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Metastability for Kawasaki dynamics at low temperature with two types of particles

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Abstract

This is the first in a series of three papers in which we study a two-dimensional lattice gas consisting of two types of particles subject to Kawasaki dynamics at low temperature in a large finite box with an open boundary. Each pair of particles occupying neighboring sites has a negative binding energy provided their types are different, while each particle has a positive activation energy that depends on its type. There is no binding energy between neighboring particles of the same type. At the boundary of the box particles are created and annihilated in a way that represents the presence of an infinite gas reservoir. We start the dynamics from the empty box and compute the transition time to the full box. This transition is triggered by a *critical droplet* appearing somewhere in the box.

We identify the region of parameters for which the system is metastable. For this region, in the limit as the temperature tends to zero, we show that the first entrance distribution on the set of critical droplets is uniform, compute the expected transition time up to a multiplicative factor that tends to one, and prove that the transition time divided by its expectation is exponentially distributed. These results are derived under *three hypotheses* on the energy landscape, which are verified in the second and the third paper for a certain subregion of the metastable region. These hypotheses involve three model-dependent quantities – the energy, the shape and the number of the critical droplets – which are identified in the second and the third paper as well.

The main motivation behind this work is to understand metastability of multi-type particle systems. It turns out that for two types of particles the *geometry* of the energy landscape is more complex than for one type of particle. Consequently, it is a somewhat delicate matter to capture the proper mechanisms behind the growing and shrinking of subcritical, critical and supercritical droplets. Our proofs in the present paper use potential theory and rely on ideas developed in Bovier, den Hollander and Nardi [6] for Kawasaki dynamics with one type of particle. Our target is to identify the *minimal* hypotheses that lead to metastable behavior for multi-type Kawasaki dynamics.

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1 Introduction and main results

Section 1.1 defines the model, Section 1.2 introduces basic notation, Section 1.3 identifies the metastable region, while Section 1.4 states the main theorems. Section 1.5 discusses the main theorems and places them in the proper context. Section 1.6 proves three geometric lemmas that are needed in the proof of the main theorems.

For an overview on metastability and droplet growth, we refer the reader to the monograph by Olivieri and Vares [23], and the review papers by Bovier [3], [4], den Hollander [14], Olivieri and Scoppola [22], Gaudillière and Scoppola [12] and Gaudillière [13].

1.1 Lattice gas subject to Kawasaki dynamics

Let $\Lambda \subset \mathbb{Z}^2$ 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 boundary, respectively, the external boundary of Λ, and put $\Lambda^- = \Lambda\backslash\partial\Lambda^-$ and $\Lambda^+ = \Lambda \cup \partial\Lambda^+$. With each site $x \in \Lambda$ we associate a variable $\eta(x) \in \{0,1,2\}$ indicating the absence of a particle or the presence of a particle of type 1 or type 2. A configuration $\eta = \{\eta(x)\colon\ x \in \Lambda\}$ is an element of $\mathcal{X} = \{0,1,2\}^\Lambda$. To each configuration η we associate an energy given by the Hamiltonian

$$H(\eta) = -U \sum_{(x,y)\in(\Lambda^-)^\star} 1_{\{\eta(x)\eta(y)=2\}} + \Delta_1 \sum_{x\in\Lambda} 1_{\{\eta(x)=1\}} + \Delta_2 \sum_{x\in\Lambda} 1_{\{\eta(x)=2\}}, \tag{1.2}$$

where $(\Lambda^-)^\star = \{(x,y)\colon\ x,y \in \Lambda^-, |x-y| = 1\}$ is the set of non-oriented bonds inside Λ^-, $-U < 0$ is the *binding energy* between neighboring particles of *different* types inside Λ^-, and $\Delta_1 > 0$ and $\Delta_2 > 0$ are the *activation energies* of particles of type 1, respectively, type 2 inside Λ. W.l.o.g. we will assume that

$$\Delta_1 \leq \Delta_2. \tag{1.3}$$

The Gibbs measure associated with H is

$$\mu_\beta(\eta) = \frac{1}{Z_\beta}\, e^{-\beta H(\eta)}, \qquad \eta \in \mathcal{X}, \tag{1.4}$$

where $\beta \in (0,\infty)$ is the inverse temperature, and Z_β is the normalizing partition sum.

Kawasaki dynamics is the continuous-time Markov process $(\eta_t)_{t\geq 0}$ with state space $\mathcal{X}$ whose transition rates are

$$c_\beta(\eta,\eta') = \begin{cases} e^{-\beta[H(\eta')-H(\eta)]_+}, & \eta,\eta' \in \mathcal{X},\ \eta \sim \eta', \\ 0, & \text{otherwise}, \end{cases} \tag{1.5}$$

(i.e., Metroplis rate w.r.t. βH), where $\eta \sim \eta'$ means that η' can be obtained from η and vice versa by one of the following moves:

- interchanging the states $0 \leftrightarrow 1$ or $0 \leftrightarrow 2$ at neighboring sites in Λ ("hopping of particles inside Λ"),

- changing the state $0 \to 1$, $0 \to 2$, $1 \to 0$ or $2 \to 0$ at single sites in $\partial^-\Lambda$ ("creation and annihilation of particles inside $\partial^-\Lambda$").

This dynamics is ergodic and reversible with respect to the Gibbs measure μ_β. Note that particles are preserved in Λ^-, but can be created and annihilated in $\partial^-\Lambda$. Think of the particles entering and exiting Λ along non-oriented edges between $\partial^-\Lambda$ and $\partial^+\Lambda$ (where we allow only one edge for each site in $\partial^-\Lambda$). The pairs (η, η') with $\eta \sim \eta'$ are called *communicating configurations*, the transitions between them are called *allowed moves*. Note that particles in $\partial^-\Lambda$ do not interact with particles anywhere in Λ.

The dynamics defined by (1.2) and (1.5) models the behavior inside Λ of a lattice gas in $\mathbb{Z}^2$, consisting of two types of particles subject to random hopping with hard core repulsion and with binding between different neighboring types. We may think of $\mathbb{Z}^2 \backslash \Lambda$ as an *infinite reservoir* that keeps the particle densities inside Λ fixed at $\rho_1 = e^{-\beta\Delta_1}$ and $\rho_2 = e^{-\beta\Delta_2}$. In our model this reservoir is replaced by an *open boundary* $\partial^-\Lambda$, where particles are created and annihilated at a rate that matches these densities. Consequently, our Kawasaki dynamics is a *finite-state* Markov process.

Note that there is *no* binding energy between neighboring particles of the *same* type. Consequently, the model does *not* reduce to Kawasaki dynamics for one type of particle when $\Delta_1 = \Delta_2$.

1.2 Notation

To identify the metastable region in Section 1.3 and state our main theorems in Section 1.4, we need some notation.

Definition 1.2.1 *(a) $n_i(\eta)$ is the number of particles of type $i = 1, 2$ in η.*
(b) $B(\eta)$ is the number of bonds in $(\Lambda^-)^\star$ connecting neighboring particles of different type in η, i.e., the number of active bonds in η.
(c) A droplet is a maximal set of particles connected by active bonds.
(d) $\square$ is the configuration where Λ is empty, $\boxplus$ is the configuration where Λ is filled as a checkerboard (see Remark 1.4.8 below).
(e) $\omega\colon \eta \to \eta'$ is any path of allowed moves from η to η'.
(f) $\tau_{\mathcal{A}} = \inf\{t \geq 0\colon \eta_t \in \mathcal{A}, \exists\, 0 < s < t\colon \eta_s \notin \mathcal{A}\}$, $\mathcal{A} \subset \mathcal{X}$, is the first hitting/return time of $\mathcal{A}$.
(g) $\mathbb{P}_\eta$ is the law of $(\eta_t)_{t \geq 0}$ given $\eta_0 = \eta$.

Definition 1.2.2 *(a) $\Phi(\eta, \eta')$ is the communication height between $\eta, \eta' \in \mathcal{X}$ defined by*

$$\Phi(\eta, \eta') = \min_{\omega\colon \eta \to \eta'} \max_{\xi \in \omega} H(\xi), \tag{1.6}$$

and $\Phi(\mathcal{A}, \mathcal{B})$ is its extension to non-empty sets $\mathcal{A}, \mathcal{B} \subset \mathcal{X}$ defined by

$$\Phi(\mathcal{A}, \mathcal{B}) = \min_{\eta \in \mathcal{A}, \eta' \in \mathcal{B}} \Phi(\eta, \eta'). \tag{1.7}$$

(b) $\mathcal{S}(\eta, \eta')$ is the communication level set between η and η' defined by

$$\mathcal{S}(\eta, \eta') = \left\{ \zeta \in \mathcal{X}\colon \exists\, \omega\colon \eta \to \eta',\, \omega \ni \zeta\colon \max_{\xi \in \omega} H(\xi) = H(\zeta) = \Phi(\eta, \eta') \right\}. \tag{1.8}$$

(c) V_η *is the stability level of* $\eta \in \mathcal{X}$ *defined by*

$$V_\eta = \Phi(\eta, \mathcal{I}_\eta) - H(\eta), \tag{1.9}$$

where $\mathcal{I}_\eta = \{\xi \in \mathcal{X}\colon\ H(\xi) < H(\eta)\}$ *is the set of configurations with energy lower than* η.
(d) $\mathcal{X}_{\rm stab} = \{\eta \in \mathcal{X}\colon\ H(\eta) = \min_{\xi\in\mathcal{X}} H(\xi)\}$ *is the set of stable configurations, i.e., the set of configurations with minimal energy.*
(e) $\mathcal{X}_{\rm meta} = \{\eta \in \mathcal{X}\colon\ V_\eta = \max_{\xi\in\mathcal{X}\backslash\mathcal{X}_{\rm stab}} V_\xi\}$ *is the set of metastable configurations, i.e., the set of non-stable configurations with maximal stability level.*
(f) $\Gamma = V_\eta$ *for* $\eta \in \mathcal{X}_{\rm meta}$ *(note that* $\eta \mapsto V_\eta$ *is constant on* $\mathcal{X}_{\rm meta}$*),* $\Gamma^\star = \Phi(\square, \boxplus) - H(\square)$ *(note that* $H(\square) = 0$*).*

Definition 1.2.3 *(a)* $(\eta \to \eta')_{\rm opt}$ *is the set of paths realizing the minimax in* $\Phi(\eta, \eta')$.
(b) A set $\mathcal{W} \subset \mathcal{X}$ *is called a gate for* $\eta \to \eta'$ *if* $\mathcal{W} \subset \mathcal{S}(\eta, \eta')$ *and* $\omega \cap \mathcal{W} \neq \emptyset$ *for all* $\omega \in (\eta \to \eta')_{\rm opt}$.
(c) A set $\mathcal{W} \subset \mathcal{X}$ *is called a minimal gate for* $\eta \to \eta'$ *if it is a gate for* $\eta \to \eta'$ *and for any* $\mathcal{W}' \subsetneq \mathcal{W}$ *there exists an* $\omega' \in (\eta \to \eta')_{\rm opt}$ *such that* $\omega' \cap \mathcal{W}' = \emptyset$.
(d) A priori there may be several (not necessarily disjoint) minimal gates. Their union is denoted by $\mathcal{G}(\eta, \eta')$ *and is called the essential gate for* $(\eta \to \eta')_{\rm opt}$*. (The configurations in* $\mathcal{S}(\eta, \eta')\backslash\mathcal{G}(\eta, \eta')$ *are called dead-ends.)*

1.3 Metastable region

We want to understand how the system tunnels from $\square$ to $\boxplus$ when the former is a local minimum and the latter is a global minimum of H. We begin by identifying the *metastable region*, i.e., the region in parameter space for which this is the case.

Lemma 1.3.1 *The condition* $\Delta_1 + \Delta_2 < 4U$ *is necessary and sufficient for* $\square$ *to be a local minimum but not a global minimum of* H.

Proof. Note that $H(\square) = 0$. We know that $\square$ is a local minimum of H, since as soon as a particle enters Λ we obtain a configuration with energy either $\Delta_1 > 0$ or $\Delta_2 > 0$. To show that there is a configuration $\hat\eta$ with $H(\hat\eta) < 0$, we write

$$H(\eta) = n_1(\eta)\Delta_1 + n_2(\eta)\Delta_2 - B(\eta)U. \tag{1.10}$$

Since $\Delta_1 \leq \Delta_2$, we may assume w.l.o.g. that $n_1(\eta) \geq n_2(\eta)$. Indeed, if $n_1(\eta) < n_2(\eta)$, then we simply take the configuration $\eta^{1\Leftrightarrow 2}$ obtained from η by interchanging the types 1 and 2, i.e.,

$$\eta^{1\Leftrightarrow 2}(x) = \begin{cases} 1 & \text{if } \eta(x) = 2, \\ 2 & \text{if } \eta(x) = 1, \\ 0 & \text{otherwise,} \end{cases} \tag{1.11}$$

which satisfies $H(\eta^{1\Leftrightarrow 2}) \leq H(\eta)$.

Since $B(\eta) \leq 4n_2(\eta)$, we have

$$H(\eta) \geq n_1(\eta)\Delta_1 + n_2(\eta)\Delta_2 - 4n_2(\eta)U \geq n_2(\eta)(\Delta_1 + \Delta_2 - 4U). \tag{1.12}$$

Hence, if $\Delta_1 + \Delta_2 \geq 4U$, then $H(\eta) \geq 0$ for all η and $H(\square) = 0$ is a global minimum. On the other hand, consider a configuration $\hat\eta$ such that $n_1(\hat\eta) = n_2(\hat\eta)$ and $n_1(\hat\eta) + n_2(\hat\eta) = \ell^2$

for some $\ell \in 2\mathbb{N}$. Arrange the particles of $\hat{\eta}$ in a checkerboard square of side length ℓ. Then a straightforward computation gives

$$H(\hat{\eta}) = \tfrac{1}{2}\ell^2\Delta_1 + \tfrac{1}{2}\ell^2\Delta_2 - 2\ell(\ell-1)U, \tag{1.13}$$

and so

$$H(\hat{\eta}) < 0 \iff \ell^2(\Delta_1+\Delta_2) < 4\ell(\ell-1)U \iff \Delta_1+\Delta_2 < (4-4\ell^{-1})U. \tag{1.14}$$

Hence, if $\Delta_1+\Delta_2 < 4U$, then there exists an $\bar{\ell} \in 2\mathbb{N}$ such that $H(\hat{\eta}) < 0$ for all $\ell \in 2\mathbb{N}$ with $\ell \geq \bar{\ell}$. Here, Λ must be taken large enough, so that a droplet of size $\bar{\ell}$ fits inside Λ^-. ■

Note that $\Gamma^\star = \Gamma^\star(U,\Delta_1,\Delta_2) \in (0,\infty)$ because of Lemma 1.3.1.

