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Alessio Troiani

Contents

Summary

Metastability is a phenomenon that may occur in a system subject to a noisy dynamics. It is characterized by the existence of different times scales on which the system evolves. On a short time scale the system is in an apparent equilibrium and explores a limited region of its state space, whereas on a long time scale it undergoes rapid transitions between different regions of the state space. In thermodynamics metastability is related to first-order phase transitions. The classical example of metastable behavior is the freezing of a supercooled liquid: the system stays for a long time in the (metastable) liquid phase before reaching the (stable) solid phase and the crossover is triggered by the appearance of a critical droplet of the solid phase inside the liquid phase. However, metastable phenomena do not only occur in physics: they appear in many fields such as biology, chemistry, economics and computer science.

A behavior of the above type can be modeled by defining an energy function H on the state space $\mathcal{X}$ of the system and by considering a dynamics on $\mathcal{X}$ that allows transitions towards states with higher energy with low probability. In this framework, the metastable and the stable state correspond, respectively, to a local and a global minimizer of the energy. The crossover time towards the stable state is determined by the depth of the deepest valley separating the stable and the metastable state.

In the context of metastability, typical questions that are addressed concern the probability distribution of the time it takes to observe the transition from the metastable to the stable state, the shape of the critical configurations that trigger the transition, and the typical trajectories the dynamics follows in order to realize the transition. Over the years, different approaches have been developed to tackle these questions. However, a unified theory is still lacking, and a detailed analysis of specific models and of model-dependent properties is required to deal with the key questions of interest.

In this thesis we consider a model of a low-temperature and low-density two-dimensional lattice gas with particles of two different types subject to Kawasaki dynamics in a large finite box Λ 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 particles of the same type. At the boundary of Λ particles are created and annihilated in a way that represents the presence of an infinite gas reservoir. We start the dynamics from the configuration where Λ is empty (denoted by $\square$) and are interested in the transition time to configuration where Λ is full (denoted by $\boxplus$). This transition is triggered by a critical droplet appearing somewhere in Λ.

The structure of the thesis is as follows. In Chapter 1 we introduce the main approaches developed in the literature to deal with metastability, and we present the most relevant results obtained for models related to ours. In Chapter 2 we introduce our model and identify the values of the parameters for which the transition from $\square$ to $\boxplus$ exhibits metastable behavior in the limit of low temperature. Under *three hypotheses*, we determine the distribution and the expectation of the transition time, and identified the so-called critical configurations that satisfy a certain "gate property". The first hypothesis assumes that configuration $\boxplus$, corresponding to the liquid phase, is a minimizer of H. The second hypothesis requires that the valleys of the energy landscape are not too deep. The third hypothesis requires that the critical configurations have an appropriate geometry. Subject to these three hypotheses, several theorems are derived, for which *three model-dependent quantities* need to be identified as well: (1) the energy barrier $\Gamma^\star$ separating $\square$ from $\boxplus$; (2) the set $\mathcal{C}^\star$ of critical configurations; (3) the cardinality $N^\star$ of the set of protocritical configurations, which can be thought of as the "entrance" set of $\mathcal{C}^\star$. In Chapter 3 the first two hypotheses are verified and the value $\Gamma^\star$ of the energy barrier separating $\square$ and $\boxplus$ is identified. These results are sufficient to establish the exponential probability distribution of the nucleation time divided by its mean, and to determine the mean nucleation time up to a multiplicative factor $1 + o(1)$ in the limit of low temperature. In Chapter 4 we show that the model satisfies the third hypothesis, and we identify the set of critical configurations. We give a geometric characterization of the configurations in $\mathcal{C}^\star$ and compute the value of $N^\star$.

Nederlandse Samenvatting

Metastabiliteit is een fenomeen dat voor kan komen in een systeem dat beïnvloed wordt door een drukke dynamiek. Het wordt gekarakteriseerd door het bestaan van verschillende tijdsschalen waarover het systeem evolueert. Op de korte termijn is het systeem ogenschijnlijk in evenwicht en verkent het slechts een beperkt gebied van de toestandsruimte, terwijl het systeem op de lange termijn snelle overgangen tussen de verschillende gebieden van de toestandsruimte ondergaat. In de thermodynamica is metastabiliteit gerelateerd aan eerste-orde fase transities. Het klassieke voorbeeld van metastabiel gedrag is het bevriezen van een supergekoelde vloeistof: het systeem blijft lang in de (metastabiele) vloeibare fase voordat het de (stabiele) vaste fase bereikt. De overgang hiertussen wordt geactiveerd door het verschijnen van een kritieke druppel van de vaste fase binnen de vloeibare fase. Daarentegen komen metastabiele fenomenen niet alleen voor in de natuurkunde, maar ook in veel andere gebieden, zoals in de biologie, scheikunde, economie en informatica.

Het gedrag van het bovenstaande soort model kan gemodelleerd worden door het definiëren van een energie functie H op de toestandsruimte $\mathcal{X}$. Deze energie functie staat met een kleine kans overgangen naar toestanden met hogere energie toe. In deze opzet corresponderen de metastabiele en de stabiele staat respectievelijk met een lokale en een globale minimizer van de energie. De overgangstijd richting een stabiele staat wordt bepaald door de diepte van het diepste dal dat de stabiele en de metastabiele staat scheidt.

Het soort vragen die gesteld kunnen worden over metastabiliteit hebben betrekking tot de kansverdeling van de tijd die nodig is om de overgang van metastabiliteit naar stabiliteit waar te nemen, de vorm van de kritische configuraties die de overgang activeren en de typische trajecten die het dynamische systeem volgt om de overgang te realiseren. Door de jaren heen zijn verschillende benaderingen ontwikkeld om deze vragen te kunnen beantwoorden. Echter, een uniforme theorie bestaat nog niet en gedetailleerde analyses van specifieke modellen en van model-afhankelijke eigenschappen zijn genoodzaakt om alleen de voor dat model belangrijkste vraag te behandelen.

In dit proefschrift bekijken we een gas model op een twee dimensionaal lattice met een lage temperatuur en lage dichtheid. Dit model heeft 2 verschillende soorten deeltjes in een grote eindige doos Λ met een open rand. Deze deeltjes worden beïnvloed door Kawasaki dynamiek. Elk tweetal deeltjes die zich bevinden op aangrenzende posities hebben een negatieve bindingsenergie wanneer hun types verschillend zijn, terwijl elk deeltje een positieve activatie energie heeft, die afhangt van zijn type. Er is geen bindingsenergie tussen deeltjes van dezelfde soort. Op de rand van Λ worden deeltjes gecreëerd en vernietigd op een manier die de aanwezigheid van een oneindig gas reservoir weergeeft. We starten deze dynamiek vanuit de configuratie waarin Λ leeg is (genoteerd met $\square$) en zijn geïnteresseerd in de overgangstijd tot de configuratie waarin Λ volledig gevuld is (genoteerd met $\boxplus$). Deze overgang wordt getriggerd door een kritieke druppel ergens in Λ.

