend the focalization to manifolds that are not magic, which is hampered by the degeneracy found in Alonso and Cerf [1] for the isoperimetric inequalities when the number of particles is not a magic number. At present it seems too difficult to handle this problem. Some further discussion is provided in Section 4.2.

3 Proof of main theorems

3.1 Proof of Theorem 1.55(a)

Upper bound:

The upper bound on the nucleation time in fact holds uniformly in the starting point.

Proposition 3.1

$$\lim_{\beta\to\infty}\min_{\eta\in\mathcal{X}} P_\eta\Big(\tau_{\blacksquare} < e^{(\Gamma+\delta)\beta}\Big) = 1 \qquad \forall\delta>0. \tag{3.2}$$

Proof. The proof is achieved by exhibiting a sufficiently probable nucleation event.

1. Fix $\eta\in\mathcal{X}$ and $\delta>0$, put $T=e^{(\Gamma+\frac{\delta}{2})\beta}$, and define the event

$$\{\tau_{\blacksquare}<T\} = \{\omega\colon \exists t\in[0,T)\colon \omega_t\in\blacksquare\}. \tag{3.3}$$

We will prove that

$$\min_{\eta\in\mathcal{X}} P_\eta(\tau_{\blacksquare}<T) \geq e^{-\frac{\delta}{4}\beta} \qquad \forall\beta>\beta_0(\delta). \tag{3.4}$$

Putting $T_+=e^{(\Gamma+\delta)\beta}$ and using (3.4) in combination with the Markov property, we get

$$\max_{\eta\in\mathcal{X}} P_\eta\Big(\tau_{\blacksquare}\geq T_+\Big) \leq \Big(1-e^{-\frac{\delta}{4}\beta}\Big)^{T_+/T} = \Big(1-e^{-\frac{\delta}{4}\beta}\Big)^{e^{\frac{\delta}{2}\beta}} = \mathrm{SES}. \tag{3.5}$$

2. To prove (3.4), we introduce an event

$$\mathbf{E}_\eta^T \subseteq \{\tau_{\blacksquare}<T\} \tag{3.6}$$

whose probability we will be able to estimate properly, namely,

$$\mathbf{E}_\eta^T = \bigcup_{t_1\in[0,\frac{T}{4}]} \Big\{\mathbf{E}_\eta^{\{\square,\blacksquare\};\blacksquare,t_1} \cup \widetilde{\mathbf{E}}_\eta^{t_1,T}\Big\} \tag{3.7}$$

with

$$\begin{aligned}
\mathbf{E}_\eta^{\{\square,\blacksquare\};\blacksquare,t_1} &= \{\omega\colon \omega_0=\eta,\ \omega_s\notin\{\square,\blacksquare\}\ \forall\,0<s<t_1,\ \omega_{t_1}\in\blacksquare\},\\
\mathbf{E}_\eta^{\{\square,\blacksquare\};\square,t_1} &= \{\omega\colon \omega_0=\eta,\ \omega_s\notin\{\square,\blacksquare\}\ \forall\,0\leq s<t_1,\ \omega_{t_1}=\square\},\\
\widetilde{\mathbf{E}}_\eta^{t_1,T} &= \bigcup_{t_2\in[t_1,\frac{T}{2}]}\ \bigcup_{t_3\in[t_2,\frac{3T}{4}]}\ \bigcup_{t_4\in[t_3,T]}\\
&\qquad \Big\{\mathbf{E}_\eta^{\{\square,\blacksquare\};\square,t_1} \cap \mathbf{E}_{\square,t_1}^{R^{2pr,fp},t_2} \cap \mathbf{E}_{R^{2pr,fp},t_2}^{R^{spr},t_3} \cap \mathbf{E}_{R^{spr},t_3}^{\blacksquare,t_4}\Big\},
\end{aligned} \tag{3.8}$$

where $R^{2pr,fp}$ is any configuration in $\mathcal{R}^{2pr,fp}_{l_c-1,l_c}(m_c-1,m_c-\delta_c,m_c)$ and R^{spr} is any configuration obtained from $R^{2pr,fp}$ by attaching the free particle to an external corner of $R^{2pr,fp}$ (both configurations are fixed arbitrarily), while, for $\zeta\in\mathcal{X}$, $B\subseteq\mathcal{X}$, $0\leq t\leq u$,

$$\mathbf{E}_{\zeta,t}^{B,u} = \{\omega\colon \omega_t=\zeta,\ \omega_s\notin B\,\forall\,t<s<u, \omega_u\in B\}. \tag{3.9}$$

Note that in (3.9) the lower index t means that time is shifted by t units.