Within the metastable region $\Delta_1+\Delta_2 < 4U$, we may as well exclude the subregion $\Delta_1,\Delta_2 < U$ (see Fig. 1). In this subregion, each time a particle of type 1 enters Λ and attaches itself to a particle of type 2 in the droplet, or vice versa, the energy goes down. Consequently, the "critical droplet" for the transition from $\square$ to $\boxplus$ consists of only two free particles, one of type 1 and one of type 2. Therefore this subregion does not exhibit proper metastable behavior.

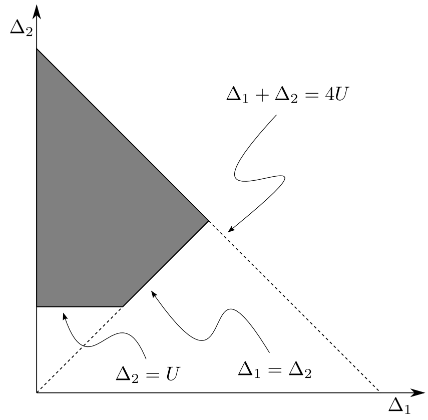

Figure 1: Proper metastable region.

1.4 Main theorems

Theorems 1.4.3–1.4.5 below will be proved in the *metastable region* subject to the following *hypotheses*:

(H1) $\mathcal{X}_{\mathrm{stab}} = \boxplus$.

(H2) There exists a $V^\star < \Gamma^\star$ such that $V_\eta \leq V^\star$ for all $\eta \in \mathcal{X}\backslash\{\square,\boxplus\}$.

The third hypothesis consists of three parts characterizing the entrance set of $\mathcal{G}(\square,\boxplus)$, the set of critical droplets, and the exit set of $\mathcal{G}(\square,\boxplus)$. To formulate this hypothesis some further definitions are needed.

Definition 1.4.1 *(a) $\mathcal{C}^\star_{\mathrm{bd}}$ is the minimal set of configurations in $\mathcal{G}(\square,\boxplus)$ such that all paths in $(\square\to\boxplus)_{\mathrm{opt}}$ enter $\mathcal{G}(\square,\boxplus)$ through $\mathcal{C}^\star_{\mathrm{bd}}$.*
(b) $\mathcal{P}$ is the set of configurations visited by these paths just prior to their first entrance of $\mathcal{G}(\square,\boxplus)$.

(H3-a) Every $\hat{\eta} \in \mathcal{P}$ consists of a *single droplet* somewhere in Λ^-. This single droplet fits inside an $L^\star \times L^\star$ square somewhere in Λ^- for some $L^\star \in \mathbb{N}$ large enough that is independent of $\hat{\eta}$ and Λ. Every $\eta \in \mathcal{C}^\star_{\mathrm{bd}}$ consists of a single droplet $\hat{\eta} \in \mathcal{P}$ and a *free particle* of type 2 somewhere in $\partial^-\Lambda$.

Definition 1.4.2 *(a) $\mathcal{C}^\star_{\mathrm{att}}$ is the set of configurations obtained from $\mathcal{P}$ by attaching a particle of type 2 to the single droplet, and decomposes as $\mathcal{C}^\star_{\mathrm{att}} = \cup_{\hat{\eta}\in\mathcal{P}} \mathcal{C}^\star_{\mathrm{att}}(\hat{\eta})$.*
(b) $\mathcal{C}^\star$ is the set of configurations obtained from $\mathcal{P}$ by adding a particle of type 2 somewhere in Λ, and decomposes as $\mathcal{C}^\star = \cup_{\hat{\eta}\in\mathcal{P}} \mathcal{C}^\star(\hat{\eta})$.

Note that $\Gamma^\star = H(\mathcal{C}^\star \backslash \mathcal{C}^\star_{\mathrm{att}}) = H(\mathcal{P}) + \Delta_2$, and that $\mathcal{C}^\star$ consists of precisely those configurations "interpolating" between $\mathcal{P}$ and $\mathcal{C}^\star_{\mathrm{att}}$: a free particle of type 2 enters $\partial^-\Lambda$ and moves to the single droplet where it attaches itself via an active bond. Think of $\mathcal{P}$ as the set of configurations where the dynamics is "almost over the hill", of $\mathcal{C}^\star$ as the set of configurations where the dynamics is "on top of the hill", and of the free particle as "achieving the crossover" when it attaches itself properly to the single droplet (the meaning of the word properly will become clear in Section 2.4).

The set $\mathcal{P}$ is referred to as the set of *protocritical droplets*. We write $N^\star$ to denote the cardinality of $\mathcal{P}$ modulo shifts of the droplet. The set $\mathcal{C}^\star \backslash \mathcal{C}^\star_{\mathrm{att}}$ is referred to as the set of *critical droplets*.

(H3-b) All transitions from $\mathcal{C}^\star$ that either add a particle in Λ or increase the number of droplets (by breaking an active bond) lead to energy $> \Gamma^\star$.

(H3-c) All $\omega \in (\mathcal{C}^\star_{\mathrm{bd}} \to \boxplus)_{\mathrm{opt}}$ pass through $\mathcal{C}^\star_{\mathrm{att}}$. For every $\hat{\eta} \in \mathcal{P}$ there exists a $\zeta \in \mathcal{C}^\star_{\mathrm{att}}(\hat{\eta})$ such that $\Phi(\zeta, \boxplus) < \Gamma^\star$.

We are now ready to state our main theorems subject to (H1)–(H3).

Theorem 1.4.3 *(a)* $\lim_{\beta\to\infty} P_\square(\tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\boxplus \mid \tau_\boxplus < \tau_\square) = 1$.
(b) $\lim_{\beta\to\infty} P_\square(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \zeta) = 1/|\mathcal{C}^\star_{\mathrm{bd}}|$ *for all* $\zeta \in \mathcal{C}^\star_{\mathrm{bd}}$.

Theorem 1.4.4 *There exists a constant $K = K(\Lambda; U, \Delta_1, \Delta_2) \in (0, \infty)$ such that*

$$\lim_{\beta\to\infty} e^{-\beta\Gamma^\star} E_\square(\tau_\boxplus) = K. \tag{1.15}$$

Moreover,

$$K \sim \frac{1}{N^\star} \frac{\log|\Lambda|}{4\pi|\Lambda|} \qquad \text{as } \Lambda \to \mathbb{Z}^2. \tag{1.16}$$

Theorem 1.4.5 $\lim_{\beta\to\infty} P_\square(\tau_\boxplus / E_\square(\tau_\boxplus) > t) = e^{-t}$ *for all* $t \geq 0$.

We close this section with a few remarks.

Remark 1.4.6 The free particle in (H3-a) is of type 2 only when $\Delta_1 < \Delta_2$. If $\Delta_1 = \Delta_2$ (recall (1.3)), then the free particle can be of type 1 or 2. Indeed, for $\Delta_1 = \Delta_2$ there is full symmetry of $\mathcal{S}(\square, \boxplus)$ under the map $1 \Leftrightarrow 2$ defined in (1.11).

Remark 1.4.7 We will see in Section 1.6 that (H1–H2) imply that

$$(\mathcal{X}_{\text{meta}}, \mathcal{X}_{\text{stab}}) = (\square, \boxplus), \qquad \Gamma = \Gamma^\star. \tag{1.17}$$

Remark 1.4.8 We will see in [17] that, depending on the shape of Λ and the choice of U, Δ_1, Δ_2, $\mathcal{X}_{\text{stab}}$ may actually consist of more than the single configuration $\boxplus$, namely, it may contain configurations that differ from $\boxplus$ in $\partial^-\Lambda$. Since this boundary effect does not affect our main theorems, we will ignore it here. A precise description of $\mathcal{X}_{\text{stab}}$ will be given in [17]. Moreover, depending on the choice of U, Δ_1, Δ_2, large droplets with minimal energy tend to have a shape that is either *square-shaped* or *rhombus-shaped*. Therefore it turns out to be expedient to choose Λ to have the same shape. Details will be given in [17].

Remark 1.4.9 As we will see in Section 2.4, the value of K is given by a *non-trivial variational formula* involving the set of all configurations where the dynamics can enter and exit $\mathcal{C}^\star$. This set includes not only the border of the "$\Gamma^\star$-valleys" around $\square$ and $\boxplus$, but also the border of "wells" inside the energy plateau $\mathcal{C}^\star$ that have energy $< \Gamma^\star$ but communication height $\Gamma^\star$ towards both $\square$ and $\boxplus$. It contains $\mathcal{P}$, $\mathcal{C}^\star_{\text{att}}$ and possibly more, as we will see in [18] (for Kawasaki dynamics with one type of particle this was shown in Bovier, den Hollander and Nardi [6], Section 2.3.2). As a result of this geometric complexity, for finite Λ only upper and lower bounds are known for K. What (1.16) says is that these bounds merge and simplify in the limit as $\Lambda \to \mathbb{Z}^2$ (after the limit $\beta \to \infty$ has already been taken), and that for the asymptotics only the simpler quantity $N^\star$ matters rather than the full geometry of critical and near critical droplets. We will see in Section 2.4 that, apart from the uniformity property expressed in Theorem 1.4.3(b), the reason behind this simplification is the fact that simple random walk (the motion of the free particle) is *recurrent* on $\mathbb{Z}^2$.

1.5 Discussion

1. Theorem 1.4.3(a) says that $\mathcal{C}^\star$ is a gate for the nucleation, i.e., on its way from $\square$ to $\boxplus$ the dynamics passes through $\mathcal{C}^\star$. Theorem 1.4.3(b) says that all protocritical droplets and all locations of the free particle in $\partial^-\Lambda$ are equally likely to be seen upon first entrance in $\mathcal{G}(\square, \boxplus)$. Theorem 1.4.4 says that the average nucleation time is asymptotic to $Ke^{\Gamma\beta}$, which is the classical Arrhenius law, and it identifies the asymptotics of the prefactor K in the limit as Λ becomes large. Theorem 1.4.5, finally, says that the nucleation time is exponentially distributed on the scale of its average.

2. Theorems 1.4.3–1.4.5 are *model-independent*, i.e., they are expected to hold in the same form for a large class of stochastic dynamics in a finite box at low temperature exhibiting metastable behavior. So far this universality has been verified for only a handful of examples, including Kawasaki dynamics with one type of particle (see also item 4 below). In Section 2 we will see that (H1)–(H3) are the *minimal* hypotheses needed for metastable behavior, in the sense that any relative of Kawasaki dynamics for which Theorems 1.4.3–1.4.5 hold must satisfy (H1)–(H3) (including multi-type Kawasaki dynamics).

The *model-dependent* ingredient of Theorems 1.4.3–1.4.5 is the triple

$$(\Gamma^\star, \mathcal{C}^\star, N^\star). \tag{1.18}$$

This triple depends on the parameters U, Δ_1, Δ_2 in a manner that will be identified in [17] and [18]. The set $\mathcal{C}^\star$ also depends on Λ, but in such a way that $|\mathcal{C}^\star| \sim N^\star|\Lambda|$ as $\Lambda \to \mathbb{Z}^2$, with the error coming from boundary effects. Clearly, Λ must be taken large enough so that critical droplets fit inside (i.e., Λ must contain an $L^\star \times L^\star$ square with $L^\star$ as in (H3-a)).

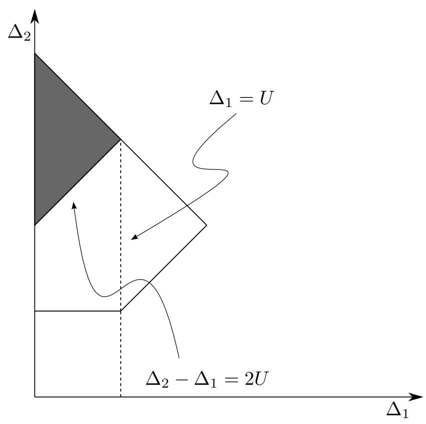

Figure 2: Subregion of the proper metastable region considered in [17] and [18].

3. In [17] and [18], we will prove (H1)–(H3), identify $(\Gamma^\star, \mathcal{C}^\star, N^\star)$ and derive an upper bound on $V^\star$ in the subregion of the proper metastable region given by (see Fig. 2)

$$\Delta_1 < U, \quad \Delta_2 - \Delta_1 > 2U. \tag{1.19}$$

More precisely, in [17] we will prove (H1), identify $\Gamma^\star$, show that $V^\star \leq 10U - \Delta_1$, and conclude that (H2) holds as soon as $\Gamma^\star > 10U - \Delta_1$, which poses further restrictions on U, Δ_1, Δ_2 on top of (1.19). In [17] we will also see that it would be possible to show that $V^\star \leq 4U + \Delta_1$ provided certain boundary effects (arising when a droplet sits close to $\partial^-\Lambda$ or when two or more droplets are close to each other) could be controlled. Since it will turn out that $\Gamma^\star > 4U + \Delta_1$ throughout the region (1.19), this upper bound would settle (H2) without further restrictions on U, Δ_1, Δ_2. In [18] we will prove (H3) and identify $\mathcal{C}^\star, N^\star$.

The simplifying features of (1.19) are the following: $\Delta_1 < U$ implies that each time a particle of type 1 enters Λ and attaches itself to a particle of type 2 in the droplet the energy goes down, while $\Delta_2 - \Delta_1 > 2U$ implies that no particle of type 2 sits on the boundary of a droplet that has minimal energy given the number of particles of type 2 in the droplet. We *conjecture* that (H1)–(H3) hold throughout the proper metastable region (see Fig. 1). However, as we will see in [17] and [18], $(\Gamma^\star, \mathcal{C}^\star, N^\star)$ is different when $\Delta_1 > U$ compared to when $\Delta_1 < U$ (because the critical droplets are square-shaped, respectively, rhombus-shaped).