Dit proefschrift is als volgt opgebouwd. In Hoofdstuk 1 introduceren we de belangrijkste benaderingen uit al bestaande literatuur om om te gaan met metastabiliteit en geven we de belangrijkste relevante resultaten die verkregen gerelateerd aan ons model. In Hoofdstuk 2 introduceren we ons model en identificeren we de waardes van de parameters waarvoor de overgang van $\square$ naar $\boxplus$ metastabiel gedrag vertoond in het limiet geval van lage temperaturen. Onder drie hypotheses, bepalen we de verdeling en de verwachting van de overgangstijd en identificeren we de zogenaamde kritische configuraties die voldoen aan een zekere "poort eigenschap". De eerste hypothese neemt aan dat configuratie $\boxplus$, die correspondeert met de vloeibare fase een minimizer van H is. De tweede hypothese stelt dat de verschillende dalen van het energie landschap niet te diep zijn. De derde hypothese eist dat de kritische configuraties een geschikte geometrie hebben. Onder deze drie hypotheses leiden we verschillende stellingen af en hiervoor is het noodzakelijk om ook de volgende drie model-afhankelijke grootheden te identificeren: (1) de energie barrière $\Gamma^\star$ die $\square$ van $\boxplus$ scheidt; (2) de verzameling $\mathcal{C}^\star$ van kritische configuraties; (3) de kardinaliteit $N^\star$ van de verzameling van protokritsche configuraties, die gezien kunnen worden als de "ingangs" verzameling van $\mathcal{C}^\star$. In Hoofdstuk 3 worden de eerste 2 hypotheses geverifieerd en de waarde $\Gamma^\star$ van de energie barrière die $\square$ en $\boxplus$ scheidt geïdentificeerd. Deze resultaten zijn voldoende om de exponentiele kansverdeling van de kernvormingstijd gedeeld door zijn gemiddelde te bepalen en om de gemiddelde kernvormingstijd te berekenen in de lage temperatuur limiet, op een multiplicatieve factor $1 + o(1)$ na. In Hoofdstuk 4 laten we zien dat het model voldoet aan de derde hypothese en we identificeren de verzameling van kritische configuraties. We geven tenslotte een geometrische karakterisatie van de configuraties in $\mathcal{C}^\star$ en berekenen de waarden van $N^\star$.

1 Introduction

In this thesis, we consider a low-temperature and low-density lattice gas with particles of two types, describing the condensation of a supersaturated gas mixture. Particles are subject to random hopping with hard-core repulsion, while particles of different types are subject to nearest-neighbor attraction and have different densities. The goal of the thesis is to study the metastable behavior of this system. In Section 1.1 we introduce the concept of metastability, in Section 1.2 we describe the mathematical approaches to metastability and the questions that are of interest. In Section 1.3 we turn to finite systems at low temperature, define Metropolis dynamics, and define the quantities that play a central role in the analysis of metastable behavior. We describe earlier work for Kawasaki dynamics with one type of particle and state our target to extend this work to two types of particles.

1.1 The concept of metastability

Metastability is a phenomenon where a system moves between different region of its state space according to a noisy dynamics. On a *short time scale*, the system explores a limited region of the state space and therefore is in a quasi-equilibrium. On a *long time scale*, the system undergoes rapid transitions between different regions of the state space, where it reaches new quasi-equilibria. The transitions between these different *phases* of the system are typically triggered by the creation of a *critical droplet*, via spontaneous fluctuations or external perturbations. Throughout the sequel, we will concentrate on the case where the transition is from a *metastable state* (a single quasi-equilibrium) to a *stable state* (a single equilibrium).

In thermodynamics, metastability is associated with a *first-order phase transition*. Examples are supercooled liquids, supersaturated gases, as well as ferromagnets in the part of the hysteresis loop where the magnetization is opposite to the external magnetic field. In all these cases the system may remain for a long time in a metastable phase that, for the given thermodynamic parameters such as temperature or magnetic field, is not stable. The appearance of a *nucleus* of the stable phase inside the unstable phase will initiate a rapid crossover.

The occurrence of metastable phenomena is not limited to thermodynamics and plays a key role in various different fields, ranging from biology and chemistry to economics and computer science.

1.2 Mathematical approaches and questions of interest

The mathematical description of metastable systems started in the 1930s and 1940s, with the work of Eyring [Eyr35] and Kramers [Kra40], who studied a one-dimensional diffusion process in a double-well potential in the context of the theory of chemical reactions. The first attempt to formulate a rigorous dynamical theory of metastability goes back to the work of Lebowitz and Penrose [PL71] on metastable states in Van der Waals theory. In the 1980s Freidlin and Wentzell [FW84] used large deviation theory to study the long-term behavior of dynamical systems with small random perturbations. They associated metastable systems with what they called a *Markov Chain with exponentially small transition probabilities*, whose states correspond to the different attractors of the underlying dynamical system. The transition probabilities of this Markov chain are computed by finding the probability of the most likely trajectory between these attractors.

Later it was noted that such Markov chains also arise in other contexts, in particular, in stochastic dynamics of interacting particle systems at low temperature, which have become the subject of intense investigation (Olivieri and Scoppola [OS95], [OS96], Ben Arous and Cerf [BAC96], Catoni and Cerf [CC97]), initially again with the help of large deviation techniques. Since then a vast literature has developed. The different models investigated can be classified according to the "size" of their state space and the "type" of dynamics governing their evolution.

From the point of view of state space, an important distinction is between *finite* and *infinite* state space. In the first case, in the low-temperature regime, the stochastic dynamics is driven by energy only and entropic effects can essentially be neglected. In the second case, however, entropic effects play an important role and must be taken into account when studying the statistical properties of the transition toward global equilibria.

From the point of view of dynamics, an important distinction is between *non-conservative* dynamics and *conservative* dynamics. In the first case, the total number of particles or spins (of a given type) is not conserved. Examples are spin-flip dynamics in magnets, either sequentially (Glauber dynamics) or parallel dynamics (cellular automata). Models of Glauber dynamics in finite volume are

Neves and Schonmann [NS91] and Bovier and Manzo [BM02], and in infinite volume Dehghanpour and Schonmann [DS97] and Schonmann and Shlosman [SS98], while models of cellular automata can be found in Cirillo and Nardi [CN03], Cirillo Nardi and Spitoni [CNS08b] and [CNS08a]. In the second case, the total number of particle or spins stays fixed, which places a severe restriction on the evolution. In general, models with conservative dynamics are more difficult to analyze because of long-range effects introduced by the conservation law. Examples are hopping dynamics in lattice gases, either sequentially (Kawasaki dynamics) or parallel dynamics (cellular automata) Models of Kawasaki dynamics in finite volume are den Hollander Olivieri and Scoppola [dOS00], [dHNOS03] and Bovier den Hollander and Nardi [BdN06], and in infinite volume Gaudillière, den Hollander, Nardi, Olivieri and Scoppola [GdHN$^+$a], [GdHN$^+$b] and Bovier den Hollander and Spitoni [BdHS10]. An example of a parallel conservative dynamics can be found in Gaudillière, Scoppola, Scoppola and Viale [GSSV11]. Typical questions addressed in the context of metastability are: What is the probability distribution of the time it takes to observe the transition from the metastable to the stable state (nucleation time)? What are the critical configurations that trigger the transition (critical droplets)? What are the typical trajectories the dynamics follows in order to realize the transition (tube of trajectories)? Different approaches have been developed to tackle these questions. We will see what are the questions these approaches manage to answer. A unified theory is still lacking, and a detailed analysis of specific models and of model-dependent properties is therefore crucial to make progress on the key issues of interest.

1.2.1 Pathwise approach

The pathwise approach, in essence, exploits the large deviation techniques developed in the theory of Friedlin and Wentzell. This approach was initiated by Cassandro, Galves, Olivieri, Vares [CGOV84] in 1984, who applied large deviation techniques to a dynamics with Metropolis transition probabilities, i.e., probabilities depending on the difference of the energy of the configurations immediately before and after the transition. The equilibrium properties of the system are described by a probability measure that is determined by the Hamiltonian defined on the state space of the Markov chain. In the limit of inverse temperature β tending to ∞, it is hard for trajectories to climb out of wells in the energy landscape, and the local minima of the Hamiltonian correspond to the metastable states.

In the framework of the pathwise approach, it is natural to study the typical trajectories realizing the tunneling between the metastable and the stable configuration. In this description, a central role is played by the optimal paths, i.e., the paths realizing the minimax between the metastable state and the stable state. The transition time is determined by the largest energy barrier separating these two states. A comprehensive overview of this method can be found in the monograph on large deviations and metastability by Olivieri and Vares [OV05]. The essential features of metastability have been listed in Manzo, Nardi, Olivieri, and Scoppola [MNOS04]. Here, the asymptotic behavior of the transition time is separated from the study of the typical trajectories realizing the transition. Results on the transition times are obtained via control on the depth of the wells of the energy landscape and the saddles connecting them.