3. Since t_1, t_2, t_3, t_4 in (3.8) are first hitting times, we have

$$P\left(\bigcup_{t_1\in[0,\frac{T}{4}]}\left\{\mathbf{E}_\eta^{\{\square,\blacksquare\};\blacksquare,t_1}\cup\widetilde{\mathbf{E}}_\eta^{t_1,T}\right\}\right)=\sum_{t_1\in[0,\frac{T}{4}]}\{P(\mathbf{E}_\eta^{\{\square,\blacksquare\};\blacksquare,t_1})+P(\widetilde{\mathbf{E}}_\eta^{t_1,T})\} \tag{3.10}$$

and

$$P(\widetilde{\mathbf{E}}_\eta^{t_1,T})=P(\mathbf{E}_\eta^{\{\square,\blacksquare\};\square,t_1}) \times\sum_{t_2\in[t_1,\frac{T}{2}]}\sum_{t_3\in[t_2,\frac{3T}{4}]}\sum_{t_4\in[t_3,T]}P\left(\mathbf{E}_{\square,t_1}^{R^{2pr,fp},t_2}\right)P\left(\mathbf{E}_{R^{2pr,fp},t_2}^{R^{spr},t_3}\right)P\left(\mathbf{E}_{R^{spr},t_3}^{\blacksquare,t_4}\right). \tag{3.11}$$

On the other hand,

$$\begin{aligned}P(\mathbf{E}_\eta^{\{\square,\blacksquare\};\square,t_1}) &= P_\eta(\tau_{\{\square,\blacksquare\}}=t_1)q_{t_1}(\eta),\\ P(\mathbf{E}_\eta^{\{\square,\blacksquare\};\blacksquare,t_1}) &= P_\eta(\tau_{\{\square,\blacksquare\}}=t_1)(1-q_{t_1}(\eta)),\end{aligned} \tag{3.12}$$

with

$$q_{t_1}(\eta)=P_\eta\left(\eta_{\tau_{\{\square,\blacksquare\}}}=\square\mid\tau_{\{\square,\blacksquare\}}=t_1\right). \tag{3.13}$$

We may therefore write

$$\sum_{t_1\in[0,\frac{T}{4}]}\{P(\mathbf{E}_\eta^{\{\square,\blacksquare\};\blacksquare,t_1})+P(\widetilde{\mathbf{E}}_\eta^{t_1,T})\}\geq\sum_{t_1\in[0,\frac{T}{4}]}P_\eta(\tau_{\{\square,\blacksquare\}}=t_1)[(1-q_{t_1}(\eta))+q_{t_1}(\eta)r_T] \tag{3.14}$$

with

$$r_T=P\left(\mathbf{E}_\square^{R^{2pr,fp},\leq\frac{T}{4}}\right)P\left(\mathbf{E}_{R^{2pr,fp}}^{R^{spr},\leq\frac{T}{4}}\right)P\left(\mathbf{E}_{R^{spr}}^{\blacksquare,\leq\frac{T}{4}}\right), \tag{3.15}$$

where

$$\mathbf{E}_\zeta^{\xi,\leq t}=\{\omega\colon\omega_0=\zeta,\exists\,0\leq s\leq t\colon\omega_s=\xi\}. \tag{3.16}$$

From (3.7), (3.10) and (3.14) we get

$$P(\mathbf{E}_\eta^T)\geq P_\eta\left(\tau_{\{\square,\blacksquare\}}\leq\frac{T}{4}\right)\,r_T. \tag{3.17}$$

4. Propositions 2.34 and 2.47 imply that

$$\lim_{\beta\to\infty}\min_{\eta\in\mathcal{X}}P_\eta\left(\tau_{\{\square,\blacksquare\}}<e^{(\Gamma_0+\gamma)\beta}\right)=1\qquad\forall\gamma>0. \tag{3.18}$$

Put $\gamma=(\Gamma-\Gamma_0)/2$. Then $e^{(\Gamma_0+\gamma)\beta}<\frac{T}{4}$ for β sufficiently large and so it follows from (3.18) that

$$\min_{\eta\in\mathcal{X}}P_\eta\left(\tau_{\{\square,\blacksquare\}}\leq\frac{T}{4}\right)\geq\frac{1}{2}\qquad\forall\beta>\beta_0(\delta). \tag{3.19}$$

Thus, it remains to get a lower bound on r_T.