4. Theorems 1.4.3–1.4.5 generalize what was obtained for Kawasaki dynamics with one type of particle in den Hollander, Olivieri and Scoppola [16], and Bovier, den Hollander and Nardi [6]. In these papers, the analogues of (H1)–(H3) were proved, $(\Gamma^\star, \mathcal{C}^\star, N^\star)$ was identified, and bounds on K were derived that become sharp in the limit as $\Lambda \to \mathbb{Z}^2$. What makes the model with one type of particle more tractable is that the stochastic dynamics follows a *skeleton* of subcritical droplets that are *squares or quasi-squares*, as a result of a *standard isoperimetric inequality* for two-dimensional droplets. For the model with two types of particles this tool is no longer applicable and the geometry is much harder, as will become clear in [17] and [18].

Similar results hold for Ising spins subject to *Glauber dynamics*, as shown in Neves and Schonmann [21], and Bovier and Manzo [8]. For this system, K has a simple explicit form.

Theorems 1.4.3–1.4.5 are close in spirit to the extension for Glauber dynamics when an alternating external field is included, as carried out in Nardi and Olivieri [19], and to the extension for Kawakasi dynamics with one type of particle when the interaction between particles is different in the horizontal and the vertical direction, as carried out in Nardi, Olivieri and Scoppola [20].

Our results can in principle be extended from $\mathbb{Z}^2$ to $\mathbb{Z}^3$. For one type of particle this extension was achieved in den Hollander, Nardi, Olivieri and Scoppola [15], and Bovier, den Hollander and Nardi [6]. For one type of particle the geometry of the critical droplet is more complex in $\mathbb{Z}^3$ than in $\mathbb{Z}^2$. This will also be the case for two types of particles, and hence it will be hard to identify $\mathcal{C}^\star$ and $N^\star$. Again, only upper and lower bounds can be derived for K. Moreover, since simple random walk on $\mathbb{Z}^3$ is *transient*, these bounds do *not* merge in the limit as $\Lambda \to \mathbb{Z}^3$. For Glauber dynamics the extension from $\mathbb{Z}^2$ to $\mathbb{Z}^3$ was achieved in Ben Arous and Cerf [1], and Bovier and Manzo [8], and K again has a simple explicit form.

5. In Gaudillière, den Hollander, Nardi, Olivieri and Scoppola [9], [10], [11], and Bovier, den Hollander and Spitoni [7], the result for Kawasaki dynamics (with one type of particle) on a finite box with an open boundary obtained in den Hollander, Olivieri and Scoppola [16] and Bovier, den Hollander and Nardi [6] have been extended to Kawasaki dynamics (with one type of particle) on a *large box* $\Lambda = \Lambda_\beta$ with a *closed boundary*. The volume of Λ_β grows exponentially fast with β, so that Λ_β itself acts as a gas reservoir for the growing and shrinking of subcritical droplets. The focus is on the time of the first appearance of a critical droplet *anywhere* in Λ_β. It turns out that the nucleation time in Λ_β roughly equals the nucleation time in a finite box Λ divided by the volume of Λ_β, i.e., *spatial entropy* enters into the game. A challenge is to derive a similar result for Kawasaki dynamics with two types of particles.

6. The model in the present paper can be extended by introducing three binding energies $U_{11}, U_{22}, U_{12} < 0$ for the three different pairs of types that can occur in a pair of neighboring particles. Clearly, this will further complicate the analysis, and consequently both $(\mathcal{X}_{\rm meta}, \mathcal{X}_{\rm stab})$ and $(\Gamma^\star, \mathcal{C}^\star, N^\star)$ will in general be different. The model is interesting even when $\Delta_1, \Delta_2 < 0$ and $U < 0$, since this corresponds to a situation where the infinite gas reservoir is very dense and tends to push particles into the box. When $\Delta_1 < \Delta_2$, particles of type 1 tend to fill Λ before particles of type 2 appear, but this is not the configuration of lowest energy. Indeed, if $\Delta_2 - \Delta_1 < 4U$, then the binding energy is strong enough to still favor configurations with a checkerboard structure (modulo boundary effects). Identifying $(\Gamma^\star, \mathcal{C}^\star, N^\star)$ seems a complicated task.

1.6 Consequences of (H1)–(H3)

Lemmas 1.6.1–1.6.4 below are immediate consequences of (H1)–(H3) and will be needed in the proof of Theorems 1.4.3–1.4.5 in Section 2.

Lemma 1.6.1 (H1)–(H2) *imply that* $V_\square = \Gamma^\star$.

Proof. By Definitions 1.2.2(c–f) and (H1), $\boxplus \in \mathcal{I}_\square$, which implies that $V_\square \leq \Gamma^\star$. We show that (H2) implies $V_\square = \Gamma^\star$. The proof is by contradiction. Suppose that $V_\square < \Gamma^\star$. Then, by Definition 1.2.2(c) and (H2), there exists an $\eta \in \mathcal{I}_\square \backslash \boxplus$ such that $\Phi(\square, \eta) - H(\square) < \Gamma^\star$. But, by (H2) and the finiteness of $\mathcal{X}$, there exist an $m \in \mathbb{N}$ and a sequence $\eta_0, \ldots, \eta_m \in \mathcal{X}$ with

$\eta_0 = \eta$ and $\eta_m = \boxplus$ such that $\eta_{i+1} \in \mathcal{I}_{\eta_i}$ and $\Phi(\eta_i, \eta_{i+1}) \leq H(\eta_i) + V^\star$ for $i = 0, \ldots, m-1$. Therefore

$$\Phi(\eta, \boxplus) \leq \max_{i=0,\ldots,m-1} \Phi(\eta_i, \eta_{i+1}) \leq \max_{i=0,\ldots,m-1} [H(\eta_i) + V^\star] = H(\eta) + V^\star < H(\square) + \Gamma^\star, \quad (1.20)$$

where in the first inequality we use that

$$\Phi(\eta, \sigma) \leq \max\{\Phi(\eta, \xi), \Phi(\xi, \sigma)\} \qquad \forall\, \eta, \sigma, \xi \in \mathcal{X}, \quad (1.21)$$

and in the last inequality that $\eta \in \mathcal{I}_\square$ and $V^\star < \Gamma^\star$. It follows that

$$\Gamma^\star = \Phi(\square, \boxplus) - H(\square) \leq \max\{\Phi(\square, \eta), \Phi(\eta, \boxplus)\} - H(\square) < \Gamma^\star, \quad (1.22)$$

which is a contradiction. ■

Lemma 1.6.2 (H2) *implies that* $\Phi(\eta, \{\square, \boxplus\}) - H(\eta) \leq V^\star$ *for all* $\eta \in \mathcal{X} \backslash \{\square, \boxplus\}$.

Proof. Fix $\eta \in \mathcal{X} \backslash \{\square, \boxplus\}$. By (H2) and the finiteness of $\mathcal{X}$, there exist an $m \in \mathbb{N}$ and a sequence $\eta_0, \ldots, \eta_m \in \mathcal{X}$ with $\eta_0 = \eta$ and $\eta_m \in \{\square, \boxplus\}$ such that $\eta_{i+1} \in \mathcal{I}_{\eta_i}$ and $\Phi(\eta_i, \eta_{i+1}) \leq H(\eta_i) + V^\star$ for $i = 0, \ldots, m-1$. Therefore, as in (1.20), we get $\Phi(\eta, \{\square, \boxplus\}) \leq H(\eta) + V^\star$. ■

Lemma 1.6.3 (H1)–(H2) *imply that* $H(\eta) > H(\square)$ *for all* $\eta \in \mathcal{X} \backslash \square$ *such that* $\Phi(\eta, \square) \leq \Phi(\eta, \boxplus)$.

Proof. By (H1), $\boxplus \in \mathcal{I}_\eta$ for all $\eta \neq \boxplus$. The proof is by contradiction. Fix $\eta \in \mathcal{X} \backslash \square$ and suppose that $H(\eta) \leq H(\square) = 0$. Then $\square \notin \mathcal{I}_\eta$. By (H2) and the finiteness of $\mathcal{X}$, there exist an $m \in \mathbb{N}$ and a sequence $\eta_0, \ldots, \eta_m \in \mathcal{X}$ with $\eta_0 = \eta$ and $\eta_m = \boxplus$ such that $\eta_{i+1} \in \mathcal{I}_{\eta_i}$ and $\Phi(\eta_i, \eta_{i+1}) \leq H(\eta_i) + V^\star$ for $i = 0, \ldots, m-1$. Therefore, as in (1.20), we get $\Phi(\eta, \boxplus) \leq H(\eta) + V^\star \leq H(\square) + V^\star < H(\square) + \Gamma^\star$. Hence

$$\begin{aligned} \Gamma^\star &= \Phi(\square, \boxplus) - H(\square) \leq \max\{\Phi(\square, \eta), \Phi(\eta, \boxplus)\} - H(\square) \\ &= \max\{\Phi(\eta, \square), \Phi(\eta, \boxplus)\} - H(\square) = \Phi(\eta, \boxplus) - H(\square) < \Gamma^\star, \end{aligned} \quad (1.23)$$

which is a contradiction. ■

Lemma 1.6.4 (H3a), (H3-c) *and Definition* 1.4.2(a) *imply that for every* $\eta \in \mathcal{C}^\star_{\mathrm{att}}$ *all paths in* $(\eta \to \square)_{\mathrm{opt}}$ *pass through* $\mathcal{C}^\star_{\mathrm{bd}}$.

Proof. Let η be any configuration in $\mathcal{C}^\star_{\mathrm{att}}$. Then, by (H3-a) and Definition 1.4.2(a), there is a configuration ξ, consisting of a single *protocritical* droplet, say, D and a free particle (of type 2) next to the border of D, such that η is obtained from ξ in a single move: the free particle attaches itself *somewhere* to D. Now, consider any path starting at η, ending at $\square$, and not exceeding energy level $\Gamma^\star$. The reverse of this path, starting at $\square$ and ending at η, can be extended by the single move from η to ξ to obtain a path from $\square$ to ξ that is also not exceeding energy level $\Gamma^\star$. Moreover, this path can be further extended from ξ to $\boxplus$ without exceeding energy level $\Gamma^\star$ as well. To see the latter, note that, by (H3-c), there is *some* location x on the border of D such that the configuration $\zeta \in \mathcal{C}^\star_{\mathrm{att}}$ consisting of D with the free particle attached at x is such that there is a path from ζ to $\boxplus$ that stays *below* energy level $\Gamma^\star$. Furthermore, we can move from ξ (with $H(\xi) = \Gamma^\star$) to ζ (with $H(\zeta) < \Gamma^\star$) at constant energy level $\Gamma^\star$, dropping below $\Gamma^\star$ only at ζ, simply by moving the free particle to x without letting it hit $\partial^-\Lambda$. (By (H3-a), there is room for the free particle to do so because D fits inside an $L^\star \times L^\star$ square somewhere in Λ^-. Even when D touches $\partial^-\Lambda$ the free particle can still avoid $\partial^-\Lambda$, because x can never be in $\partial^-\Lambda$: particles in $\partial^-\Lambda$ do not interact with particles in Λ^-.) The resulting path from $\square$ to $\boxplus$ (via η, ξ and ζ) is a path in $(\square \to \boxplus)_{\text{opt}}$. However, by Definition 1.4.1(a), *any* path in $(\square \to \boxplus)_{\text{opt}}$ must hit $\mathcal{C}^\star_{\text{bd}}$. Hence, the piece of the path from η to $\square$ must hit $\mathcal{C}^\star_{\text{bd}}$, because the piece of the path from η to $\boxplus$ (via ξ and ζ) does not. ■

2 Proof of main theorems

In this section we prove Theorems 1.4.3–1.4.5 subject to hypotheses (H1)–(H3). Sections 2.1–2.3 introduce the basic ingredients, while Sections 2.4–2.6 provide the proofs.

We will follow the *potential-theoretic* argument that was used in Bovier, den Hollander and Nardi [6] for Kawasaki dynamics with one type of particle. In fact, we will see that (H1)–(H3) are the *minimal* assumptions needed to prove Theorems 1.4.3–1.4.5.

2.1 Dirichlet form and capacity

The key ingredient of the potential-theoretic approach to metastability is the *Dirichlet form*

$$\mathcal{E}_\beta(h) = \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}} \mu_\beta(\eta) c_\beta(\eta,\eta')[h(\eta) - h(\eta')]^2, \qquad h\colon\ \mathcal{X} \to [0,1], \tag{2.1}$$

where μ_β is the Gibbs measure defined in (1.4) and c_β is the kernel of transition rates defined in (1.5). Given a pair of non-empty disjoint sets $\mathcal{A},\mathcal{B} \subset \mathcal{X}$, the *capacity* of the pair $\mathcal{A},\mathcal{B}$ is defined by

$$\text{CAP}_\beta(\mathcal{A},\mathcal{B}) = \min_{\substack{h\colon\ \mathcal{X}\to[0,1] \\ h|_{\mathcal{A}}\equiv 1, h|_{\mathcal{B}}\equiv 0}} \mathcal{E}_\beta(h), \tag{2.2}$$

where $h|_{\mathcal{A}} \equiv 1$ means that $h(\eta) = 1$ for all $\eta \in \mathcal{A}$ and $h|_{\mathcal{B}} \equiv 0$ means that $h(\eta) = 0$ for all $\eta \in \mathcal{B}$. The unique minimizer $h^\star_{\mathcal{A},\mathcal{B}}$ of (2.2), called the *equilibrium potential* of the pair $\mathcal{A},\mathcal{B}$, is given by

$$h^\star_{\mathcal{A},\mathcal{B}}(\eta) = P_\eta(\tau_{\mathcal{A}} < \tau_{\mathcal{B}}), \qquad \eta \in \mathcal{X}\backslash(\mathcal{A} \cup \mathcal{B}), \tag{2.3}$$

and is the solution of the equation

$$\begin{aligned} (c_\beta h)(\eta) &= 0, && \eta \in \mathcal{X}\backslash(\mathcal{A} \cup \mathcal{B}), \\ h(\eta) &= 1, && \eta \in \mathcal{A}, \\ h(\eta) &= 0, && \eta \in \mathcal{B}, \end{aligned} \tag{2.4}$$

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

$$\text{CAP}_\beta(\mathcal{A},\mathcal{B}) = \sum_{\eta \in \mathcal{A}} \mu_\beta(\eta)\, c_\beta(\eta, \mathcal{X}\backslash\eta)\, \mathbb{P}_\eta(\tau_{\mathcal{B}} < \tau_{\mathcal{A}}) \tag{2.5}$$

with $c_\beta(\eta,\mathcal{X}\backslash\eta) = \sum_{\eta' \in \mathcal{X}\backslash\eta} c_\beta(\eta,\eta')$ the rate of moving out of η. This rate enters because $\tau_{\mathcal{A}}$ is the first hitting time of $\mathcal{A}$ after the initial configuration is left (recall Definition 1.2.1(f)). Note that the reversibility of the dynamics and (2.1–2.2) imply

$$\text{CAP}_\beta(\mathcal{A},\mathcal{B}) = \text{CAP}_\beta(\mathcal{B},\mathcal{A}). \tag{2.6}$$

The following lemma establishes bounds on the capacity of two disjoint sets. These bounds are referred to as *a priori estimates* and will serve as the starting point for more refined estimates later on.