1.2.2 Potential-theoretic approach

The potential-theoretic approach has been developed around 2000 in the works of Bovier, Eckhoff, Gayrard and Klein [BEGK01]. It exploits the link between potential theory and Markov processes. The Markov chain is regarded as an electric network, where the nodes of the network represent the configurations the Markov chain can visit and the edges of the network represent the possible transitions. The electric potential corresponds to the hitting probabilities, while the conductances associated with the edges correspond to the transitions rate between the configurations.

The potential-theoretic apporach largely discards the trajectories that play a central role in the theory of Freidlin and Wentzell. Nevertheless, this lack of information is compensated by the capability of computing sharp asymptotic bounds for the transition time. These bounds are obtained via the computation of capacities, which can be estimated with the help of powerful variational principles involving the potential and the current of the electric network associated with the Markov chain. Applications of the potential-theoretic approach can be found in Bovier and Manzo [BM02], Bovier, Eckhoff, Gayrard and Klein [BEGK04], Bovier, den Hollander and Nardi [BdN06], Bovier den Hollander and Spitoni [BdHS10]. For an overview, see Bovier [Bov06] and [Bov09].

1.3 Finite systems at low temperature

In the rest of this introduction we will focus on *Metropolis dynamics* in *finite volume* at *low temperature*. In words, we will take a finite state space, consider the asymptotic regime where the inverse temperature β tends to infinity, and use "updating rules" that only depend on the change in the energy associated with the transition. In this setting, the transition from the metastable to the stable state is essentially driven by the energy landscape on the configuration space in which the system evolves. Many models in this class have been investigated over the past twenty years. The general setting is the following.

Let $\Lambda \subset \mathbb{Z}^d$, $d \geq 1$, and let S be a finite set. With each site $x \in \Lambda$ we associated a variable $\eta(x) \in S$. A configuration $\eta = \{\eta(x)\colon x \in \Lambda\}$ is an element of the state space $\mathcal{X} = S^\Lambda$. With each configuration we associate an energy given by a Hamiltonian $H\colon \mathcal{X} \to \mathbb{R}$ depending on one or more parameters. The equilibrium properties of the system are described by the *Gibbs measure*

$$\mu_\beta(\eta) = \frac{e^{-\beta H(\xi)}}{Z_\beta}, \qquad \eta \in \mathcal{X}, \tag{1.1}$$

where $\beta \in (0, \infty)$ is the inverse temperature, and Z_β is the normalizing partition sum. In the limit of low temperature the measure is concentrated on the global minimizer of H.

As dynamics we consider the continuous-time Markov process $(\eta_t)_{t\geq 0}$ with state space $\mathcal{X}$ whose transition rates are given by

$$c_\beta(\eta, \eta') = \begin{cases} e^{-\beta[H(\eta')-H(\eta)]_+}, & \eta, \eta' \in \mathcal{X},\ \eta \neq \eta',\ \eta \sim \eta', \\ 0, & \text{otherwise,} \end{cases} \tag{1.2}$$

where $\eta \sim \eta'$ means that η' can be obtained from η via a single draw from a *set of allowed moves* satisfying the following assumptions:

- $\sim$ is reflective, i.e., the reverse of an allowed move is allowed too.
- $\mathcal{X}$ is connected with respect to $\sim$, i.e., any two configurations are connected by a path of allowed moves.

This dynamics is called the *Metropolis dynamics* with respect to H at inverse temperature β. It is ergodic and reversible with respect to μ_β:

$$\mu_\beta(\eta) c_\beta(\eta, \eta') = \mu_\beta(\eta') c_\beta(\eta', \eta) \qquad \forall\, \eta, \eta' \in \mathcal{X}. \tag{1.3}$$

Choosing a particular model amounts to choosing Λ, S, H, β and $\sim$.

In this setting the following quantities are key for the analysis of the transition from a local minimizer of the Hamiltonian $\mathbf{m}$ to a global minimizer $\mathbf{s}$.

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

$$\Phi(\eta, \eta') = \min_{\omega\colon\, \eta \to \eta'} \max_{\sigma \in \omega} H(\sigma), \tag{1.4}$$

where $\omega\colon\ \eta \to \eta'$ is any path of allowed moves from η to η'. For non-empty sets $\mathcal{A}, \mathcal{B} \subseteq \mathcal{X}$ put

$$\Phi(\mathcal{A}, \mathcal{B}) = \min_{\eta \in \mathcal{A}, \eta' \in \mathcal{B}} \Phi(\eta, \eta'). \tag{1.5}$$

- $\mathcal{S}(\eta, \eta')$ is the *communication level set* between $\eta, \eta' \in \mathcal{X}$ defined by

$$\mathcal{S}(\eta, \eta') = \left\{\chi \in \mathcal{X}\colon\ \exists\, \omega\colon\ \eta \to \eta',\, \omega \ni \chi\colon\ \max_{\zeta \in \omega} H(\zeta) = H(\chi) = \Phi(\eta, \eta')\right\}. \tag{1.6}$$

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

$$V_\eta = \Phi(\eta, I_\eta) - H(\eta), \tag{1.7}$$

where $I_\eta = \{\zeta \in \mathcal{X}\colon\ H(\zeta) < H(\eta)\}$ is the set of configurations with energy lower than η.

- $(\mathbf{m} \to \mathbf{s})_{\mathrm{opt}}$ is the set of paths realizing the minimax in $\Phi(\mathbf{m}, \mathbf{s})$.

In words, the communication height between configurations η and η' is the minimal energy the path needs to reach in order to achieve the transition between configurations η and η', whereas the stability level of a configuration is the height of the energy barrier separating a configuration η from the set of configurations with lower energy.

If the condition

$$V_\eta < V_{\mathbf{m}} \quad \forall \eta \in \mathcal{X} \setminus \{\mathbf{s}\} \tag{1.8}$$

holds, then the local minimum $\mathbf{m}$ is called a metastable configuration. The energy barrier separating $\mathbf{m}$ and $\mathbf{s}$ is denoted by

$$\Gamma^\star = \Phi(\mathbf{m}, \mathbf{s}) - H(\mathbf{m}). \tag{1.9}$$

If the energy landscape is sufficiently "well behaved" (for instance if $\mathbf{m}$ is metastable in the sense of (1.8)), then

$$\lim_{\beta \to \infty} \frac{1}{\beta} \log \mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = \Gamma^\star. \tag{1.10}$$

Furthermore, the probability distribution of the nucleation time divided by its mean is exponential with mean 1. This is due to the fact that uphill transitions are improbable and each time the dynamics does not manage to climb over the hill it falls back to the bottom of the valley in the energy landscape where it came from and it starts afresh. For a detailed analysis, see [MNOS04].