5. Let

$$\mathcal{A}_\square=\left\{\eta\in\mathcal{X}\colon\exists\,\omega\colon\eta\to\square\colon\max_i H(\omega_i)<\Gamma\right\}. \tag{3.20}$$

This set is a cycle with $\mathcal{F}(\partial\mathcal{A}_\square) \supseteq R^{2pr,fp-}$, the subset of $R^{2pr,fp}$ where the free particle is in the boundary $\partial^-\Lambda$ (because $H(R^{2pr,fp-}) = \Gamma$ and removal of the free particle in $R^{2pr,fp-}$ leads to a configuration in $\mathcal{A}_\square$). Hence Proposition 2.42(a,c) and (3.18) yield

$$P\left(\mathbf{E}_\square^{R^{2pr,fp},\leq\frac{T}{4}}\right) \geq e^{-\delta'\beta} \qquad \forall\delta'>0 \quad \forall\beta>\beta_0(\delta'). \tag{3.21}$$

Next, since there is a finite downhill path from $R^{2pr,fp}$ to R^{spr}, there exists a constant $a>0$, independent of β, such that

$$P\left(\mathbf{E}_{R^{2pr,fp}}^{R^{spr},\leq\frac{T}{4}}\right) \geq a. \tag{3.22}$$

Next, let

$$\mathcal{A}_\blacksquare = \left\{\eta\in\mathcal{X}\colon \exists\,\omega\colon \eta\to\blacksquare\colon \max_i H(\omega_i) < \Gamma\right\}. \tag{3.23}$$

This set is a cycle, and $R^{spr}\subseteq\mathcal{A}_\blacksquare$ (as can be deduced by looking at the reference path ω^K defined in Section 2.2). Since $\square\notin\mathcal{A}_\blacksquare$, Proposition 2.42(b) and (3.19) yield

$$P\left(\mathbf{E}_{R^{spr}}^{\blacksquare,\leq\frac{T}{4}}\right) \geq \frac{1}{2} \qquad \forall\beta>\beta_0(\delta). \tag{3.24}$$

Combining (3.15), (3.21–3.22) and (3.24) we find that

$$r_T \geq \frac{1}{2}ae^{-\delta'\beta} \qquad \forall\delta'>0 \quad \forall\beta>\beta_0(\delta,\delta'). \tag{3.25}$$

From (3.6), (3.17), (3.19) and (3.25) we conclude that,

$$\min_{\eta\in\mathcal{X}} P(\mathbf{E}_\eta^T) \geq e^{-\delta''\beta} \qquad \forall\delta''>0 \quad \forall\beta>\beta_0(\delta,\delta''), \tag{3.26}$$

which proves (3.4). ♡

Lower bound:

Proposition 3.27 $\lim_{\beta\to\infty} P_\square\left(\tau_\blacksquare > e^{(\Gamma-\delta)\beta}\right) = 1$ *for all* $\delta>0$.

Proof. We know from Proposition 2.13 that

$$\Phi(\square,\blacksquare) = \Gamma. \tag{3.28}$$

Hence the claim follows from reversibility. Indeed, put $T_- = e^{(\Gamma-\delta)\beta}$. Since every path $\omega\colon\square\to\blacksquare$ has to cross $\partial\mathcal{A}_\square$, we can write

$$P_\square(\tau_\blacksquare\leq T_-) \leq P_\square(\tau_{\partial\mathcal{A}_\square}\leq T_-) = \sum_{t=1}^{T_-}\sum_{\xi\in\partial\mathcal{A}_\square} P_\square(\tau_{\partial\mathcal{A}_\square}=t,\,\eta_t=\xi). \tag{3.29}$$

By reversibility, we have

$$P_\square(\tau_{\partial\mathcal{A}_\square}=t,\,\eta_t=\xi) = e^{-\beta[H(\xi)-H(\square)]}P_\xi(\eta_s\in\mathcal{A}_\square\,\forall\,0<s<t,\,\eta_t=\square). \tag{3.30}$$