Lemma 2.1.1 *For every pair of non-empty disjoint sets $\mathcal{A},\mathcal{B}\subset\mathcal{X}$ there exist constants $0 < C_1 \leq C_2 < \infty$ (depending on Λ and $\mathcal{A},\mathcal{B}$) such that*

$$C_1 \leq e^{\beta\Phi(\mathcal{A},\mathcal{B})} Z_\beta \mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) \leq C_2 \qquad \forall\,\beta\in(0,\infty). \tag{2.7}$$

Proof. The proof is given in [6], Lemma 3.1.1. We repeat it here, because it uses basic properties of communication heights that provide useful insight.

Upper bound: The upper bound is obtained from (2.2) by picking $h = 1_{K(\mathcal{A},\mathcal{B})}$ with

$$K(\mathcal{A},\mathcal{B}) = \{\eta\in\mathcal{X}\colon\ \Phi(\eta,\mathcal{A}) \leq \Phi(\eta,\mathcal{B})\}. \tag{2.8}$$

The key observation is that if $\eta\sim\eta'$ with $\eta\in K(\mathcal{A},\mathcal{B})$ and $\eta'\in\mathcal{X}\backslash K(\mathcal{A},\mathcal{B})$, then

$$\begin{array}{ll} (1) & H(\eta') < H(\eta), \\ (2) & H(\eta) \geq \Phi(\mathcal{A},\mathcal{B}). \end{array} \tag{2.9}$$

To see (1), suppose that $H(\eta')\geq H(\eta)$. Clearly,

$$H(\eta') \geq H(\eta) \qquad \Longleftrightarrow \qquad \Phi(\eta',\mathcal{F}) = \Phi(\eta,\mathcal{F}) \vee H(\eta')\ \ \forall\,\mathcal{F}\subset\mathcal{X}. \tag{2.10}$$

But $\eta\in K(\mathcal{A},\mathcal{B})$ tells us that $\Phi(\eta,\mathcal{A})\leq\Phi(\eta,\mathcal{B})$, hence $\Phi(\eta',\mathcal{A})\leq\Phi(\eta',\mathcal{B})$ by (2.10), and hence $\eta'\in K(\mathcal{A},\mathcal{B})$, which is a contradiction.

To see (2), note that (1) implies the reverse of (2.10):

$$H(\eta) \geq H(\eta') \qquad \Longleftrightarrow \qquad \Phi(\eta,\mathcal{F}) = \Phi(\eta',\mathcal{F}) \vee H(\eta)\ \ \forall\,\mathcal{F}\subset\mathcal{X}. \tag{2.11}$$

Trivially, $\Phi(\eta,\mathcal{B})\geq H(\eta)$. We claim that equality holds. Indeed, suppose that equality fails. Then we get

$$H(\eta) < \Phi(\eta,\mathcal{B}) = \Phi(\eta',\mathcal{B}) < \Phi(\eta',\mathcal{A}) = \Phi(\eta,\mathcal{A}), \tag{2.12}$$

where the equalities come from (2.11), while the second inequality uses that $\eta'\in\mathcal{X}\backslash K(\mathcal{A},\mathcal{B})$. Thus, $\Phi(\eta,\mathcal{A})>\Phi(\eta,\mathcal{B})$, which contradicts $\eta\in K(\mathcal{A},\mathcal{B})$. From $\Phi(\eta,\mathcal{B})=H(\eta)$ we obtain $\Phi(\mathcal{A},\mathcal{B})\leq\Phi(\mathcal{A},\eta)\vee\Phi(\eta,\mathcal{B})=\Phi(\eta,\mathcal{B})=H(\eta)$, which proves (2).

Combining (2.9) with (1.4–1.5) and using reversibility, we find that

$$\mu_\beta(\eta)c_\beta(\eta,\eta') \leq \frac{1}{Z_\beta}e^{-\beta\Phi(\mathcal{A},\mathcal{B})} \qquad \forall\,\eta\in K(\mathcal{A},\mathcal{B}),\ \eta'\in\mathcal{X}\backslash K(\mathcal{A},\mathcal{B}),\ \eta\sim\eta'. \tag{2.13}$$

Hence

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) \leq \mathcal{E}_\beta(1_{K(\mathcal{A},\mathcal{B})}) \leq C_2\frac{1}{Z_\beta}\,e^{-\beta\Phi(\mathcal{A},\mathcal{B})} \tag{2.14}$$

with $C_2 = |\{(\eta,\eta')\in\mathcal{X}^2\colon\ \eta\in K(\mathcal{A},\mathcal{B}),\eta'\in\mathcal{X}\backslash K(\mathcal{A},\mathcal{B}),\eta\sim\eta'\}|$.

Lower bound: The lower bound is obtained by picking any path $\omega=(\omega_0,\omega_1,\dots,\omega_L)$ that realizes the minimax in $\Phi(\mathcal{A},\mathcal{B})$ and ignoring all the transitions that are not in this path, i.e.,

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) \geq \min_{\substack{h\colon\,\omega\to[0,1]\\ h(\omega_0)=1,h(\omega_L)=0}} \mathcal{E}^\omega_\beta(h), \tag{2.15}$$

where the Dirichlet form $\mathcal{E}^{\omega}_{\beta}$ is defined as $\mathcal{E}_{\beta}$ in (2.1) but with $\mathcal{X}$ replaced by ω. Due to the one-dimensional nature of the set ω, the variational problem in the right-hand side can be solved explicitly by elementary computations. One finds that the minimum equals

$$M = \left[\sum_{l=0}^{L-1} \frac{1}{\mu_\beta(\omega_l)c_\beta(\omega_l,\omega_{l+1})}\right]^{-1}, \tag{2.16}$$

and is uniquely attained at h given by

$$h(\omega_l) = M \sum_{k=0}^{l-1} \frac{1}{\mu_\beta(\omega_k)c_\beta(\omega_k,\omega_{k+1})}, \qquad l = 0,1,\dots,L. \tag{2.17}$$

We thus have

$$\begin{aligned} \mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) &\geq M \\ &\geq \frac{1}{L} \min_{l=0,1,\dots,L-1} \mu_\beta(\omega_l)c_\beta(\omega_l,\omega_{l+1}) \\ &= \frac{1}{K}\frac{1}{Z_\beta} \min_{l=0,1,\dots,L-1} e^{-\beta[H(\omega_l)\vee H(\omega_{l+1})]} \\ &= C_1 \frac{1}{Z_\beta}\, e^{-\beta\Phi(\mathcal{A},\mathcal{B})} \end{aligned} \tag{2.18}$$

with $C_1 = 1/L$. ■

2.2 Graph structure of the energy landscape

View $\mathcal{X}$ as a graph whose *vertices* are the configurations and whose *edges* connect communicating configurations, i.e., (η,η') is an edge if and only if $\eta \sim \eta'$. Define

- $\mathcal{X}^\star$ is the subgraph of $\mathcal{X}$ obtained by removing all vertices η with $H(\eta) > \Gamma^\star$ and all edges incident to these vertices;
- $\mathcal{X}^{\star\star}$ is the subgraph of $\mathcal{X}^\star$ obtained by removing all vertices η with $H(\eta) = \Gamma^\star$ and all edges incident to these vertices;
- $\mathcal{X}_\square$ and $\mathcal{X}_\boxplus$ are the connected components of $\mathcal{X}^{\star\star}$ containing $\square$ and $\boxplus$, respectively.

Lemma 2.2.1 *The sets $\mathcal{X}_\square$ and $\mathcal{X}_\boxplus$ are disjoint (and hence are disconnected in $\mathcal{X}^{\star\star}$), and*

$$\begin{aligned} \mathcal{X}_\square &= \{\eta \in \mathcal{X}\colon\ \Phi(\eta,\square) < \Phi(\eta,\boxplus) = \Gamma^\star\}, \\ \mathcal{X}_\boxplus &= \{\eta \in \mathcal{X}\colon\ \Phi(\eta,\boxplus) < \Phi(\eta,\square) = \Gamma^\star\}. \end{aligned} \tag{2.19}$$

Moreover, $\mathcal{P} \subset \mathcal{X}_\square$, and $\mathcal{C}^\star_{\mathrm{att}}(\hat\eta) \cap \mathcal{X}_\boxplus \neq \emptyset$ for all $\hat\eta \in \mathcal{P}$.

Proof. By Definition 1.2.2(f), all paths connecting $\square$ and $\boxplus$ reach energy level $\geq \Gamma^\star$. Therefore $\mathcal{X}_\square$ and $\mathcal{X}_\boxplus$ are disconnected in $\mathcal{X}^{\star\star}$ (because $\mathcal{X}^{\star\star}$ does not contain vertices with energy $\geq \Gamma^\star$).

First note that, by (H2) and (1.21), $\Gamma^\star = \Phi(\square,\boxplus) \leq \max\{\Phi(\eta,\square),\Phi(\eta,\boxplus)\} \leq \Gamma^\star$, and hence either $\Phi(\eta,\square) = \Gamma^\star$ or $\Phi(\eta,\boxplus) = \Gamma^\star$ or both. To check the first line of (2.19) we argue as follows. For any $\eta \in \mathcal{X}_\square$, we have $H(\eta) < \Gamma^\star$ (because $\mathcal{X}_\square \subset \mathcal{X}^{\star\star}$) and $\Phi(\eta,\square) < \Gamma^\star$ (because $\mathcal{X}$ is connected). Conversely, let η be such that $\Phi(\eta,\square) < \Gamma^\star$. Then $H(\eta) < \Gamma^\star$, hence $\eta \in \mathcal{X}^{\star\star}$, and there is a path connecting η and $\square$ that stays below energy level $\Gamma^\star$. Therefore η belongs to the connected component of $\mathcal{X}^{\star\star}$ containing $\square$, i.e., $\eta \in \mathcal{X}_\square$. The second line of (2.19) is checked in an analogous manner.

To prove that $\mathcal{P} \subset \mathcal{X}_\square$, we must show that $\Phi(\square, \hat\eta) < \Gamma^\star$ for all $\hat\eta \in \mathcal{P}$. Pick any $\hat\eta \in \mathcal{P}$, and let $\eta \in \mathcal{C}^\star_{\mathrm{bd}}$ be any configuration obtained from $\hat\eta$ by adding a particle of type 2 somewhere in $\partial^-\Lambda$. Denote by $\Omega(\eta)$ the set of optimal paths from $\square$ to $\boxplus$ that enter $\mathcal{G}(\square,\boxplus)$ via η (note that this set is non-empty because $\mathcal{C}^\star_{\mathrm{bd}}$ is a minimal gate by Definition 1.4.1(a)). By Definition 1.4.1(b), $\omega_i \in \Omega(\eta)$ visits $\hat\eta$ before η for all $i \in 1,\dots,|\Omega(\eta)|$. The proof proceeds via contradiction. Suppose that $\max_{\sigma\in\omega_i\backslash S_i(\eta)} H(\sigma) = \Gamma^\star$ for all $i \in 1,\dots,|\Omega(\eta)|$, where $S_i(\eta)$ consists of η and all its successors in ω_i. Let $\sigma_i^\star(\eta)$ be the last configuration $\sigma \in \omega_i\backslash S_i(\eta)$ such that $H(\sigma) = \Gamma^\star$, and put $\mathcal{L}(\eta) = \{\sigma_1^\star(\eta),\dots,\sigma^\star_{|\Omega(\eta)|}(\eta)\}$. Then the set $(\mathcal{C}^\star_{\mathrm{bd}}\backslash\eta) \cup \mathcal{L}(\eta)$ is a minimal gate. But ω_i hits $\sigma_i^\star(\eta)$ before η, and so this contradicts the fact that $\mathcal{C}^\star_{\mathrm{bd}}$ is the entrance set of $\mathcal{G}(\square,\boxplus)$.

The claim that $\mathcal{C}^\star_{\mathrm{att}}(\hat\eta) \cap \mathcal{X}_\boxplus \neq \emptyset$ for all $\hat\eta \in \mathcal{P}$ is immediate from (H3-c). ■

We now have all the geometric ingredients that are necessary for the proof of Theorems 1.4.3–1.4.5 along the lines of [6], Section 3. Our hypotheses (H1)–(H3) replace the somewhat delicate and model-dependent geometric analysis for Kawasaki dynamics with one type of particle that was carried out in [6], Section 2. They are the *minimal hypotheses* that are necessary to carry out the proof below. Their verification will be given in [17] and [18].

2.3 Metastable set, link between average nucleation time and capacity

Bovier, Eckhoff, Gayrard and Klein [5] define metastable sets in terms of capacities:

Definition 2.3.1 *A non-empty set $\mathcal{A} \subset \mathcal{X}$ is called metastable if*

$$\lim_{\beta\to\infty} \frac{\max_{\eta\notin\mathcal{A}} \mu_\beta(\eta)/\mathrm{CAP}_\beta(\eta,\mathcal{A})}{\min_{\eta\in\mathcal{A}} \mu_\beta(\eta)/\mathrm{CAP}_\beta(\eta,\mathcal{A}\backslash\eta)} = 0. \tag{2.20}$$

In order to apply the theory in [5], we need the following.