Applying potential theory in this framework allows us to sharpen the results in (1.10). The key object in the potential-theoretic approach to metastability is the *Dirichlet form*

$$\mathcal{E}_\beta(h) = \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}} \mu_\beta(\eta) c_\beta(\eta,\eta')[h(\eta) - h(\eta')]^2, \qquad h\colon \mathcal{X} \to [0,1], \tag{1.11}$$

where μ_β is the Gibbs measure defined in (1.1) and c_β is the kernel of transition rates defined in (1.2). Given a pair of non-empty disjoint sets $\mathcal{A}, \mathcal{B} \subseteq \mathcal{X}$, the *capacity* of the pair $\mathcal{A}, \mathcal{B}$ is defined by

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) = \min_{\substack{h\colon \mathcal{X} \to [0,1] \\ h|_{\mathcal{A}} \equiv 1, h|_{\mathcal{B}} \equiv 0}} \mathcal{E}_\beta(h), \tag{1.12}$$

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 (1.11) is called the *equilibrium potential* of the pair $\mathcal{A}, \mathcal{B}$ and is given by

$$h^\star_{\mathcal{A},\mathcal{B}}(\eta) = P_\eta(\tau_{\mathcal{A}} < \tau_{\mathcal{B}}), \qquad \eta \in \mathcal{X} \backslash (\mathcal{A} \cup \mathcal{B}). \tag{1.13}$$

This is the solution of the equation

$$\begin{aligned} (c_\beta h)(\eta) &= 0, \qquad && \eta \in \mathcal{X} \setminus (\mathcal{A} \cup \mathcal{B}), && (1.14)\\ h(\eta) &= 1, && \eta \in \mathcal{A}, && (1.15)\\ h(\eta) &= 0, && \eta \in \mathcal{B}, && (1.16) \end{aligned}$$

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

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) = \sum_{\eta \in \mathcal{A}} \mu_\beta(\eta)\, c_\beta(\eta, \mathcal{X} \setminus \{\eta\})\, \mathbb{P}_\eta(\tau_{\mathcal{B}} < \tau_{\mathcal{A}}) \tag{1.17}$$

with $c_\beta(\eta, \mathcal{X} \backslash \{\eta\}) = \sum_{\eta' \in \mathcal{X} \backslash \{\eta\}} c_\beta(\eta,\eta')$ the rate to move out of η. This rate enters because $\tau_{\mathcal{A}}$ is the first hitting time of $\mathcal{A}$ after the initial configuration is left.

As shown in [BEGK02],

$$\mathbb{E}_{\mathbf{m}}(\tau_{\mathbf{s}}) = \frac{\mu_\beta(\mathcal{R}_{\mathbf{m}})}{\mathrm{CAP}_\beta(\mathbf{m},\mathbf{s})} \, [1 + o(1)] \quad \text{as } \beta \to \infty, \tag{1.18}$$

where

$$\mathcal{R}_{\mathbf{m}} = \{\eta \in \mathcal{X} \colon \mathbb{P}_\eta(\tau_{\mathbf{m}} < \tau_{\mathbf{s}}) \geq \mathbb{P}_\eta(\tau_{\mathbf{s}} < \tau_{\mathbf{m}})\} \tag{1.19}$$

is the set of configuration from which it is more likely to reach $\mathbf{m}$ before $\mathbf{s}$. Sharp estimates on the capacity therefore translate into sharp estimates on the nucleation time, provided the states $\mathbf{m}$ and $\mathbf{s}$ satisfy:

$$\lim_{\beta\to\infty} \frac{\max_{\eta\notin\{\mathbf{m},\mathbf{s}\}} \mu_{\beta(\eta)}/\mathrm{CAP}_{\beta(\eta,\{\mathbf{m},\mathbf{s}\})}}{\min_{\eta\in\{\mathbf{m},\mathbf{s}\}} \mu_{\beta(\eta)}/\mathrm{CAP}_{\beta(\eta,\{\mathbf{m},\mathbf{s}\})}} = 0. \tag{1.20}$$

If the previous equality holds, then the pair $(\mathbf{m}, \mathbf{s})$ is called a *metastable pair* according to Bovier, Eckhoff, Gayrard and Klein [BEGK02]. The estimates on the capacity can then be obtained via *variational principles*. In [dHNT11] it is shown that (1.8) indeed implies (1.20). Works where this approach is exploited are Bovier and Manzo [BM02], and Bovier, den Hollander and Nardi [BdN06].

1.3.1 Kawasaki dynamics on a finite box with open boundary for one type of particle

In this section we will explain what results have been obtained with the help of the potential-theoretic approach for the lattice gas subject to Kawasaki dynamics. Since this thesis focusses on Kawasaki dynamics with two types of particles, a review of this work provides the necessary background.

In [BdN06], Kawasaki dynamics on a large finite box $\Lambda \subset \mathbb{Z}^2$ is considered with an *open boundary condition* that mimics the presence of an infinite gas reservoir outside Λ with density $e^{-\beta\Delta}$, $\Delta > 0$. Particles are conserved inside Λ, and are created and annihilated at the boundary. In this sense, the dynamics is *locally conservative*. The set of critical configurations is identified, the expected value of the nucleation time is computed up to a multiplicative factor that tends to one, and it is shown that the nucleation time divied by its mean has exponential probability distribution with mean 1, all in the limit as $\beta \to \infty$. Moreover, sharp bounds are derived for the proportionality constant of the average nucleation time in term of capacities associated with simple random walk, and the asymptotic behavior of this constant is computed as the system size tends to infinity. These results sharpen those obtained by den Hollander, Olivieri and Scoppola [dOS00] on $\mathbb{Z}^2$ and den Hollander, Nardi, Olivieri and Scoppola [dHNOS03] on $\mathbb{Z}^3$ with the help of the pathwise approach.

The results in [BdN06] are comparable with those obtained by Bovier and Manzo

[BM02] for the Ising model on a finite box in two and three dimensions with periodic boundary conditions subject to Glauber dynamics at low temperature. This work, in terms, sharpened the results obtained by Neves and Schonmann [NS92] on $\mathbb{Z}^2$ and by Ben Arous and Cerf [BAC96] on $\mathbb{Z}^3$.

Since inside Λ the number of particles is conserved, controlling the growing and shrinking of a droplet is complicated because particles have to travel between the boundary of the box and the boundary of the droplet. Moreover, it turns out that particles move along the droplet faster than they arrive from the boundary of the box, and this makes the shape of the critical droplets more complicated than those for Ising spins subject to Glauber dynamics.

For the purpose of this introduction, we will only refer to the analysis in the two-dimensional case. Let $\Lambda \subset \mathbb{Z}^2$ be a large finite box. Let

$$\partial^- \Lambda = \{x \in \Lambda\colon\ \exists\, y \notin \Lambda\colon\ |y - x| = 1\}, \tag{1.21}$$
$$\partial^+ \Lambda = \{x \notin \Lambda\colon\ \exists\, y \in \Lambda\colon\ |y - x| = 1\}, \tag{1.22}$$

be the internal boundary, respectively, the external boundary of Λ, and put $\Lambda^- = \Lambda \backslash \partial^- \Lambda$ and $\Lambda^+ = \Lambda \cup \partial^+ \Lambda$. Let $S = \{0, 1\}$. A configuration η is an element of the space $\{0, 1\}^\Lambda$, where $\eta(x) = 1$ and $\eta(x) = 0$ denote, respectively, the presence or the absence of a particle at site x. As Hamiltonian, choose

$$H(\eta) = -U \sum_{x,y \in (\Lambda^-)^\star} \eta(x)\eta(y) + \Delta \sum_{x \in \Lambda} \eta(x), \tag{1.23}$$

where $(\Lambda^-)^\star = \{(x, y)\colon\ x, y \in \Lambda^-, |x - y| = 1\}$ is the set of non-oriented bonds inside Λ^- (with $|\cdot|$ the Euclidean norm), $-U < 0$ is the *binding energy* between neighboring particles Λ^-, and $\Delta \in (U, 2U)$ the *activation energy* for each particle in Λ.

Let $\square \equiv 0$ and $\blacksquare \equiv 1$. These configurations are associated, respectively, to the gas phase and the liquid phase. It is easy to see that $\blacksquare$ is the global minimizer of the Hamiltonian. In [dOS00] it is proven that $\mathbf{m} = \square$ and the value of $\Gamma^\star = \varPhi(\square, \blacksquare) - H(\square)$ is determined. Note that, since $H(\square) = 0$, $\Gamma^\star$ coincide with the energy of a critical configuration.