From (3.29–3.30) we get

$$P_\square(\tau_\blacksquare\leq T_-) \leq T_-|\partial\mathcal{A}_\square|e^{-\beta[H(\mathcal{F}(\partial\mathcal{A}_\square))-H(\square)]} = |\partial\mathcal{A}_\square|e^{-\delta\beta} \tag{3.31}$$

(recall that $H(\square)=0$, $H(\mathcal{F}(\partial\mathcal{A}_\square))=\Gamma$), from which the claim follows. ♡

3.2 Proof of Theorem 1.55(b)

By considering the magic number $\bar{n}_{i_c} = m_c(m_c - \delta_c)(m_c - 1) + l_c(l_c - 1)$, we have

$$\mathbb{P}_\square(\tau_{\square,\mathcal{C}^*,\blacksquare} > \tau_\blacksquare) \leq \mathbb{P}_\square(\eta_{\tau_{\mathcal{V}_{\bar{n}_{i_c}+2}}} \notin \mathcal{C}^*) \leq \mathbb{P}_\square(\tau_{\mathcal{A}_{>\Gamma}} < \tau_\blacksquare), \tag{3.32}$$

where $\mathcal{A}_{>\Gamma} = \{\eta \in \mathcal{X}: H(\eta) > \Gamma\}$. The second inequality holds because, by Proposition 2.75(a), if $\eta_{\tau_{\mathcal{V}_{\bar{n}_{i_c}+2}}} \notin \mathcal{C}^*$, then $\max_s H(\eta_s) > H(\mathcal{C}^*) = \Gamma$. Estimate

$$\mathbb{P}_\square(\tau_{\mathcal{A}_{>\Gamma}} < \tau_\blacksquare) \leq \mathbb{P}_\square(\tau_\blacksquare > e^{(\Gamma+\delta)\beta}) + \mathbb{P}_\square(\tau_{\mathcal{A}_{>\Gamma}} < e^{(\Gamma+\delta)\beta}). \tag{3.33}$$

The first term in the right-hand side tends to zero as $\beta \to \infty$ by Proposition 3.1. Let $\epsilon_0 > 0$ be such that $\min_{\eta \in \mathcal{A}_{>\Gamma}} H(\eta) \geq \Gamma + \epsilon_0$. Then, by using reversibility as in (3.29–3.31), we may estimate the second term in the right-hand side by

$$\mathbb{P}_\square(\tau_{\mathcal{A}_{>\Gamma}} < e^{(\Gamma+\delta)\beta}) \leq |\mathcal{A}_{>\Gamma}| e^{(\Gamma+\delta)\beta} e^{-(\Gamma+\epsilon_0)\beta}, \tag{3.34}$$

which also tends to zero as $\beta \to \infty$ when we pick $0 < \delta < \epsilon_0$.

3.3 Proof of Theorem 1.58

Let $\eta \subsetneq P(m_c - 1, m_c - \delta_c, m_c)$. Then, by Proposition 2.19(a), we have $\Phi(\eta, \square) < \Phi(\eta, \blacksquare)$. Fix $0 < \epsilon_0 < \Phi(\eta, \blacksquare) - \Phi(\eta, \square)$. Then

$$\mathcal{A}_\square^{\Phi(\eta,\square)+\epsilon_0} = \{\eta' \in \mathcal{X}\colon \Phi(\eta', \square) < \Phi(\eta, \square) + \epsilon_0\} \tag{3.35}$$

is a non-trivial cycle containing η and $\square$, but not $\blacksquare$. By applying the general result on cycles in Proposition 2.42(b), we obtain the first line in (1.59). The proof of the second line in (1.59) for the case $\eta \supsetneq P(m_c - 1, m_c - \delta_c, m_c)$ is similar.

4 Additional path properties

In Section 1.5, Item 8, we introduced two types of sets of configurations: those denoted by $\mathcal{R}$, which are given explicitly in terms of a geometric description, and those denoted by $\mathcal{D}$, which have a more complicated definition in terms of communication height, namely, configurations that can be reached from a configuration of type $\mathcal{R}$ by a path on a manifold $\mathcal{V}_n$, for a suitable n, with a maximal energy threshold $2U$. In particular, the set of critical configurations $\mathcal{C}^*$, which plays a crucial role in the present paper, is a set of type $\mathcal{D}$ (recall (1.43) and (1.45)). Thus, in order to obtain geometric information on $\mathcal{C}^*$ we need to investigate the effect of allowing this threshold $2U$, which results in a motion of particles along the border of a droplet.