Lemma 2.3.2 *The set $\{\square,\boxplus\}$ is metastable in the sense of Definition* 2.3.1.

Proof. By (1.4), Lemma 1.6.2 and the lower bound in (2.7), the numerator is bounded from above by $e^{V^\star\beta}/C_1 = e^{(\Gamma^\star-\delta)\beta}/C_1$ for some $\delta > 0$. By (1.4), the definition of $\Gamma^\star$ and the upper bound in (2.7), the denominator is bounded from below by $e^{\Gamma^\star\beta}/C_2$ (with the minimum being attained at $\square$). ■

Lemma 2.3.2 has an important consequence:

Lemma 2.3.3 $\mathbb{E}_\square(\tau_\boxplus) = [Z_\beta \mathrm{CAP}_\beta(\square,\boxplus)]^{-1}\,[1+o(1)]$ *as $\beta\to\infty$.*

Proof. According to [5], Theorem 1.3(i), we have

$$\mathbb{E}_\square(\tau_\boxplus) = \frac{\mu_\beta(\mathcal{R}_\square)}{\mathrm{CAP}_\beta(\square,\boxplus)}\,[1+o(1)] \qquad \text{as } \beta\to\infty, \tag{2.21}$$

where

$$\mathcal{R}_\square = \big\{\eta \in \mathcal{X}\colon\ \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) \geq \mathbb{P}_\eta(\tau_\boxplus < \tau_\square)\big\}. \tag{2.22}$$

Recalling (2.3), we can rewrite (2.22) as $\mathcal{R}_\square = \{\eta \in \mathcal{X}\colon\ h^\star_{\square,\boxplus}(\eta) \geq \frac{1}{2}\}$. It follows from Lemma 2.4.1 below that

$$\lim_{\beta\to\infty} \min_{\eta\in\mathcal{X}_\square} h^\star_{\square,\boxplus}(\eta) = 1, \qquad \lim_{\beta\to\infty} \max_{\eta\in\mathcal{X}_\boxplus} h^\star_{\square,\boxplus}(\eta) = 0. \tag{2.23}$$

Hence, for β large enough,

$$\mathcal{X}_\square \subset \mathcal{R}_\square \subset \mathcal{X}\backslash\mathcal{X}_\boxplus. \tag{2.24}$$

By Lemma 2.2.1, the second inclusion implies that $\Phi(\eta,\square) \leq \Phi(\eta,\boxplus)$ for all $\eta \in \mathcal{R}_\square$. Therefore Lemma 1.6.3 yields

$$\min_{\eta\in\mathcal{R}_\square\backslash\square} H(\eta) > H(\square) = 0, \tag{2.25}$$

which implies that $\mu_\beta(\mathcal{R}_\square)/\mu_\beta(\square) = 1 + o(1)$. Since $\mu_\beta(\square) = 1/Z_\beta$, the claim follows. ■

Lemma 2.3.3 shows that the proof of Theorem 1.4.4 revolves around getting sharp bounds on $Z_\beta \mathrm{CAP}_\beta(\square,\boxplus)$. The a priori estimates in Lemma 2.1.1 serve as a jump board for the derivation of these bounds.

2.4 Proof of Theorem 1.4.4

Our starting point is Lemma 2.3.3. Recalling (2.1–2.3), our task is to show that

$$\begin{aligned} Z_\beta \mathrm{CAP}_\beta(\square,\boxplus) &= \tfrac{1}{2} \sum_{\eta,\eta'\in\mathcal{X}} Z_\beta \mu_\beta(\eta) c_\beta(\eta,\eta')\,[h^\star_{\square,\boxplus}(\eta) - h^\star_{\square,\boxplus}(\eta')]^2 \\ &= [1+o(1)]\,\Theta\, e^{-\Gamma^\star\beta} \qquad \text{as } \beta\to\infty, \end{aligned} \tag{2.26}$$

and to identify the constant Θ, since (2.26) will imply (1.15) with $\Theta = 1/K$. This is done in four steps, organized in Sections 2.4.1–2.4.4.

2.4.1 Step 1: Triviality of $h^\star_{\square,\boxplus}$ on $\mathcal{X}_\square$, $\mathcal{X}_\boxplus$ and $\mathcal{X}^{\star\star}\backslash(\mathcal{X}_\square \cup \mathcal{X}_\boxplus)$

For all $\eta \in \mathcal{X}\backslash\mathcal{X}^\star$ we have $H(\eta) > \Gamma^\star$, and so there exists a $\delta > 0$ such that $Z_\beta\mu_\beta(\eta) \leq e^{-(\Gamma^\star+\delta)\beta}$. Therefore, we can replace $\mathcal{X}$ by $\mathcal{X}^\star$ in the sum in (2.26) at the cost of a prefactor $1 + O(e^{-\delta\beta})$. Moreover, we have the following analogue of [6], Lemma 3.3.1.

Lemma 2.4.1 *There exist $C < \infty$ and $\delta > 0$ such that*

$$\min_{\eta\in\mathcal{X}_\square} h^\star_{\square,\boxplus}(\eta) \geq 1 - Ce^{-\delta\beta}, \qquad \max_{\eta\in\mathcal{X}_\boxplus} h^\star_{\square,\boxplus}(\eta) \leq Ce^{-\delta\beta}, \qquad \forall\,\beta\in(0,\infty). \tag{2.27}$$

Proof. A standard renewal argument gives the relations, valid for $\eta \notin \{\square,\boxplus\}$,

$$\mathbb{P}_\eta(\tau_\boxplus < \tau_\square) = \frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_{\square\cup\eta})}{1 - \mathbb{P}_\eta(\tau_{\square\cup\boxplus} > \tau_\eta)}, \qquad \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) = \frac{\mathbb{P}_\eta(\tau_\square < \tau_{\boxplus\cup\eta})}{1 - \mathbb{P}_\eta(\tau_{\square\cup\boxplus} > \tau_\eta)}. \tag{2.28}$$

For $\eta \in \mathcal{X}_\square\backslash\square$, we estimate

$$h^\star_{\square,\boxplus}(\eta) = 1 - \mathbb{P}_\eta(\tau_\boxplus < \tau_\square) = 1 - \frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_{\square\cup\eta})}{\mathbb{P}_\eta(\tau_{\square\cup\boxplus} < \tau_\eta)} \geq 1 - \frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_\eta)}{\mathbb{P}_\eta(\tau_\square < \tau_\eta)} \tag{2.29}$$

and, with the help of (2.5) and Lemma 2.1.1,

$$\frac{\mathbb{P}_\eta(\tau_{\boxplus} < \tau_\eta)}{\mathbb{P}_\eta(\tau_{\square} < \tau_\eta)} = \frac{Z_\beta \, \mathrm{CAP}_\beta(\eta, \boxplus)}{Z_\beta \, \mathrm{CAP}_\beta(\eta, \square)} \leq C(\eta) \, e^{-[\Phi(\eta,\boxplus)-\Phi(\eta,\square)]\beta} \leq C(\eta) \, e^{-\delta\beta}, \tag{2.30}$$

which proves the first claim with $C = \max_{\eta \in \mathcal{X}_\square \backslash \square} C(\eta)$. Note that $h^\star_{\square,\boxplus}(\square)$ is a convex combination of $h^\star_{\square,\boxplus}(\eta)$ with $\eta \in \mathcal{X}_\square \backslash \square$, and so the claim includes $\eta = \square$.

For $\eta \in \mathcal{X}_\boxplus \backslash \boxplus$, we estimate

$$h^\star_{\square,\boxplus}(\eta) = \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) = \frac{\mathbb{P}_\eta(\tau_\square < \tau_{\boxplus \cup \eta})}{\mathbb{P}_\eta(\tau_{\square \cup \boxplus} < \tau_\eta)} \leq \frac{\mathbb{P}_\eta(\tau_\square < \tau_\eta)}{\mathbb{P}_\eta(\tau_\boxplus < \tau_\eta)} \tag{2.31}$$

and, with the help of (2.5) and Lemma 2.1.1,

$$\frac{\mathbb{P}_\eta(\tau_{\square} < \tau_\eta)}{\mathbb{P}_\eta(\tau_{\boxplus} < \tau_\eta)} = \frac{Z_\beta \, \mathrm{CAP}_\beta(\eta, \square)}{Z_\beta \, \mathrm{CAP}_\beta(\eta, \boxplus)} \leq C(\eta) \, e^{-[\Phi(\eta,\square)-\Phi(\eta,\boxplus)]\beta} \leq C(\eta) \, e^{-\delta\beta}, \tag{2.32}$$

which proves the second claim with $C = \max_{\eta \in \mathcal{X}_\boxplus \backslash \boxplus} C(\eta)$. ■

In view of Lemma 2.4.1, $h^\star_{\square,\boxplus}$ is trivial on the set $\mathcal{X}_\square \cup \mathcal{X}_\boxplus$, and its contribution to the sum in (2.26), which is $O(e^{-\delta\beta})$, can be accounted for by the prefactor $1 + o(1)$. Consequently, all that is needed is to understand what $h^\star_{\square,\boxplus}$ looks like on the set

$$\mathcal{X}^\star \backslash (\mathcal{X}_\square \cup \mathcal{X}_\boxplus) = \{\eta \in \mathcal{X}^\star \colon \; \Phi(\eta, \square) = \Phi(\eta, \boxplus) = \Gamma^\star\}. \tag{2.33}$$

However, $h^\star_{\square,\boxplus}$ is also trivial on the set

$$\mathcal{X}^{\star\star} \backslash (\mathcal{X}_\square \cup \mathcal{X}_\boxplus) = \bigcup_{i=1}^{I} \mathcal{X}_i, \tag{2.34}$$

which is a union of wells $\mathcal{X}_i$, $i = 1, \ldots, I$, in $\mathcal{S}(\square, \boxplus)$ for some $I \in \mathbb{N}$. (Each $\mathcal{X}_i$ is a maximal set of communicating configurations with energy $< \Gamma^\star$ and with communication height $\Gamma^\star$ towards both $\square$ and $\boxplus$.) Namely, we have the following analogue of [6], Lemma 3.3.2.

Lemma 2.4.2 *There exist $C < \infty$ and $\delta > 0$ such that*

$$\max_{\eta, \eta' \in \mathcal{X}_i} |h^\star_{\square,\boxplus}(\eta) - h^\star_{\square,\boxplus}(\eta')| \leq C e^{-\delta\beta} \qquad \forall \, i = 1, \ldots, I, \; \beta \in (0, \infty). \tag{2.35}$$

Proof. Fix i. Let $\eta' \in \mathcal{X}_i$ be such that $\min_{\sigma \in \mathcal{X}_i} H(\sigma) = H(\eta_i)$ and pick $\eta \in \mathcal{X}_i$. Estimate

$$h^\star_{\square,\boxplus}(\eta) = \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) \leq \mathbb{P}_\eta(\tau_\square < \tau_{\eta'}) + \mathbb{P}_\eta(\tau_{\eta'} < \tau_\square < \tau_\boxplus). \tag{2.36}$$

First, as in the proof of Lemma 2.4.1, we have

$$\begin{aligned} \mathbb{P}_\eta(\tau_\square < \tau_{\eta'}) &= \frac{\mathbb{P}_\eta(\tau_\square < \tau_{\eta \cup \eta'})}{1 - \mathbb{P}_\eta(\tau_{\square \cup \eta'} > \tau_\eta)} \leq \frac{\mathbb{P}_\eta(\tau_\square < \tau_\eta)}{\mathbb{P}_\eta(\tau_{\eta'} < \tau_\eta)} \\ &= \frac{Z_\beta \mathrm{CAP}_\beta(\eta, \square)}{Z_\beta \mathrm{CAP}_\beta(\eta, \eta')} \leq C(\eta, \eta') \, e^{-[\Phi(\eta,\square)-\Phi(\eta,\eta')]\beta} \leq C(\eta, \eta') \, e^{-\delta\beta}, \end{aligned} \tag{2.37}$$

where we use that $\Phi(\eta, \square) = \Gamma^\star$ and $\Phi(\eta, \eta') < \Gamma^\star$. Second,

$$\mathbb{P}_\eta(\tau_{\eta'} < \tau_\square < \tau_\boxplus) = \mathbb{P}_\eta(\tau_{\eta'} < \tau_{\square \cup \boxplus}) \mathbb{P}_{\eta'}(\tau_\square < \tau_\boxplus) \leq \mathbb{P}_{\eta'}(\tau_\square < \tau_\boxplus) = h^\star_{\square,\boxplus}(\eta'). \tag{2.38}$$

Combining (2.36–2.38), we get

$$h^\star_{\square,\boxplus}(\eta) \leq C(\eta,\eta')\, e^{-\delta\beta} + h^\star_{\square,\boxplus}(\eta') \tag{2.39}$$

Interchanging η and η',we get the claim with $C = \max_i \max_{\eta,\eta' \in \mathcal{X}_i} C(\eta,\eta')$. ■

In view of Lemma 2.4.2, the contribution to the sum in (2.26) of the transitions inside a well can also be put into the prefactor $1 + o(1)$. Thus, only the transitions *in and out of wells* contribute.

2.4.2 Step 2: Variational formula for K

By Step 1, the estimation of $Z_\beta \mathrm{CAP}_\beta(\square,\boxplus)$ reduces to the study of a simpler variational problem. The following is the analogue of [6], Proposition 3.3.3.