The paradigmatic shape of critical configurations was identified in [dOS00]. It consist of a droplet whose support is quasi-square of side lengths $(\ell_c, \ell_c - 1)$ plus a protuberance on the longest side of the rectangle plus a particle at $\partial^- \Lambda$, where

$$\ell_c = \left\lceil \frac{U}{2U - \Delta} \right\rceil \tag{1.24}$$

(the condition $\frac{U}{2U-\Delta} \notin \mathbb{N}$ is assumed in order to avoid ties). In [BdN06] the full geometry of the set of critical configurations has been determined. It consists of all the configurations obtained by adding a particle in a site in $\partial^-\Lambda$ to a configuration belonging to a set $\mathcal{D}$ defined as $\mathcal{D} = \bar{\mathcal{D}} \cup \widetilde{\mathcal{D}}$ where

- $\bar{\mathcal{D}}$ is the set of configurations with a single cluster anywhere in Λ^- whose support consists of an $(\ell_c - 2) \times (\ell_c - 2)$ square with four bars of lengths $\bar{k}_i$, $i = 1, 2, 3, 4$, attached to its four sides satisfying

$$1 \leq \bar{k}_i \leq \ell_c - 1, \qquad \sum_i \bar{k}_i = 3\ell_c - 3; \tag{1.25}$$

- $\widetilde{\mathcal{D}}$ is the set of configurations with a single cluster anywhere in Λ^- whose support consists of an $(\ell_c - 3) \times (\ell_c - 1)$ rectangle with four bars of lengths $\widetilde{k}_i$, $i = 1, 2, 3, 4$, attached to its four sides satisfying

$$1 \leq \widetilde{k}_i \leq \ell_c - 1, \qquad \sum_i \widetilde{k}_i = 3\ell_c - 2. \tag{1.26}$$

Configurations in $\mathcal{D}$ are called protocritical. The set of critical configurations is denoted by $\mathcal{D}^{\mathrm{fp}}$. It is proven that the dynamics visits the set of critical configurations with probability 1,

$$\lim_{\beta\to\infty} P_{\square}(\tau_{\mathcal{D}^{\mathrm{fp}}} < \tau_{\boxplus} \mid \tau_{\boxplus} < \tau_{\square}) = 1, \tag{1.27}$$

and that all critical configurations are equally likely to be visited,

$$\lim_{\beta\to\infty} P_{\square}(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \zeta) = 1/|\mathcal{D}^{\mathrm{fp}}| \quad \forall\, \zeta \in \mathcal{D}^{\mathrm{fp}}, \tag{1.28}$$

when the dynamics reaches for the first time the set $\mathcal{D}^{\mathrm{fp}}$.

Application of potential theory to the estimation of the expected nucleation time allows for a proof that there is a constant $K = K(\ell_c, \Lambda)$ such that

$$\mathbb{E}_{\square}(\tau_{\blacksquare}) = K e^{\beta\Gamma^\star}[1 + o(1)] \quad \text{as } \beta \to \infty. \tag{1.29}$$

For the value of K a variational formula is derived whose exact computation is

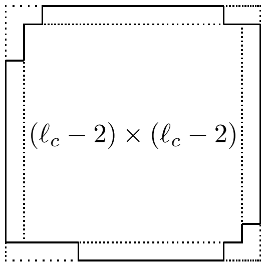

Figure 1.1: A configuration in $\bar{\mathcal{D}}$ with an $(\ell_c - 2) \times (\ell_c - 2)$ square in the center and four bars attached to it. A similar picture applies for $\widetilde{\mathcal{D}}$ with an $(\ell_c - 3) \times (\ell_c - 1)$ rectangle in the center.

highly non-trivial. However, as $\Lambda \to \mathbb{Z}^2$,

$$K \sim \frac{1}{4\pi N(\ell_c)} \frac{\log|\Lambda|}{|\Lambda|} \tag{1.30}$$

with

$$N(\ell_c) = \sum_{k=1,2,3,4} \binom{4}{k} \left[\binom{\ell_c + k - 2}{2k-1} + 2\binom{\ell_c + k - 3}{2k-1} \right] \tag{1.31}$$

being the cardinality of the set $\mathcal{D}$ modulo shifts.

1.3.2 Kawasaki dynamics on a finite box with open boundary for two types of particles

The model studied in this thesis constitutes a first attempt to generalize the results in [BdN06] for two dimensions to *multi-type particles systems*. We take a large finite box $\Lambda \subset \mathbb{Z}^2$. Particles come in two types: type 1 and type 2. Particles hop around subject to hard-core repulsion, and are conserved inside Λ. At the boundary of Λ particles are created and annihilated as in a gas reservoir, where the two types of particles have different densities $e^{-\beta\Delta_1}$ and $e^{-\beta\Delta_2}$. Also in this case the dynamics is locally conservative. The Hamiltonian is

$$H(\eta) = -U_{12} \sum_{x,y\in(\Lambda^-)^\star} 1_{\eta(x)\eta(y)=2} - U_{11} \sum_{x,y\in(\Lambda^-)^\star} 1_{\eta(x)\eta(y)=1} - U_{22} \sum_{x,y\in(\Lambda^-)^\star} 1_{\eta(x)\eta(y)=4} \tag{1.32}$$

$$+ \Delta_1 \sum_{x\in\Lambda} 1_{\eta(x)=1} + \Delta_2 \sum_{x\in\Lambda} 1_{\eta(x)=2}, \tag{1.33}$$

where $U_{i,j} > 0$ is the binding energy between particles of type i and j and Δ_i is the activation energy of particles of type i. This dynamics can be seen as a conservative analogue of the Blume-Capel model investigated by Cirillo and Olivieri [CO96].

The phase diagram of this model turns out to be very rich: we have to take into account different metastable states. In our analysis, though, we only consider the simplified version of the model obtained by setting $U_{11} = U_{22} = 0$. In order to lighten the notation, we will write $U_{12} = U$. Thus, the Hamiltonian becomes

$$H(\eta) = -U \sum_{x,y\in(\Lambda^-)^\star} 1_{\eta(x)\eta(y)=2} + \Delta_1 \sum_{x\in\Lambda} 1_{\eta(x)=1} + \Delta_2 \sum_{x\in\Lambda} 1_{\eta(x)=2}. \tag{1.34}$$

We will see that for this simplified version of the model the geometry of the local minimizers of the Hamiltonian and saddle points connecting them is already very involved and heavily depends on the values of Δ_1 and Δ_2. The main goal of the thesis is to classify the metastable behavior in different parameter regimes.

1.4 Overview of the main results in the thesis

In Chapter 2 we define the model that is the object of our study. We identify the values of the parameters for which the model properly describes the condensation of a supersaturated gas and exhibits a metastable behavior. Under *three hypotheses*, we determine the distribution and the expectation of the nucleation time, and identify the so-called critical configurations that satisfy a certain "gate property". The first hypothesis assumes that a configuration corresponding to the liquid phase is a minimizer of the Hamiltonian. The second hypothesis requires that the valleys of the energy landscape are not too deep. The third hypothesis requires that the critical configurations have an appropriate geometry. Subject to the three hypotheses, several theorems are derived, for which *three model-dependent quantities* need to be identified as well: (1) the energy barrier $\Gamma^\star$ separating the configuration $\square$ consisting of the empty box and the set $\mathcal{X}_{\text{stab}}$ of global minimizers of the Hamiltonian; (2) the set $\mathcal{C}^\star$ of critical configurations; (3) the cardinality $N^\star$ of the

the set of protocritical configurations. This set can be thought as the "entrance" of $\mathcal{C}^\star$. These quantities are identified in Chapters 3 and 4 via a detailed analysis of the energy landscape that combines combinatorial and geometric techniques.

In Chapter 3 it is shown that the first two hypotheses are satisfied and the first model-dependent quantity is identified.