In Section 4.1 we describe the border motion, both for the two- and for the three-dimensional model. In Section 4.2 we obtain some information on the geometry of configurations in $\mathcal{C}^*$, while in Section 4.3 we offer some reflections on the tube of typical nucleation paths.

4.1 Motion along border of droplet

A particle can move away from a droplet, travel as a free particle for awhile and then return to the droplet, but it can also move along the border of the droplet. In fact, it can either move on a face of the droplet, following a two-dimensional border motion, or it can move from one face to another while staying attached to the droplet, following a three-dimensional border motion. This border motion is a special feature of Kawasaki dynamics and plays an important role in determining the geometry of the critical configurations and of the typical nucleation path.

4.1.1 Two dimensions

Let us first consider the two-dimensional model, which was studied in den Hollander, Olivieri and Scoppola [5], [6]. Here the metastable regime is $\Delta \in (U, 2U)$. The two-dimensional border motion is illustrated in Fig. 6: with the help of a free particle, particles can slide from one side to another at maximal energy cost U (replacing the maximal energy cost $2U$ in three dimensions).

FIG. 6. Two-dimensional motion along the border of the droplet.

In Fig. 6, pictures 3–13 show the border motion triggered by a free particle between its arrival to (pictures 1–2) and departure from (pictures 14-15) the droplet. Note that the configurations in pictures 3, 6, 8, 10 and 13 all have the same energy, while the energy of the configurations in pictures 4, 5, 7, 9, 11 and 12 is U higher.

Due to this border motion, the gate for the nucleation and the tube of typical nucleation paths are completely different from those for Glauber dynamics, where the gate is given by an $l_c \times (l_c - 1)$ quasi-square with a protuberance on one of the longest sides. The configurations given by the same quasi-square but with the protuberance on one of the shortest sides are dead-ends (see Ben Arous and Cerf [2]). In contrast, for Kawasaki dynamics the gate for the nucleation is given by a larger set of configurations, containing the configuration given by an $(l_c-1)\times l_c$ quasi-square with a protuberance on one of the longest sides plus a free particle, but also containing the configuration given by the same quasi-square with the protuberance on one of the shortest sides plus a free particle. Indeed, the latter is not a dead-end, since it is easy to check that the path obtained by completing the shortest side to obtain an $(l_c-1)\times(l_c+1)$ rectangle, adding a protuberance on one of the longest sides of this rectangle and sliding particles along the border from the shortest side to the side of the protuberance (as shown in Fig. 6) is made up of configurations having an energy smaller than the initial one.

4.1.2 Three dimensions

For the three-dimensional model studied in the present paper, the situation is more complex. The three-dimensional border motion is illustrated in Fig. 7: when a two-dimensional droplet with a protuberance is attached to a face near the boundary of the face, particles can slide into this face at a maximal energy cost $2U$.

FIG. 7. Three-dimensional motion along the border of the droplet.

In Fig. 7, the configurations in pictures 1, 3, 5 and 6 all have the same energy, while the energy of the configurations in pictures 2, 4, 8 and 10 is U higher and in pictures 7 and 9 is $2U$ higher. Between pictures 2 and 3, particles slide one by one along the edge of the cube. Between pictures 5 and 6, the border motion connecting pictures 1 and 5 is repeated until one bar of the two-dimensional droplet attached to the face has been completed. In pictures 7, 8, 9 and 10 a bar is moved from one side of the two-dimensional droplet to another, so as to reach a situation similar to picture 1: a two-dimensional droplet with a protuberance that helps to slide into the face the rest of the particles on the edge of the cube (not depicted further). Since picture 10 has energy U higher than picture 1, this sliding can only follow a border motion similar to the one connecting pictures 1 and 6, but cannot continue further.

In Section 4.2 we will show that the border motion cannot really deform the critical droplet, in the sense that all the configurations of minimal energy obtained by this border motion have the same circumscribing parallelepiped. This is only limited information, but a first step towards understanding the geometry of $\mathcal{C}^*$.