Lemma 2.4.3 $Z_\beta \mathrm{CAP}_\beta(\square,\boxplus) = [1+o(1)]\, \Theta\, e^{-\Gamma^\star\beta}$ *as* $\beta \to \infty$ *with*

$$\Theta = \min_{C_1\dots,C_I} \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h|_{\mathcal{X}_\square} \equiv 1,\, h|_{\mathcal{X}_\boxplus} \equiv 0,\, h|_{\mathcal{X}_i} \equiv C_i\ \forall\, i=1,\dots,I}} \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}^\star} 1_{\{\eta \sim \eta'\}}\, [h(\eta) - h(\eta')]^2. \tag{2.40}$$

Proof. First, recalling (1.4–1.5) and (2.1–2.2), we have

$$\begin{aligned} Z_\beta\, \mathrm{CAP}_\beta(\square,\boxplus) &= Z_\beta \min_{\substack{h:\ \mathcal{X} \to [0,1] \\ h(\square)=1,\, h(\boxplus)=0}} \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}} \mu_\beta(\eta) c_\beta(\eta,\eta') [h(\eta) - h(\eta')]^2 \\ &= O\left(e^{-(\Gamma^\star+\delta)\beta}\right) + Z_\beta \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h(\square)=1,\, h(\boxplus)=0}} \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta,\eta') [h(\eta) - h(\eta')]^2. \end{aligned} \tag{2.41}$$

Next, with the help of Lemmas 2.4.1–2.4.2, we get

$$\begin{aligned} &\min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h(\square)=1,\, h(\boxplus)=0}} \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta,\eta') [h(\eta) - h(\eta')]^2 \\ &= \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h = h^\star_{\square,\boxplus} \text{ on } \mathcal{X}_\square \cup \mathcal{X}_\boxplus \cup (\mathcal{X}_1,\dots,\mathcal{X}_I)}} \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta,\eta') [h(\eta) - h(\eta')]^2 \\ &= [1 + O(e^{-\delta\beta})] \min_{C_1,\dots,C_I} \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h|_{\mathcal{X}_\square} \equiv 1,\, h|_{\mathcal{X}_\boxplus} \equiv 0,\, h|_{\mathcal{X}_i} \equiv C_i\ \forall\, i=1,\dots,I}} \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta,\eta') [h(\eta) - h(\eta')]^2, \end{aligned} \tag{2.42}$$

where the error term $O(e^{-\delta\beta})$ arises after we replace the *approximate* boundary conditions

$$h = \begin{cases} 1 - O(e^{-\delta\beta}) & \text{on } \mathcal{X}_\square, \\ O(e^{-\delta\beta}) & \text{on } \mathcal{X}_\boxplus, \\ C_i + O(e^{-\delta\beta}) & \text{on } \mathcal{X}_i,\ i = 1,\dots,I, \end{cases} \tag{2.43}$$

by the *sharp* boundary conditions

$$h = \begin{cases} 1 & \text{on } \mathcal{X}_\square, \\ 0 & \text{on } \mathcal{X}_\boxplus, \\ C_i & \text{on } \mathcal{X}_i,\ i = 1,\dots,I. \end{cases} \tag{2.44}$$

Finally, by (1.4–1.5) and reversibility, we have

$$Z_\beta \mu_\beta(\eta) c_\beta(\eta, \eta') = 1_{\{\eta \sim \eta'\}}\, e^{-\Gamma^\star \beta} \text{ for all } \eta, \eta' \in \mathcal{X}^\star \text{ that are not either both in } \mathcal{X}_\square \text{ or both in } \mathcal{X}_\boxplus \text{ or both in } \mathcal{X}_i \text{ for some } i = 1, \ldots, I. \tag{2.45}$$

To check the latter, note that there are no allowed moves between these sets, so that either $H(\eta) = \Gamma^\star > H(\eta')$ or $H(\eta) < \Gamma^\star = H(\eta')$ for allowed moves in and out of these sets. ■

Combining Lemmas 2.3.3 and 2.4.3, we see that we have completed the proof of (1.15) with $K = 1/\Theta$. The variational formula for $\Theta = \Theta(\Lambda; U, \Delta_1, \Delta_2)$ is *non-trivial* because it depends on the geometry of the wells $\mathcal{X}_i$, $i = 1, \ldots, I$.

2.4.3 Step 3: Bounds on K in terms of capacities of simple random walk

So far we have only used (H1)–(H2). In the remainder of the proof we use (H3) to prove (1.16). The intuition behind (1.16) is the following. When the free particle attaches itself to the protocritial droplet, the dynamics enters the set $\mathcal{C}^\star_{\text{att}}$. The entrance configurations of $\mathcal{C}^\star_{\text{att}}$ are either in $\mathcal{X}_\boxplus$ or in one of the $\mathcal{X}_i$'s. In the former case the path can reach $\boxplus$ while staying below $\Gamma^\star$ in energy, in the latter case it cannot. By Lemma 1.6.4, if the path exits an $\mathcal{X}_i$, then for it to return to $\mathcal{X}_\square$ it must pass through $\mathcal{C}^\star_{\text{bd}}$, i.e., it must go through a series of configurations consisting of a single protocritical droplet and a free particle moving away from that protocritical droplet towards $\partial^-\Lambda$. Now, this backward motion has a small probability because simple random walk in $\mathbb{Z}^2$ is *recurrent*, namely, the probability is $[1 + o(1)]\, 4\pi/\log|\Lambda|$ as $\Lambda \to \mathbb{Z}^2$ (see [6], Equation (3.4.5)). Therefore, the free particle is likely to re-attach itself to the protocritical droplet before it manages to reach $\partial^-\Lambda$. Consequently, with a probability tending to 1 as $\Lambda \to \mathbb{Z}^2$, before the free particle manages to reach $\partial^-\Lambda$ it will re-attach itself to the protocritical droplet in all possible ways, which must include a way such that the dynamics enters $\mathcal{X}_\boxplus$. In other words, after entering $\mathcal{C}^\star_{\text{att}}$ the path is likely to reach $\mathcal{X}_\boxplus$ before it returns to $\mathcal{X}_\square$, i.e., it "goes over the hill". Thus, in the limit as $\Lambda \to \mathbb{Z}^2$, the $\mathcal{X}_i$'s become *irrelevant*, and the dominant role is played by the transitions in and out of $\mathcal{X}_\square$ and by the simple random walk performed by the free particle.

Remark 2.4.4 The protocritical droplet may change each time the path enters and exits an $\mathcal{X}_i$. There are $\mathcal{X}_i$'s from which the path can reach $\boxplus$ without going back to $\mathcal{C}^\star$ and without exceeding $\Gamma^\star$ in energy (see the proof of [6], Theorem 1.4.3, where this is shown for Kawasaki dynamics with one type of particle).

In order to make the above intuition precise, we need some further notation.

Definition 2.4.5 *(a) For $F \subset \mathbb{Z}^2$, ∂^+F and ∂^-F are the external, respectively, internal boundary of F.*
(b) For $\eta \in \mathcal{X}$, $\mathrm{supp}(\eta)$ is the set of occupied sites of η.
(c) For $\eta \in \mathcal{C}^\star \cup \mathcal{C}^\star_{\text{att}}$, write $\eta = (\hat\eta, x)$ with $\hat\eta \in \mathcal{P}$ the protocritical droplet and $x \in \Lambda$ the location of the free/attached particle of type 2.
(d) For $\hat\eta \in \mathcal{P}$, $A(\hat\eta) = \{x \in \partial^+\mathrm{supp}(\hat\eta)\colon H(\hat\eta, x) < \Gamma^\star\}$ is the set of sites where the free particle of type 2 can attach itself to a particle of type 1 in $\partial^-\mathrm{supp}(\eta)$ to form an active bond. Note that $x \in A(\hat\eta)$ if and only if $\eta = (\hat\eta, x) \in \mathcal{C}^\star_{\text{att}}$, and that for every $\eta \in \mathcal{C}^\star_{\text{att}}$ either $\eta \in \mathcal{X}_\boxplus$

or $\eta \in \mathcal{X}_i$ for some $i = 1, \dots, I$.
(e) For $\hat\eta \in \mathcal{P}$, let

$$\begin{aligned} G(\hat\eta) &= \{x \in A(\hat\eta)\colon\ (\hat\eta, x) \in \mathcal{X}_{\boxplus}\}, \\ B(\hat\eta) &= \{x \in A(\hat\eta)\colon\ \exists\, i = 1, \dots, I\colon\ (\hat\eta, x) \in \mathcal{X}_i\}, \end{aligned} \tag{2.46}$$

be called the set of good sites, respectively, bad sites. Note that $(\hat\eta, x)$ may be in the same $\mathcal{X}_i$ for different $x \in B(\hat\eta)$.
(f) For $\hat\eta \in \mathcal{P}$, let

$$I(\hat\eta) = \{i \in 1, \dots, I\colon\ \exists\, x \in B(\hat\eta)\colon\ (\hat\eta, x) \in \mathcal{X}_i\}. \tag{2.47}$$

Note that $B(\hat\eta)$ can be partitioned into disjoint sets $B_1(\hat\eta), \dots, B_{|I(\hat\eta)|}(\hat\eta)$ according to which $\mathcal{X}_i$ the configuration $(\hat\eta, x)$ belongs to.
(g) Write $\mathrm{CS}(\hat\eta) = \mathrm{supp}(\hat\eta) \cup G(\hat\eta)$, $\mathrm{CS}^+(\hat\eta) = \partial^+\mathrm{CS}(\hat\eta)$ and $\mathrm{CS}^{++}(\hat\eta) = \partial^+\mathrm{CS}^+(\hat\eta)$.

Note that Definitions 2.4.5(c–d) rely on (H3-a), and that $G(\hat\eta) \neq \emptyset$ for all $\hat\eta \in \mathcal{P}$ by (H3-c) and Lemma 2.2.1. For the argument below it is of no relevance whether $B(\hat\eta) \neq \emptyset$ for some or all $\hat\eta \in \mathcal{P}$.

The following lemma is the analogue of [6], Proposition 3.3.4.

Lemma 2.4.6 *$\Theta \in [\Theta_1, \Theta_2]$ with*

$$\begin{aligned} \Theta_1 &= [1 + o(1)] \sum_{\hat\eta \in \mathcal{P}} \mathrm{CAP}^{\Lambda^+}\left(\partial^+\Lambda, \mathrm{CS}(\hat\eta)\right), \\ \Theta_2 &= \sum_{\hat\eta \in \mathcal{P}} \mathrm{CAP}^{\Lambda^+}\left(\partial^+\Lambda, \mathrm{CS}^{++}(\hat\eta)\right), \end{aligned} \tag{2.48}$$

where

$$\mathrm{CAP}^{\Lambda^+}\left(\partial^+\Lambda, F\right) = \min_{\substack{g\colon\ \Lambda^+ \to [0,1] \\ g|_{\partial^+\Lambda} \equiv 1,\ g|_F \equiv 0}} \tfrac{1}{2} \sum_{(x,x') \in (\Lambda^+)^\star} [g(x) - g(x')]^2, \qquad F \subset \Lambda, \tag{2.49}$$

with $(\Lambda^+)^\star = \{(x,y)\colon\ x, y \in \Lambda^+, |x - y| = 1\}$, and $o(1)$ an error term that tends to zero as $\Lambda \to \mathbb{Z}^2$.

Proof. The variational problem in (2.40) decomposes into disjoint variational problems for the maximally connected components of $\mathcal{X}^\star$. Only those components that contain $\mathcal{X}_\square$ or $\mathcal{X}_\boxplus$ contribute, since for the other components the minimum is achieved by picking h constant.

$\underline{\Theta \geq \Theta_1}$: A lower bound is obtained from (2.40) by removing all transitions that do not involve a fixed protocritical droplet and a move of the free/attached particle of type 2. This removal gives

$$\begin{aligned} \Theta \geq \sum_{\hat\eta \in \mathcal{P}} \min_{C_i(\hat\eta),\, i \in I(\hat\eta)} & \min_{\substack{g\colon\ \Lambda^+ \to [0,1] \\ g|_{G(\hat\eta)} \equiv 0,\ g|_{B_i(\hat\eta)} \equiv C_i(\hat\eta),\ i \in I(\hat\eta),\ g|_{\partial^+\Lambda} \equiv 1}} \\ & \tfrac{1}{2} \sum_{(x,x') \in [\Lambda^+ \backslash \mathrm{supp}(\hat\eta)]^\star} [g(x) - g(x')]^2. \end{aligned} \tag{2.50}$$

To see how this bound arises from (2.40), pick h in (2.40) and g in (2.50) such that

$$h(\eta) = h(\hat\eta, x) = g(x), \qquad \hat\eta \in \mathcal{P},\ x \in \Lambda^+ \backslash \mathrm{supp}(\hat\eta), \tag{2.51}$$

and use that, by Definitions 2.4.5(c–f), for every $\hat\eta \in \mathcal{P}$ (recall Lemma 2.2.1)

$$\begin{array}{ll} (\hat\eta, x) \in \mathcal{X}_{\boxplus}, & x \in G(\hat\eta), \\ (\hat\eta, x) \in \mathcal{X}_i & x \in B_i(\hat\eta),\ i \in I(\hat\eta), \\ (\hat\eta, x) \in \mathcal{P} \subset \mathcal{X}_{\square}, & x \in \partial^+\Lambda. \end{array} \tag{2.52}$$

A further lower bound is obtained by removing from the right-hand side of (2.52) the boundary condition on the sets $B_i(\hat\eta)$, $i \in I(\hat\eta)$. This gives

$$\begin{aligned} \Theta &\geq \sum_{\hat\eta\in\mathcal{P}} \min_{\substack{g\colon \Lambda^+\to[0,1] \\ g|_{G(\hat\eta)}\equiv 0,\ g|_{\partial^+\Lambda}\equiv 1}} \tfrac12 \sum_{(x,x')\in[\Lambda^+\backslash\mathrm{supp}(\hat\eta)]^\star} [g(x)-g(x')]^2 \\ &= \sum_{\hat\eta\in\mathcal{P}} \mathrm{CAP}^{\,\Lambda^+\backslash\mathrm{supp}(\hat\eta)}\left(\partial^+\Lambda, G(\hat\eta)\right), \end{aligned} \tag{2.53}$$

where the upper index $\Lambda^+\backslash\mathrm{supp}(\hat\eta)$ refers to the fact that no moves in and out of $\mathrm{supp}(\hat\eta)$ are allowed (i.e., this set acts as an obstacle for the free particle). To complete the proof we show that, in the limit as $\Lambda \to \mathbb{Z}^2$,

$$\begin{aligned} &\mathrm{CAP}^{\,\Lambda^+}\left(\partial^+\Lambda, \mathrm{supp}(\hat\eta)\cup G(\hat\eta)\right) \geq \mathrm{CAP}^{\,\Lambda^+\backslash\mathrm{supp}(\hat\eta)}\left(\partial^+\Lambda, G(\hat\eta)\right) \\ &\geq \mathrm{CAP}^{\,\Lambda^+}\left(\partial^+\Lambda, \mathrm{supp}(\hat\eta)\cup G(\hat\eta)\right) - O([1/\log|\Lambda|]^2). \end{aligned} \tag{2.54}$$

Since $\mathrm{CS}(\hat\eta) = \mathrm{supp}(\hat\eta)\cup G(\hat\eta)$ and, as we will show in Step 4 below, $\mathrm{CAP}^{\,\Lambda^+}(\partial^+\Lambda, \mathrm{CS}(\hat\eta))$ decays like $1/\log|\Lambda|$, the lower bound follows.