- In the first part of this chapter we prove that a configuration $\boxplus$, consisting of a large checkerboard filling the volume Λ, minimizes the Hamiltonian, and we identify the energy barrier $\Gamma^\star$ separating the configuration $\square$ from the set $\mathcal{X}_{\mathrm{stab}}$ of global minimizers of the Hamiltonian. To carry out this task, the number of particles of type 2 is identified as a key quantity, and the configurations of minimal energy for a fixed number of particle of type 2 is identified. This is achieved by observing that in configurations of minimal energy, since we will assume that $\Delta_1 < U$, particles of type 2 must be surrounded by particles of type 1. This allows us to look at configurations of minimal energy not as clusters of single particles, but as clusters of "tiles": particles of type 2 surrounded by particles of type 1. To deal with tiles, it is convenient to look at the representation of configurations on a dual lattice. With this dual representation, a tile correspond to a unit square and the configurations of minimal energy are those where these unit squares are arranged in an "optimal" manner. It turns out that for a fixed number of particles of type 2 the quantity over which the optimization must be performed is the number of particles of type 1. This number is linked to the perimeter and the shape of the "polyomino" (union of unit squares) associated with the tiles in a configuration. It turns out that, in order to minimize the energy, the polyomino must be a convex polyomino of minimal perimeter. With this observation, the ground state is easily identified to be a configuration $\boxplus$ consisting of the largest checkerboard configuration fitting inside the box Λ. The prototype shape of critical configurations and the value of $\Gamma^\star$ are then easily derived by considering a foliation of the state space according to the number of particles of type 2 in Λ. Note that all these results only require us to analyze the model from a static point of view.
- In the second part of this chapter we derive an upper bound for the stability level of all the configurations in $\mathcal{X}$, i.e., (loosely speaking) for the depth of the valleys of the energy landscape, and we make sure that close to the phase transition curve the depth of these valleys is smaller than $\Gamma^\star$. Here the particular dynamics that has been chosen plays a crucial role. In order to show that each configuration η other than $\square$ and $\boxplus$ is separated from a configuration with lower energy by a barrier smaller than $\Gamma^\star$, a path leading to $\mathcal{I}_\eta$ is constructed. The complication arises from the fact that particles

can only be created and annihilated at the boundary of Λ, and that the path they follow inside Λ is constrained by the presence of other particles. Furthermore, the fact that only particles of different types feel an attractive interaction poses the problem of parity of clusters: when clusters are close to each other they cannot merge when they have different parity. As a consequence, the transition from one configuration η to a configuration η' that differs from η only at a single site x may require the motion of many particle occupying sites possibly far from x. To achieve this we will make use of a recursive algorithm that, starting from any configuration η, allows us to find a sequence of configurations whose energy is non-increasing that eventually reaches the set $\mathcal{I}_\eta$.

The results derived in Chapter 3 are sufficient to establish the exponential probability distribution of the nucleation time divided by its mean and to determine the mean nucleation time up to a multiplicative factor of order $1+o(1)$ as $\beta \to \infty$.

In Chapter 4 it is shown that the model satisfies the third hypothesis, and the set of critical configurations is identified. We give a geometric characterization of the configurations $\mathcal{C}^\star$ and compute the value of $N^\star$. A prototype of the critical configuration is already identified in Chapter 3, and consists of a configuration of minimal energy with $\ell^\star(\ell^\star - 1) + 1$ particles of type 2 arranged in a cluster of minimal energy plus a particle of type 2. The difficult task is to characterize the *full* set of critical configurations. Also this part of the analysis uses the specific dynamical aspects of the model, which are investigated in detail in a neighborhood of the saddle configurations $\mathcal{S}(\square, \boxplus)$.

The tiles making up the cluster can travel around the cluster faster than particles of type 2 can appear at the boundary of Λ. This motion of tiles along the border gives the dynamics the opportunity to extend the set of critical configurations. Different mechanism are identified that allow tiles to travel around a cluster. The energy barrier that must be overcome in order to activate these mechanisms is determined, and is compared with the energy barrier the dynamics has to climb in order to let a particle enter Λ. How rich the set of critical configurations is depends on the relative magnitude of these barriers. Consequently, the geometry of this set is highly sensitive to the choice of parameters: the set of critical configurations is indeed very different in different regions of the parameter space.

The problem of computing the value $N^\star$, i.e., the cardinality of the set of protocritical configurations, is reduced to counting the number of polyominoes of minimal perimeter belonging to certain classes of configurations that depend on the values of the parameters Δ_1 and Δ_2. This is a non-trivial problem that is interesting in its own right. With these results we are able to derive the sharp asymptotics for the nucleation time and to find the entrance distribution of the set of critical configurations.

Results in this chapter are derived using a foliation of the state space according to the number of particles of type 1 in Λ and the fact that configurations in $\mathcal{C}^{\star}$ must satisfy a "gate property", i.e., they must be visited by all optimal paths. These results allow us to derive appropriate variational formulas for $\mathrm{CAP}(\square, \boxplus)$ and compute sharp asymptotic values for the expected nucleation time.

2 Kawasaki dynamics with two types of particles

This chapter is based on:
F. den Hollander, F. R. Nardi, A. Troiani, *Metastability for Kawasaki dynamics at low temperature with two types of particles*, Electronic Journal of Probability, 17(2), 1–26, 2012.

2.1 Introduction and main results

The main motivation behind this work is to understand metastability of *multi-type particle systems* subject to *conservative stochastic dynamics*. In the past ten years a good understanding was achieved of the metastable behavior of the lattice gas subject to Kawasaki dynamics, i.e., random hopping of particles of a single type with hardcore repulsion and nearest-neighbor attraction. The analysis was based on a combination of techniques coming from large deviation theory, potential theory, geometry and combinatorics. In particular, a precise description was obtained of the time to nucleation (from the "gas phase" to the "liquid phase"), the critical droplet triggering the nucleation, and the typical nucleation path, i.e., the typical growing and shrinking of droplets. For an overview we refer the reader to two recent papers presented at the 12th Brazilian School of Probability: Gaudillière and Scoppola [GS08] and Gaudillière [Gau09]. For an overview on metastability and droplet growth in a broader context, we refer the reader to the monograph by Olivieri and Vares [OV05], and the review papers by Bovier [Bov09], [Bov11], den Hollander [den09], Olivieri and Scoppola [OS10].

It turns out that for systems with two types of particles, as considered in this chapter, the *geometry* of the energy landscape is much 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 droplets. Our proofs in this chapter use potential theory and rely on ideas developed in Bovier, den Hollander and Nardi [BdN06] for Kawasaki dynamics with one type of particle.

Our target is to identify the *minimal* hypotheses that lead to metastable behavior. We will argue that these hypotheses, stated in the context of our specific model, also suffice for Kawasaki dynamics with more than two types of particles and are robust against variations of the interaction.

The model studied in the present work falls in the class of variations on Ising spins subject to Glauber dynamics and lattice gas particles subject to Kawasaki dynamics. These variations include Blume–Capel, anisotropic interactions, staggered magnetic field, next-nearest-neighbor interactions, and probabilistic cellular automata. In all these models the geometry of the energy landscape is complex and needs to be controlled in order to arrive at a complete description of metastability. For an overview, see the monograph by Olivieri and Vares [OV05], chapter 7.

Section 2.1.1 defines the model, Section 2.1.2 introduces basic notation, Section 2.1.3 identifies the metastable region, while Section 2.2.1 states the main theorems. Section 2.2.2 discusses the main theorems, *places them in their proper context and provides further motivation.* Section 2.2.3 proves three geometric lemmas that are needed in the proof of the main theorems, which is provided in Section 2.3.