4.2 Some geometry of critical configurations

Let $\bar{n} = m_c(m_c-\delta_c)(m_c-1) + l_c(l_c-1) + 1$. For $\bar{\eta} \in \mathcal{R}^{2pr}_{l_c-1,l_c}(m_c-1, m_c-\delta_c, m_c)$, let $C^{2U}_{\bar{\eta}}$ be the set of configurations η that can be reached from $\bar{\eta}$ by a path $\omega = (\omega_1, \ldots, \omega_k)$, $k \in \mathbb{N}$, in $\mathcal{V}_{\bar{n}}$ such that

$$\omega_1 = \bar{\eta}, \quad \omega_k = \eta, \quad \max_{1\le i\le k} H(\omega_i) \le H(\bar{\eta}) + 2U. \tag{4.1}$$

From Theorem 2.4(a) we know that $\bar{\eta} \in \mathcal{F}(C^{2U}_{\bar{\eta}})$. Hence we have (recall (1.45) and (2.84))

$$\mathcal{C}^* = \left(\bigcup_{\bar{\eta}\in\mathcal{R}^{2pr}_{l_c-1,l_c}(m_c-1,m_c-\delta_c,m_c)} \mathcal{F}(C^{2U}_{\bar{\eta}}) \right)^{fp}. \tag{4.2}$$

Proposition 4.3 *For any $\bar{\eta} \in \mathcal{R}^{2pr}_{l_c-1,l_c}(m_c-1, m_c-\delta_c, m_c)$ and any $\eta \in \mathcal{F}(C^{2U}_{\bar{\eta}})$,*

$$P(\bar{\eta}) = P(\eta), \tag{4.4}$$

where $P(\bar{\eta}), P(\eta)$ are the parallelepipeds circumscribing $\bar{\eta}, \eta$.

Proof. Let $\eta \in \mathcal{F}(C^{2U}_{\bar{\eta}})$ with $\eta \neq \bar{\eta}$. Then there exists a path $\omega = (\omega_1, \ldots, \omega_k)$, $k \in \mathbb{N}$, in $\mathcal{V}_{\bar{n}}$ such that

$$\omega_1 = \bar{\eta}, \quad \omega_k = \eta, \quad \max_{1\le i<k} H(\omega_i) \le H(\bar{\eta}) + 2U, \quad H(\bar{\eta}) = H(\eta). \tag{4.5}$$

First we show that, for any such ω,

$$\min_{1\le i\le k} |\omega_i \cap P(\bar{\eta})| \ge \bar{n} - 1. \tag{4.6}$$

Indeed, if (4.6) fails, then there exists $1 \le i_0 \le k$ such that $|\omega_{i_0} \cap P(\bar{\eta})| = \bar{n} - 2$ and $|\omega_i \cap P(\bar{\eta})| \ge \bar{n} - 1$ for all $1 \le i < i_0$. We have

$$H(\omega_{i_0}) \ge H(\omega_{i_0} \cap P(\bar{\eta})) + 2\Delta - 2U. \tag{4.7}$$

Namely, in ω_{i_0}, the particle that has moved outside $P(\bar{\eta})$ in the transition from ω_{i_0-1} to ω_{i_0} has no nearest-neighbor particles inside $P(\bar{\eta})$, while the other particle outside $P(\bar{\eta})$ has at most one nearest-neighbor particle inside $P(\bar{\eta})$. Therefore these two particles can at most form a dimer touching a single particle inside $P(\bar{\eta})$, which gives (4.7). Now, by Theorem 2.4(b), we have

$$H(\omega_{i_0} \cap P(\bar{\eta})) \ge \min_{\eta'\in\mathcal{V}_{\bar{n}-2}} H(\eta') = H(\bar{\eta}) - \Delta + 2U - \Delta + 3U, \tag{4.8}$$

so that

$$H(\omega_{i_0}) \ge H(\bar{\eta}) - 2\Delta + 5U + 2\Delta - 2U = H(\bar{\eta}) + 3U, \tag{4.9}$$

which contradicts (4.5).