Before we prove (2.54), note that the capacity in the right-hand side of (2.54) includes more transitions than the capacity in the left-hand side, namely, all transitions from $\mathrm{supp}(\hat\eta)$ to $B(\hat\eta)$. Let

$$g^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}_{\partial^+\Lambda, G(\hat\eta)}(x) = \text{ equilibrium potential for } \mathrm{CAP}^{\,\Lambda^+\backslash\mathrm{supp}(\hat\eta)}\left(\partial^+\Lambda, G(\hat\eta)\right) \text{ at } x. \tag{2.55}$$

Below we will show that $g^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}_{\partial^+\Lambda, G(\hat\eta)}(x) \leq C/\log|\Lambda|$ for all $x \in B(\hat\eta)$ and some $C < \infty$. Since in the Dirichlet form in (2.49) the equilibrium potential appears squared, the error made by adding to the capacity in the left-hand side of (2.54) the transitions from $\mathrm{supp}(\hat\eta)$ to $B(\hat\eta)$ therefore is of order $[1/\log|\Lambda|]^2$ times $|B(\hat\eta)|$, which explains how (2.54) arises.

Formally, let $\mathbb{P}^{\hat\eta}_x$ be the law of the simple random walk that starts at $x \in B(\hat\eta)$ and is forbidden to visit the sites in $\mathrm{supp}(\hat\eta)$. Let $y \in G(\hat\eta)$. Using a renewal argument similar to the one used in the proof of Lemma 2.4.1, and recalling the probabilistic interpretation of the equilibrium potential in (2.3) and of the capacity in (2.5), we get

$$\begin{aligned} g^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}_{\partial^+\Lambda, G(\hat\eta)}(x) &= \mathbb{P}^{\hat\eta}_x(\tau_{\partial^+\Lambda} < \tau_{G(\hat\eta)}) = \frac{\mathbb{P}^{\hat\eta}_x(\tau_{\partial^+\Lambda} < \tau_{G(\hat\eta)\cup x})}{\mathbb{P}^{\hat\eta}_x(\tau_{G(\hat\eta)\cup\partial^+\Lambda} < \tau_x)} \\ &\leq \frac{\mathbb{P}^{\hat\eta}_x(\tau_{\partial^+\Lambda} < \tau_x)}{\mathbb{P}^{\hat\eta}_x(\tau_y < \tau_x)} = \frac{\mathrm{CAP}^{\,\Lambda^+\backslash\mathrm{supp}(\hat\eta)}(x, \partial^+\Lambda)}{\mathrm{CAP}^{\,\Lambda^+\backslash\mathrm{supp}(\hat\eta)}(x, y)}. \end{aligned} \tag{2.56}$$

The denominator of (2.56) can be bounded from below by some $C' > 0$ that is independent of x, y and $\mathrm{supp}(\hat\eta)$. To see why, pick a path from x to y that avoids $\mathrm{supp}(\hat\eta)$ but stays inside an $L^\star \times L^\star$ square around $\hat\eta$ (recall (H3-a)), and argue as in the proof of the lower bound of Lemma 2.1.1. On the other hand, the numerator is bounded from above by $\mathrm{CAP}^{\,\Lambda^+}(\partial^+\Lambda, G(\hat\eta))$, i.e., by the capacity of the same sets for a random walk that is not forbidden to visit $\mathrm{supp}(\hat\eta)$, since the Dirichlet problem associated to the latter has the same boundary conditions, but includes more transitions. In the proof of Lemma 2.4.7 below, we will see that $\mathrm{CAP}^{\Lambda^+}(\partial^+\Lambda, G(\hat\eta))$ decays like $C''/\log|\Lambda|$ for some $C''<\infty$ (see (2.63–2.64) below). We therefore conclude that indeed $g^{\mathrm{supp}(\hat\eta)}_{\partial^+\Lambda,G(\hat\eta)}(x) \leq C/\log|\Lambda|$ for all $x\in B(\hat\eta)$ with $C = C''/C'$.

$\underline{\Theta \leq \Theta_2}$: The upper bound is obtained from (2.40) by picking $C_i = 0$, $i=1,\dots,I$, and

$$h(\eta) = \begin{cases} 1 & \text{for } \eta \in \mathcal{X}_\square, \\ g(x) & \text{for } \eta = (\hat\eta, x) \in \mathcal{C}^{++}, \\ 0 & \text{for } \eta \in \mathcal{X}^\star \backslash [\mathcal{X}_\square \cup \mathcal{C}^{++}], \end{cases} \tag{2.57}$$

where

$$\mathcal{C}^{++} = \{\eta = (\hat\eta, x)\colon\ \hat\eta \in \mathcal{P},\ x\in \Lambda\backslash \mathrm{CS}^{++}(\hat\eta)\} \tag{2.58}$$

consists of those configurations in $\mathcal{C}^\star$ for which the free particle is at distance ≥ 2 of the protocritical droplet. The choice in (2.57) gives

$$\Theta \leq \sum_{\hat\eta\in\mathcal{P}} \mathrm{CAP}^{\Lambda^+}\left(\partial^+\Lambda, \mathrm{CS}^{++}(\hat\eta)\right). \tag{2.59}$$

To see how this upper bound arises, note that:

- The choice in (2.57) satisfies the boundary conditions in (2.40) because (recall (2.33–2.34))

$$\mathcal{C}^{++} \subset \mathcal{C}^\star,\ [\mathcal{X}_\square \cup \mathcal{C}^\star] \cap [\mathcal{X}_\boxplus \cup (\cup_{i=1}^I \mathcal{X}_i)] = \emptyset \quad \Longrightarrow \quad \mathcal{X}^\star\backslash[\mathcal{X}_\square \cup \mathcal{C}^{++}] \supset [\mathcal{X}_\boxplus \cup (\cup_{i=1}^I \mathcal{X}_i)]. \tag{2.60}$$

- By Lemma 2.2.1, $\mathcal{P}\subset\mathcal{X}_\square$. Therefore the first line of (2.57) implies that $h(\eta)=1$ for $\eta = (\hat\eta,x)$ with $\hat\eta\in\mathcal{P}$ and $x\in\partial^+\Lambda$, which is consistent with the boundary condition $g|_{\partial^+\Lambda}\equiv 1$ in (2.49).
- The third line of (2.57) implies that $h(\eta)=0$ for $\eta=(\hat\eta,x)$ with $\hat\eta\in\mathcal{P}$ and $x\in\mathrm{CS}^{++}(\hat\eta)$, which is consistent with the boundary condition $g|_F\equiv 0$ in (2.49) for $F=\mathrm{CS}^{++}(\hat\eta)$.

Further note that:

- By Definitions 1.4.1–1.4.2 and (H3-b), the only transitions in $\mathcal{X}^\star$ between $\mathcal{X}_\square$ and $\mathcal{C}^{++}$ are those where a free particle enters $\partial^-\Lambda$.
- The only transitions in $\mathcal{X}^\star$ between $\mathcal{C}^{++}$ and $\mathcal{X}^\star\backslash[\mathcal{X}_\square\cup\mathcal{C}^{++}]$ are those where the free particle moves from distance 2 to distance 1 of the protocritical droplet. All other transitions either involve a detachment of a particle from the protocritical droplet (which raises the number of droplets) or an increase in the number of particles in Λ. By (H3-b), such transitions lead to energy $>\Gamma^\star$, which is not possible in $\mathcal{X}^\star$.
- There are no transitions between $\mathcal{X}_\square$ and $\mathcal{X}^\star\backslash[\mathcal{X}_\square\cup\mathcal{C}^{++}]$.

The latter show that (2.49) includes all the transitions in (2.40). ■

2.4.4 Step 4: Sharp asymptotics for capacities of simple random walk

With Lemma 2.4.6 we have obtained upper and lower bounds on Θ in terms of capacities for simple random walk on $\mathbb{Z}^2$ of the pairs of sets $\partial^+\Lambda$ and $\mathrm{CS}(\hat\eta)$, respectively, $\mathrm{CS}^{++}(\hat\eta)$, with $\hat\eta$ summed over $\mathcal{P}$. The transition rates of the simple random walk are 1 between neighboring pairs of sites. Lemma 2.4.7 below, which is the analogue of [6], Lemma 3.4.1, shows that, in the limit as $\Lambda \to \mathbb{Z}^2$, each of these capacities has the same asymptotic behavior, namely, $[1+o(1)]\,4\pi/\log|\Lambda|$, *irrespective* of the location and shape of the protocritical droplet (provided it is not too close to $\partial^+\Lambda$, which is a negligible fraction of the possible locations). In what follows we pretend that $\Lambda = B_M = [-M,+M]^2 \cap \mathbb{Z}^2$ for some $M \in \mathbb{N}$ large enough. It is straightforward to extend the proof to other shapes of Λ (see van den Berg [2] for relevant estimates).

Lemma 2.4.7 *For any $\varepsilon > 0$,*

$$\begin{aligned}
&\lim_{M\to\infty} \max_{\substack{\hat\eta\in\mathcal{P}\\ d(\partial^+B_M,\mathrm{supp}(\hat\eta))\geq\varepsilon M}} \left|\frac{\log M}{2\pi}\,\mathrm{CAP}^{B_M^+}\big(\partial^+B_M,\mathrm{CS}(\hat\eta)\big)-1\right| = 0,\\
&\lim_{M\to\infty} \max_{\substack{\hat\eta\in\mathcal{P}\\ d(\partial^+B_M,\mathrm{supp}(\hat\eta))\geq\varepsilon M}} \left|\frac{\log M}{2\pi}\,\mathrm{CAP}^{B_M^+}\big(\partial^+B_M,\mathrm{CS}^{++}(\hat\eta)\big)-1\right| = 0,
\end{aligned} \tag{2.61}$$

where $d(\partial^+B_M,\mathrm{supp}(\hat\eta)) = \min\{|x-y|\colon x\in\partial^+B_M,\ y\in\mathrm{supp}(\hat\eta)\}$.

Proof. We only prove the first line of (2.61). The proof of the second line is similar.

Lower bound: For $\hat\eta\in\mathcal{P}$, let $y\in\mathrm{CS}(\hat\eta)\subset B_M$ denote the site closest to the center of $\mathrm{CS}(\hat\eta)$. The capacity decreases when we enlarge the set over which the Dirichlet form is minimized. Therefore we have

$$\begin{aligned}
\mathrm{CAP}^{B_M^+}(\partial^+B_M,\mathrm{CS}(\hat\eta)) &\geq \mathrm{CAP}^{B_M^+}(\partial^+B_M,y)\\
&= \mathrm{CAP}^{(B_M-y)^+}(\partial^+(B_M-y),0) \geq \mathrm{CAP}^{B_{2M}^+}(\partial^+B_{2M},0),
\end{aligned} \tag{2.62}$$

where the last equality uses that $(B_M-y)^+\subset B_{2M}^+$ because $y\in B_M$. By the analogue of (2.5–2.6) for simple random walk, we have (compare (2.49) with (2.1–2.2))

$$\mathrm{CAP}^{B_{2M}^+}(\partial^+B_{2M},0) = \mathrm{CAP}^{B_{2M}^+}(0,\partial^+B_{2M}) = 4\,\mathbb{P}_0(\tau_{\partial^+B_{2M}}<\tau_0), \tag{2.63}$$

where $\mathbb{P}_0$ is the law on path space of the *discrete-time* simple random walk on $\mathbb{Z}^2$ starting at 0. According to Révész [24], Lemma 22.1, we have

$$\mathbb{P}_0(\tau_{\partial^+B_{2M}}<\tau_0) \sim \frac{\pi}{2\log(2M)}, \qquad M\to\infty. \tag{2.64}$$

Combining (2.62–2.64), we get the desired lower bound.

Upper bound: As in (2.62), we have

$$\begin{aligned}
\mathrm{CAP}^{B_M^+}(\partial^+B_M,\mathrm{CS}(\hat\eta)) &\leq \mathrm{CAP}^{B_M^+}(\partial^+B_M,S_y(\hat\eta))\\
&= \mathrm{CAP}^{(B_M-y)^+}(\partial^+(B_M-y),S_y(\hat\eta)-y) \leq \mathrm{CAP}^{B_{\varepsilon M}^+}(\partial^+B_{\varepsilon M},S_y(\hat\eta)-y),
\end{aligned} \tag{2.65}$$

where $S_y(\hat\eta)$ is the smallest square centered at y containing $\mathrm{CS}(\hat\eta)$, and the last inequality uses that $(B_M - y)^+ \supset B^+_{\varepsilon M}$ when $d(\partial^+ B_M, \mathrm{supp}(\hat\eta)) \geq \varepsilon M$. By the recurrence of simple random walk, we have

$$\mathrm{CAP}^{B^+_{\varepsilon M}}(\partial^+ B_{\varepsilon M}, S_y(\hat\eta) - y) \sim \mathrm{CAP}^{B^+_{\varepsilon M}}(\partial^+ B_{\varepsilon M}, 0), \qquad M \to \infty. \tag{2.66}$$

Combining (2.64–2.66), we get the desired upper bound. ■

Combining Lemmas 2.4.6–2.4.7, we find that $\Theta \in [\Theta_1, \Theta_2]$ with

$$\begin{aligned}\Theta_1 &= O(\varepsilon M) + \sum_{\substack{\hat\eta \in \mathcal{P} \\ d(\partial^+ B_M, \mathrm{supp}(\hat\eta)) \geq \varepsilon M}} \mathrm{CAP}^{B^+_M}(\partial^+ B_M, \mathrm{CS}(\hat\eta)) \\ &= O(\varepsilon M) + \frac{2\pi}{\log M} \left|\left\{\hat\eta \in \mathcal{P} \colon\; d(\partial^+ B_M, \mathrm{supp}(\hat\eta)) \geq \varepsilon M\right\}\right| [1 + o(1)] \\ &= O(\varepsilon M) + \frac{2\pi}{\log M} N^\star\, [2(1-\varepsilon)M]^2\, [1 + o(1)],\end{aligned} \tag{2.67}$$

and the same expression for Θ_2, where we use that (recall (H3-a))

$$\mathrm{CAP}^{B^+_M}\big(\partial^+ B_M, \mathrm{CS}(\hat\eta)\big) \leq \mathrm{CAP}^{B^+_M}\big(B^+_M \backslash \mathrm{CS}(\hat\eta), \mathrm{CS}(\hat\eta)\big) = \tfrac12 |\mathrm{CS}^+(\hat\eta)| \leq \tfrac12 (L^\star + 2)^2, \tag{2.68}$$

and we recall from Definition 1.4.1(b) that $N^\star$ is the cardinality of $\mathcal{P}$ modulo shifts of the protocritical droplets. Let $M \to \infty$ followed by $\varepsilon \downarrow 0$, to conclude that $\Theta \sim 2\pi N^\star (2M)^2/\log M$. Since $|\Lambda| = (2M+1)^2$ and $K = 1/\Theta$, this proves (1.16) in Theorem 1.4.4.