2.1.1 Lattice gas subject to Kawasaki dynamics

Let $\Lambda \subset \mathbb{Z}^2$ be a large finite box. Let

$$\begin{aligned} \partial^-\Lambda &= \{x \in \Lambda\colon\ \exists\, y \notin \Lambda\colon\ |y-x| = 1\},\\ \partial^+\Lambda &= \{x \notin \Lambda\colon\ \exists\, y \in \Lambda\colon\ |y-x| = 1\}, \end{aligned} \tag{2.1}$$

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, respectively. 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

$$H(\eta) = -U \sum_{(x,y)\in(\Lambda^-)^\star} 1_{\{\eta(x)\eta(y)=2\}} + \Delta_1 \sum_{x\in\Lambda} 1_{\{\eta(x)=1\}} + \Delta_2 \sum_{x\in\Lambda} 1_{\{\eta(x)=2\}}, \tag{2.2}$$

where $(\Lambda^-)^\star = \{(x,y)\colon\ x,y \in \Lambda^-, |x-y| = 1\}$ is the set of non-oriented bonds inside Λ^- (with $|\cdot|$ the Euclidean norm), $-U < 0$ is the *binding energy* between neighboring particles of *different* types inside Λ^-, and $\Delta_1 > 0$ a nd $\Delta_2 > 0$ are the *activation energies* of particles of type 1, respectively, type 2 inside Λ. Without loss of generality we will assume that

$$\Delta_1 \leq \Delta_2. \tag{2.3}$$

The Gibbs measure associated with H is

$$\mu_\beta(\eta) = \frac{1}{Z_\beta}\, e^{-\beta H(\eta)}, \qquad \eta \in \mathcal{X}, \tag{2.4}$$

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

$$c_\beta(\eta, \eta') = \begin{cases} e^{-\beta[H(\eta')-H(\eta)]_+}, & \eta, \eta' \in \mathcal{X},\, \eta \sim \eta', \\ 0, & \text{otherwise}, \end{cases} \tag{2.5}$$

(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, i.e.,

$$\mu_\beta(\eta) c_\beta(\eta, \eta') = \mu_\beta(\eta') c_\beta(\eta', \eta) \qquad \forall\, \eta, \eta' \in \mathcal{X}. \tag{2.6}$$

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 (see (2.2)).

The dynamics defined by (2.2) and (2.5) 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 $\Delta_1 = \Delta_2$. Further note that, whereas Kawasaki dynamics for one type of particle can be interpreted as swaps of occupation numbers along edges, such an interpretation is not possible here.

2.1.2 Notation

To identify the metastable region in Section 2.1.3 and state our main theorems in Section 2.2.1, we need some notation.

Definition 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 2.13 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 2.2 *(a) $\Phi(\eta, \eta')$ is the communication height between $\eta, \eta' \in \mathcal{X}$ defined by*

$$\Phi(\eta, \eta') = \min_{\omega\colon\ \eta \to \eta'} \max_{\xi \in \omega} H(\xi), \tag{2.7}$$

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

$$\Phi(\mathcal{A}, \mathcal{B}) = \min_{\eta \in \mathcal{A}, \eta' \in \mathcal{B}} \Phi(\eta, \eta'). \tag{2.8}$$

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

$$\mathcal{S}(\eta, \eta') = \left\{ \zeta \in \mathcal{X}\colon\ \exists\, \omega\colon\ \eta \to \eta', \omega \ni \zeta\colon\ \max_{\xi \in \omega} H(\xi) = H(\zeta) = \Phi(\eta, \eta') \right\}. \tag{2.9}$$

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

$$V_\eta = \Phi(\eta, \mathcal{I}_\eta) - H(\eta), \tag{2.10}$$

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* $\mathcal{X}_{\rm meta}$*),* $\Gamma^\star = \varPhi(\square, \boxplus) - H(\square)$ *(note that* $H(\square) = 0$*).*

Definition 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.)*

Definitions 2.2–2.3 are canonical in metastability theory and are formalized in Manzo, Nardi, Olivieri and Scoppola [MNOS04].

2.1.3 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 2.4 *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

$$H(\eta) = n_1(\eta)\Delta_1 + n_2(\eta)\Delta_2 - B(\eta)U. \tag{2.11}$$

Since $\Delta_1 \leq \Delta_2$, we may assume without loss of generality 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.,

$$\eta^{1\Leftrightarrow 2}(x) = \begin{cases} 1 & \text{if } \eta(x) = 2, \\ 2 & \text{if } \eta(x) = 1, \\ 0 & \text{otherwise,} \end{cases} \tag{2.12}$$

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

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

$$H(\eta) \geq n_1(\eta)\Delta_1 + n_2(\eta)\Delta_2 - 4n_2(\eta)U \geq n_2(\eta)(\Delta_1 + \Delta_2 - 4U). \tag{2.13}$$

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

$$H(\hat{\eta}) = \tfrac{1}{2}\ell^2\Delta_1 + \tfrac{1}{2}\ell^2\Delta_2 - 2\ell(\ell-1)U, \tag{2.14}$$

and so

$$H(\hat{\eta}) < 0 \Longleftrightarrow \ell^2(\Delta_1 + \Delta_2) < 4\ell(\ell-1)U \Longleftrightarrow \Delta_1 + \Delta_2 < (4 - 4\ell^{-1})U. \tag{2.15}$$

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 2.4.

Within the metastable region $\Delta_1 + \Delta_2 < 4U$, we may as well exclude the subregion $\Delta_1, \Delta_2 < U$ (see Fig. 2.1). 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.

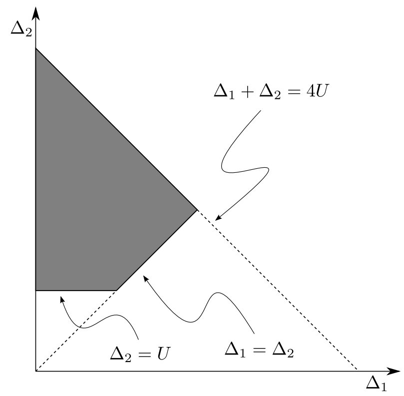

Figure 2.1: Proper metastable region.

2.2 Three theorems under three hypotheses

2.2.1 Main theorems

Theorems 2.7–2.9 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 2.5 (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 one *additional free particle* of type 2 somewhere in $\partial^-\Lambda$.

Definition 2.6 (a) $\mathcal{C}^\star_{\mathrm{att}}$ *is the set of configurations obtained from* $\mathcal{C}^\star_{\mathrm{bd}}$ *by moving the free particle of type* 2 *along a path of empty sites in* Λ *and attaching it to the single droplet (i.e., creating at least one additional active bond). This set*

decomposes as $\mathcal{C}^\star_{\rm att} = \cup_{\hat\eta \in \mathcal{P}} \mathcal{C}^\star_{\rm att}(\hat\eta)$.
(b) $\mathcal{C}^\star$ *is the set of configurations obtained from* $\mathcal{C}^\star_{\rm bd}$ *by moving the free particle of type* 2 *along a path of empty sites in* Λ. *This set decomposes as* $\mathcal{C}^\star = \cup_{\hat\eta \in \mathcal{P}} \mathcal{C}^\star(\hat\eta)$.

Note that $\Gamma^\star = H(\mathcal{C}^\star) = H(\mathcal{P}) + \Delta_2$, and that $\mathcal{C}^\star$ consists of precisely those configurations "interpolating" between $\mathcal{P}$ and $\mathcal{C}^\star_{\rm att}$: 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" before it attaches itself properly to the single droplet (the meaning of the word properly will become clear in Section 2.3.4).

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

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

Theorem 2.7 *(a)* $\lim_{\beta\to\infty} P_\square(\tau_{\mathcal{C}^\star_{\rm bd}} < \tau_\boxplus \mid \tau_\boxplus < \tau_\square) = 1$.
(b) $\lim_{\beta\to\infty} P_\square(\eta_{\tau_{\mathcal{C}^\star_{\rm bd}}} = \zeta) = 1/|\mathcal{C}^\star_{\rm bd}|$ *for all* $\zeta \in \mathcal{C}^\star_{\rm bd}$.