From (4.6) we can deduce that either $|\eta \cap P(\bar{\eta})| = \bar{n}$ or $|\eta \cap P(\bar{\eta})| = \bar{n} - 1$. In the first case, since $|\eta| = \bar{n}$, we must have $P(\eta) \subseteq P(\bar{\eta})$, and strict inclusion is not possible since all the parallelepipeds strictly contained in $P(\bar\eta)$ have a volume strictly less than $\bar n$. In the second case, we must have $\eta \notin \mathcal{F}(C^{2U}_{\bar\eta})$ since, by the same argument as above, we have

$$H(\eta) \geq H(\eta \cap P(\bar\eta)) + \Delta - U \geq H(\bar\eta) - \Delta + 2U + \Delta - U > H(\bar\eta). \tag{4.10}$$

♡

Let us add some comments:

(1) The set $C^{2U}_{\bar\eta}$ contains configurations (e.g. with a free particle or with a 1-protuberance) for which the circumscribing parallelepiped is different from $P(\bar\eta)$. However, Proposition 4.3 shows that the set $\mathcal{F}(C^{2U}_{\bar\eta})$ does not.

(2) The configuration given by an $(m_c - 1) \times (m_c - \delta_c) \times m_c$ quasi-cube with $l_c - 1$ missing particles on one edge and with an $l_c \times l_c$ square on one face is a configuration in $\mathcal{F}(C^{2U}_{\bar\eta})$. Indeed, this configuration can be obtained from $\bar\eta$ by a three-dimensional border motion (see Fig. 7).

(3) Proposition 4.3 fails in two dimensions: if we denote by $\bar\eta$ the configuration given by an $(l_c - 1) \times l_c$ quasi-square plus a protuberance, then there are configurations $\eta \in \mathcal{F}(C^{U}_{\bar\eta})$ with $P(\bar\eta) \neq P(\eta)$ (where now $P(\bar\eta), P(\eta)$ denote the rectangles circumscribing $\bar\eta, \eta$). Indeed, η can be any shift of $\bar\eta$ obtained via a path that stays inside $C^{U}_{\bar\eta}$. Fig. 8 illustrates how, with the help of a free particle, the droplet can move up/down/left/right as a result of a border motion. Due to Proposition 4.3, this shift is not possible in three dimensions.

FIG. 8. Upward movement of a 3×3 square.

In Fig. 8, pictures 3–13 show the diffusive motion triggered by a free particle between its arrival to (pictures 1–2) and departure from (pictures 14–15) the droplet. Note that the configurations in pictures 3, 6, 8, 10 and 13 all have the same energy, while the energy of the configurations in pictures 4, 5, 7, 9, 11 and 12 is U higher.

(4) Proposition 4.3 cannot be easily improved. There are configurations in $\mathcal{F}(C_{\bar\eta}^{2U})$ for which the face of the droplet in $\bar\eta$ containing the quasi-square with the 2-protuberance looks *completely different*. Such configurations can be obtained not only by completing the row, as already noted in (2), but also by producing a completely different shape on the face. In fact, the two-dimensional motion on the face below energy threshold $2U$ is even richer than the one below threshold U illustrated in Fig. 6 and can produce *all* two-dimensional droplets with the same area and perimeter (for which there is a large degeneracy: e.g. a 5×4 quasi-square with a protuberance versus a 3×7 rectangle). This degeneracy can in principle be described in full detail, but it is only part of the problem to understand the geometry of the set $\mathcal{C}^*$. Understanding the three-dimensional border motion is a much harder problem and is connected to the degeneracy found in Alonso and Cerf [1] for the isoperimetric inequalities when the number of particles is not a magic number (see the remark made below Theorem 2.4). Complete control of this degeneracy seems to be a hard problem. As noted in (3), in three dimensions the mobility of droplets is smaller than in two dimensions. However, the mobility along the border of droplets is larger. Thus, the two cases are rather different.

(5) Proposition 4.3 is not sufficient to exclude from $\mathcal{C}^*$ the configurations in which the critical two-dimensional droplet is attached to the wrong face of the quasi-cube. We believe that the three-dimensional motion along the border of the critical droplet is not rapid enough to enlarge the gate as much as it does in two dimensions, but we have no proof.

4.3 Tube of typical nucleation paths

We close this paper with a heuristic discussion of the "tube of typical nucleation paths", i.e., the typical behavior of the process in the time interval $[\theta_{\square,\blacksquare}, \tau_{\blacksquare}]$. For the case of Glauber dynamics for the Ising model, Ben Arous and Cerf [2], Theorem 7.36, contains a complete description of this tube. For the present case of Kawasaki dynamics for the lattice gas model, we have only limited reflections to offer.