2.5 Proof of Theorem 1.4.5

Proof. The proof is immediate from Lemma 2.3.2 and Bovier, Eckhoff, Gayrard and Klein [5], Theorem 1.3(iv). The main idea is that, each time the dynamics reaches the critical droplet but "fails to go over the hill and falls back into the valley around $\square$", it has a probability exponentially close to 1 to return to $\square$ (because, by (H2), $\square$ lies at the bottom of its valley (recall (2.3) and (2.27))) and to "start from scratch". Thus, the dynamics manages to grow a critical droplet and go over the hill only after a number of unsuccessful attempts that tends to infinity as $\beta \to \infty$, each having a small probability that tends to zero as $\beta \to \infty$. Consequently, the time to go over the hill is exponentially distributed on the scale of its average. ■

2.6 Proof of Theorem 1.4.3

Proof. (a) We will show that there exist $C < \infty$ and $\delta > 0$ such that

$$\mathbb{P}_\square\left(\tau_{\mathcal{C}^\star} < \tau_\boxplus \mid \tau_\boxplus < \tau_\square\right) \geq 1 - Ce^{-\delta\beta}, \qquad \forall\, \beta \in (0, \infty), \tag{2.69}$$

which implies the claim.

By (2.5), $\mathrm{CAP}_\beta(\square, \boxplus) = \mu_\beta(\square)\, c_\beta(\square, \mathcal{X}\backslash\square) \mathbb{P}_\square(\tau_\boxplus < \tau_\square)$ with $\mu_\beta(\square) = 1/Z_\beta$. From the lower bound in Lemma 2.1.1 it therefore follows that

$$\mathbb{P}_\square(\tau_\boxplus < \tau_\square) \geq C_1 e^{-\Gamma^\star\beta} \frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)}. \tag{2.70}$$

We will show that

$$\mathbb{P}_\square\left(\{\tau_{\mathcal{C}^\star} < \tau_\boxplus\}^c,\, \tau_\boxplus < \tau_\square\right) \leq C_2 e^{-(\Gamma^\star+\delta)\beta}\, \frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)}. \tag{2.71}$$

Combining (2.70–2.71), we get (2.69) with $C = C_2/C_1$.

By Definitions 1.2.2(f) and 1.2.3(d), any path from $\square$ to $\boxplus$ that does not pass through $\mathcal{C}^\star$ must hit a configuration η with $H(\eta) > \Gamma^\star$. Therefore there exists a set $\mathcal{S}$, with $H(\eta) \geq \Gamma^\star + \delta$ for all $\eta \in \mathcal{S}$ and some $\delta > 0$, such that

$$\mathbb{P}_\square\left(\{\tau_{\mathcal{C}^\star} < \tau_\boxplus\}^c,\, \tau_\boxplus < \tau_\square\right) \leq \mathbb{P}_\square\left(\tau_{\mathcal{S}} < \tau_\square\right). \tag{2.72}$$

Now estimate, with the help of reversibility,

$$\begin{aligned}
\mathbb{P}_\square\left(\tau_{\mathcal{S}} < \tau_\square\right) &\leq \sum_{\eta\in\mathcal{S}} \mathbb{P}_\square\left(\tau_\eta < \tau_\square\right)\\
&= \sum_{\eta\in\mathcal{S}} \frac{\mu_\beta(\eta) c_\beta(\eta, \mathcal{X}\backslash\eta)}{\mu_\beta(\square) c_\beta(\square, \mathcal{X}\backslash\square)}\, \mathbb{P}_\eta\left(\tau_\square < \tau_\eta\right)\\
&\leq \frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)} \sum_{\eta\in\mathcal{S}} |\{\eta' \in \mathcal{X}\backslash\eta\colon\ \eta \sim \eta'\}|\, e^{-\beta H(\eta)}\\
&\leq \frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)}\, C_2\, e^{-(\Gamma^\star+\delta)\beta}
\end{aligned} \tag{2.73}$$

with $C_2 = |\{(\eta, \eta') \in \mathcal{S} \times \mathcal{X}\backslash\{\eta\}\colon\ \eta \sim \eta'\}|$, where we use that $c_\beta(\eta, \eta') \leq 1$. Combine (2.72–2.73) to get the claim in (2.71).

(b) Write

$$\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta \mid \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big) = \frac{\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta,\, \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big)}{\mathbb{P}_\square\big(\tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big)}, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.74}$$

By reversibility,

$$\begin{aligned}
\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta,\, \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big) &= \frac{\mu_\beta(\eta) c_\beta(\eta, \mathcal{X}\backslash\eta)}{\mu_\beta(\square) c_\beta(\square, \mathcal{X}\backslash\square)}\, \mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big)\\
&= e^{-\Gamma^\star\beta}\, \frac{c_\beta(\eta, \mathcal{X}\backslash\eta)}{c_\beta(\square, \mathcal{X}\backslash\square)}\, \mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big), \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}.
\end{aligned} \tag{2.75}$$

Moreover (recall (2.3–2.4)),

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) = \sum_{\substack{\eta' \in \mathcal{X}\backslash\mathcal{C}^\star_{\mathrm{bd}}\\ \eta\sim\eta'}} \frac{c_\beta(\eta, \eta')}{c_\beta(\eta, \mathcal{X}\backslash\eta)}\, h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta'), \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}, \tag{2.76}$$

where

$$h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') = \begin{cases} 0 & \text{if } \eta' \in \mathcal{C}^\star_{\mathrm{bd}},\\ 1 & \text{if } \eta' = \square,\\ \mathbb{P}_{\eta'}(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}) & \text{otherwise.} \end{cases} \tag{2.77}$$

Because $\mathcal{P} \subset \mathcal{X}_\square$ by Lemma 2.2.1 and $\mathcal{C}^\star_{\mathrm{bd}} \subset \mathcal{G}(\square, \boxplus)$ by Definition 1.4.1(a), for all $\eta' \in \mathcal{P}$ we have $\Phi(\eta', \mathcal{C}^\star_{\mathrm{bd}}) - \Phi(\eta', \square) = \Gamma^\star - \Phi(\eta', \square) \geq \delta > 0$. Therefore, as in the proof of Lemma 2.4.1, it follows that

$$\min_{\eta' \in \mathcal{P}} h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') \geq 1 - Ce^{-\delta\beta}, \tag{2.78}$$

Moreover, letting $\bar{\mathcal{C}}^\star$ be the set of configurations that can be reached from $\mathcal{C}^\star_{\mathrm{bd}}$ via an allowed move that does not return to $\mathcal{P}$, we have

$$\max_{\eta' \in \bar{\mathcal{C}}^\star} h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') \leq Ce^{-\delta\beta}. \tag{2.79}$$

Indeed, $h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') = 0$ for $\eta' \in \mathcal{C}^\star_{\mathrm{bd}}$, while

$$\text{any path from } \bar{\mathcal{C}}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}} \text{ to } \square \text{ that avoids } \mathcal{C}^\star_{\mathrm{bd}} \text{ must reach an energy level } > \Gamma^\star. \tag{2.80}$$

To obtain (2.79) from (2.80), we can do an estimate similar to (2.29–2.30) for $\eta' \in \bar{\mathcal{C}}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}}$.

To prove (2.80) we argue as follows. Let $\zeta \in \bar{\mathcal{C}}^\star$, and let η be the configuration in $\mathcal{C}^\star_{\mathrm{bd}}$ from which ζ is obtained in a single transition. If $\zeta \in \mathcal{C}^\star_{\mathrm{bd}}$, then any path from ζ to $\square$ already starts from $\mathcal{C}^\star_{\mathrm{bd}}$ and there is nothing to prove. Therefore, let $\zeta \in \bar{\mathcal{C}}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}}$. Note that, by (H3-a), η consists of a single (protocritical) droplet in Λ^- plus a particle of type 2 in $\partial^-\Lambda$. Recalling that particles in $\partial^-\Lambda$ do not interact with other particles, we see that any configuration obtained from η by detaching a particle from the (protocritical) droplet increases the number of droplets and, by (H3-b), raises the energy above $\Gamma^\star$. Therefore, ζ can only be obtained from η by moving the free particle from $\partial^-\Lambda$ to Λ^-. Only two cases are possible: either $\zeta \in \mathcal{C}^\star_{\mathrm{att}}$ or $\zeta \in \mathcal{C}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}}$. In the former case, the claim follows via Lemma 1.6.4. In the latter case, we must show that if there is a path $\omega\colon \zeta \to \square$ that avoids $\mathcal{C}^\star_{\mathrm{bd}}$ such that $\max_{\sigma \in \omega} H(\sigma) \leq \Gamma^\star$, then a contradiction occurs.

Indeed, if ω is such a path, then the reversed path ω' is a path from $\square \to \zeta$ such that $\max_{\sigma \in \omega'} H(\sigma) \leq \Gamma^\star$. But ω' can be extended by the single move from ζ to η to obtain a path $\omega''\colon \square \to \eta$ such that $\max_{\sigma \in \omega''} H(\sigma) \leq \Gamma^\star$. Moreover, since $\eta \in \mathcal{C}^\star_{\mathrm{bd}}$, there exists a path $\gamma\colon \eta \to \boxplus$ such that $\max_{\sigma \in \gamma} H(\sigma) \leq \Gamma^\star$. But then the path obtained by joining ω'' and γ is a path in $(\square \to \boxplus)_{\mathrm{opt}}$ such that the configuration ζ visited just before $\eta \in \mathcal{C}^\star_{\mathrm{bd}}$ belongs to $\mathcal{C}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}} \subset \mathcal{C}^\star$. However, by Definitions 1.4.1–1.4.2, this implies that $\zeta \in \mathcal{P}$, which is impossible because $\mathcal{P} \cap \mathcal{C}^\star = \emptyset$.

The estimates in (2.78–2.79) can be used as follows. By restricting the sum in (2.76) to $\eta' \in \mathcal{P}$ and inserting (2.78), we get

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) \geq (1 - Ce^{-\delta\beta})\, \frac{c_\beta(\eta, \mathcal{P})}{c_\beta(\eta, \mathcal{X} \backslash \eta)}, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.81}$$

On the other hand, by inserting (2.79), we get

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) \leq \frac{c_\beta(\eta, \mathcal{P})}{c_\beta(\eta, \mathcal{X} \backslash \eta)} + Ce^{-\delta\beta} |\bar{\mathcal{C}}^\star|, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.82}$$

Because $H(\mathcal{P}) < H(\mathcal{C}^\star_{\mathrm{bd}}) = \Gamma^\star$, we have

$$c_\beta(\eta, \mathcal{P}) = \sum_{\eta' \in \mathcal{P}} c_\beta(\eta, \eta') = |\{\eta' \in \mathcal{P}\colon\, \eta \sim \eta'\}|, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}, \tag{2.83}$$

and, since $c_\beta(\eta,\mathcal{X}\backslash\eta) \le |\mathcal{X}|$, it follows that $\eta \mapsto c_\beta(\eta,\mathcal{P})/c_\beta(\eta,\mathcal{X}\backslash\eta)$ is bounded from below. Combine this observation with (2.81–2.82), to get

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\rm bd}}\big) = [1+O(e^{-\delta\beta})]\,\frac{c_\beta(\eta,\mathcal{P})}{c_\beta(\eta,\mathcal{X}\backslash\eta)}, \qquad \eta \in \mathcal{C}^\star_{\rm bd}. \tag{2.84}$$

Combining this in turn with (2.74–2.75), we arrive at

$$\begin{aligned}\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\rm bd}}} = \eta \mid \tau_{\mathcal{C}^\star_{\rm bd}} < \tau_\square\big) &= \frac{c_\beta(\eta,\mathcal{X}\backslash\eta)\,\mathbb{P}_\eta(\tau_\square < \tau_{\mathcal{C}^\star_{\rm bd}})}{\sum_{\eta'\in\mathcal{C}^\star_{\rm bd}} c_\beta(\eta',\mathcal{X}\backslash\eta')\,\mathbb{P}_{\eta'}(\tau_\square < \tau_{\mathcal{C}^\star_{\rm bd}})}\\ &= [1+O(e^{-\delta\beta})]\,\frac{c_\beta(\eta,\mathcal{P})}{\sum_{\eta'\in\mathcal{C}^\star_{\rm bd}} c_\beta(\eta',\mathcal{P})}, \qquad \eta\in\mathcal{C}^\star_{\rm bd}.\end{aligned} \tag{2.85}$$

Finally, each site in $\partial^-\Lambda$ has one edge towards $\partial^+\Lambda$ and hence, by (2.83), $\eta \mapsto c_\beta(\eta,\mathcal{P})$ is constant on $\mathcal{C}^\star_{\rm bd}$. Together with (2.85) this proves the claim. ■

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