Because of (1.57), we can divide the nucleation time interval in a subcritical part and a supercritical part:

$$[\theta_{\square,\blacksquare}, \tau_{\blacksquare}] = [\theta_{\square,\blacksquare}, \tau_{\square,\mathcal{C}^*,\blacksquare}] \cup (\tau_{\square,\mathcal{C}^*,\blacksquare}, \tau_{\blacksquare}]. \tag{4.11}$$

We have some control over the subcritical part, due to our identification in Proposition 2.75 of the minimal saddles between consecutive magic manifolds. However, the supercritical part, which is relatively simple for Glauber dynamics, is more complicated for Kawasaki dynamics.

- *Supercritical*: In two dimensions the supercritical growth for Kawasaki dynamics is qualitatively different from that of Glauber dynamics. There are arguments showing that, for Kawasaki dynamics, the two-dimensional motion along the border of the droplet rapidly turns a rectangle into a square or a quasi-square, while for Glauber dynamics this mechanism is absent. Therefore, the supercritical growth follows squares and quasi-squares for Kawasaki, while it follows (randomly growing) rectangles for Glauber (see Ben Arous and Cerf [2]). In three dimensions, as noted in (4) in Section 4.2, the motion along the border of a droplet is less rapid than in two dimensions. We therefore believe that the supercritical growth for Kawasaki dynamics is similar to that of Glauber dynamics.

– *Subcritical*: For the subcritical growth we can apply Olivieri and Scoppola [9], Theorem 2, to study the first exit from the set $\mathcal{A}_\square$ in (3.20), i.e., the maximal connected set of configurations containing $\square$ and having energy $< \Gamma$. The rough idea is the following. Look at the configurations in $\mathcal{F}(\partial\mathcal{A}_\square)$ and look at the first descent from these configurations to $\mathcal{F}(\mathcal{A}_\square) = \square$. The tube of typical paths making up this first descent defines a "standard cascade", consisting of a sequence of minimax's towards $\square$, decreasing in energy and interspersed with sequences of downhill paths and "permanence sets" (which are a kind of generalized cycles). By using reversibility, we find that the exiting tube, starting from $\square$ and ending in $\partial\mathcal{A}_\square$, can be obtained via a time-reversal transformation from the tube describing the first descent to $\square$. More precisely, by Theorem 1.55, we know that the minimal energy on $\partial\mathcal{A}_\square$ is attained in $\mathcal{C}^*$ and that $\mathcal{A}_\square$ only contains configurations with a number of particles $< n^* = m_c^2(m_c-1)+l_c(l_c-1)+2$. To construct the "standard cascade" from $\mathcal{C}^*$ to $\square$, we note that each configuration $\bar\eta \in \mathcal{A}_\square$ that is uphill connected to $\mathcal{C}^*$ is obtained by removing the free particle, i.e., $\bar\eta \in \mathcal{D}^{2pr}_{l_c-1,l_c}(m_c-1, m_c, m_c)$. Let $\hat n = n^* - 2 = m_c^2(m_c-1) + l_c(l_c-1)$, and let $(\bar n_i)$ be a decreasing sequence of magic numbers with $\bar n_1 = \hat n$. Because of Proposition 2.75, we know

$$\Phi(\mathcal{V}_{\bar n_{i-1}}, \mathcal{V}_{\bar n_i}) = \Gamma_i \tag{4.12}$$

and a gate for the transition $\mathcal{V}_{\bar n_{i-1}} \to \mathcal{V}_{\bar n_i}$. Therefore we also know

$$\Phi(\square, \mathcal{V}_{\bar n_i}) = \max_{1\le j\le i} \Gamma_j. \tag{4.13}$$

Consider the first minimal saddle, $\Phi(\square, \mathcal{V}_{\hat n}) = \Gamma_1 < \Gamma$. We note that there exists $\hat\eta \in \mathcal{F}(\mathcal{V}_{\hat n})$ such that $\bar\eta$ is contained in the maximal connected set of configurations with energy $< \Gamma_1$ containing $\hat\eta$, say $C_{\hat\eta}^{\Gamma_1}$. This set is the first "permanence set" of the "standard cascade". By considering all the successive values of i, we can proceed in a similar way and find the whole standard cascade. This is the rough idea, but it seems hard to fill in the mathematical details, again because of lack of control of what happens on non-magic manifolds.

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