Theorem 2.8 *There exists a constant* $K = K(\Lambda; U, \Delta_1, \Delta_2) \in (0,\infty)$ *such that*

$$\lim_{\beta\to\infty} e^{-\beta\Gamma^\star} E_\square(\tau_\boxplus) = K. \tag{2.16}$$

Moreover,

$$K \sim \frac{1}{N^\star}\frac{\log|\Lambda|}{4\pi|\Lambda|} \qquad \text{as } \Lambda \to \mathbb{Z}^2. \tag{2.17}$$

Theorem 2.9 $\lim_{\beta\to\infty} P_\square(\tau_\boxplus / E_\square(\tau_\boxplus) > t) = e^{-t}$ *for all* $t \geq 0$.

We close this section with a few remarks.

Remark 2.10 The free particle in (H3-a) is of type 2 only when $\Delta_1 < \Delta_2$. If $\Delta_1 = \Delta_2$ (recall (2.3)), 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 (2.12).

Remark 2.11 We will see in Section 2.2.3 that (H1–H2) imply that

$$(\mathcal{X}_{\rm meta}, \mathcal{X}_{\rm stab}) = (\square, \boxplus), \qquad \Gamma = \Gamma^\star. \tag{2.18}$$

The reason that $\boxplus$ is the configuration with lowest energy comes from the "anti-ferromagnetic" nature of the interaction in (2.2).

Remark 2.12 Note that (H2) and Lemma 2.4 imply (H1). Indeed, (H2) says that $\square$ and $\boxplus$ have the highest stability level in the sense of Definition 2.2(c), so that $\mathcal{X}_{\text{stab}} \subset \{\square, \boxplus\}$, while Lemma 2.4 says that $\square$ is not the global minimum of H, so that $\boxplus$ must be the global minumum of H, and hence $\mathcal{X}_{\text{stab}} = \boxplus$ according to Definition 2.2(d). One reason why we state (H1)–(H2) as separate hypotheses is that we will later place them in a more general context (see Section 2.2.2, item 8). Another reason is that they are the key ingredients in the proof of Theorems 2.7–2.9 in Section 2.3.

Remark 2.13 We will see in Chapter 3 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 Chapter 3. 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 Chapter 3.

Remark 2.14 As we will see in Section 2.3.4, 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 $\mathcal{G}(\square, \boxplus)$" that have energy $< \Gamma^\star$ but communication height $\Gamma^\star$ towards both $\square$ and $\boxplus$. This set contains $\mathcal{P}$, $\mathcal{C}^\star_{\text{att}}$ and possibly more, as we will see in Chapter 4 (for Kawasaki dynamics with one type of particle this was shown in Bovier, den Hollander and Nardi [BdN06], Section 2.3.2). As a result of this geometric complexity, for finite Λ only upper and lower bounds are known for K. What (2.17) 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 2.3.4 that, apart from the uniformity property expressed in Theorem 2.7(b), the reason behind this simplification is the fact that simple random walk (the motion of the free particle) is *recurrent* on $\mathbb{Z}^2$.

2.2.2 Discussion

1. Theorem 2.7(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 2.7(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 2.8 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 2.9, finally, says that the nucleation time is exponentially distributed on the scale of its average.

2. Theorems 2.7–2.9 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 2.3 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 2.7–2.9 hold must satisfy appropriate analogues of (H1)–(H3) (including multi-type Kawasaki dynamics).

The *model-dependent* ingredient of Theorems 2.7–2.9 is the triple

$$(\Gamma^\star, \mathcal{C}^\star, N^\star). \tag{2.19}$$

This triple depends on the parameters U, Δ_1, Δ_2 in a manner that will be identified in Chapter 3 and Chapter 4. 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)).

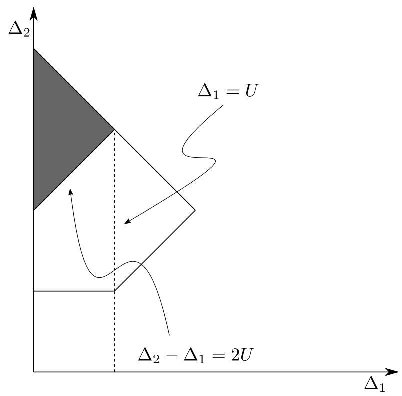

Figure 2.2: Subregion of the proper metastable region considered in Chapter 3 and Chapter 4.

3. In Chapter 3 and Chapter 4, 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. 2.2)

$$0 < \Delta_1 < U, \quad \Delta_2 - \Delta_1 > 2U. \tag{2.20}$$

More precisely, in Chapter 3 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 (2.20). In Chapter 3 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 (2.20), this upper bound would settle (H2) without further restrictions on U, Δ_1, Δ_2. In Chapter 4 we will prove (H3) and identify $\mathcal{C}^\star, N^\star$.

The simplifying features of (2.20) 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. 2.1). However, as we will see in Chapter 3 and Chapter 4, $(\Gamma^\star, \mathcal{C}^\star, N^\star)$ is different when $\Delta_1 > U$ compared to when $\Delta_1 < U$ (because the critical droplets are square-shaped, respectively, rhombus-shaped).

4. Theorems 2.7–2.9 generalize what was obtained for Kawasaki dynamics with one type of particle in den Hollander, Olivieri and Scoppola [dOS00], and Bovier, den Hollander and Nardi [BdN06]. 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 Chapter 3 and Chapter 4.

Similar results hold for Ising spins subject to *Glauber dynamics*, as shown in Neves and Schonmann [NS91], and Bovier and Manzo [BM02]. For this system, K has a simple explicit form. Theorems 2.7–2.9 are close in spirit to the extension for Glauber dynamics of Ising spins when an alternating external field is included, as carried out in Nardi and Olivieri [NO96], for Kawakasi dynamics of lattice gases 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 [NOS05], and for Glauber dynamics with three–state spins (Blume–Capel model), as carried out in Cirillo and Olivieri [CO96]

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 [dHNOS03], and Bovier, den Hollander and Nardi [BdN06]. 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 [BAC96], and Bovier and Manzo [BM02], and K again has a simple explicit form.

5. In Gaudillière, den Hollander, Nardi, Olivieri and Scoppola [GDHN+09], [GdHN+a], [GdHN+b], and Bovier, den Hollander and Spitoni [BdHS10], 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 [dOS00] and Bovier, den Hollander and Nardi [BdN06] 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 chapter 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 $(\mathcal{X}_{\text{meta}}, \mathcal{X}_{\text{stab}})$ 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.

7. We will see in Section 2.3 that (H1)–(H2) alone are enough to prove Theorems 2.7–2.9, with the exception of the uniform entrance distribution of $\mathcal{C}^\star_{\text{bd}}$ and the scaling of K in (2.17). The latter require (H3) and come out of a closer analysis of the energy landscape near $\mathcal{C}^\star$, respectively, a *variational formula* for $1/K$ that is derived on the basis of (H1)–(H2) alone.

In Manzo, Nardi, Olivieri and Scoppola [MNOS04] an "axiomatic approach" to metastability similar to the one in this chapter was put forward, but the results that were obtained (for a general dynamics) based on hypotheses similar to (H1)–(H2) were cruder, e.g. the nucleation time was shown to be $\exp[\beta\Gamma^\star + o(\beta)]$, which fails to capture the fine asymptotics in (2.16) and consequently also the scaling in (2.17). Also the uniform entrance distribution was not established. These finer details come out of the potential-theoretic approach to metastability developed in Bovier, Eckhoff, Gayrard and Klein [BEGK02] explained in Section 2.3.

8. Hypotheses (H1)–(H3) are the *minimal hypotheses* in the following sense. If we consider Kawasaki dynamics with more than two types of particles and/or change the details of the interaction (e.g. by adding to (2.2) also interactions between particles of different type), then all that changes is that $\square$ and $\boxplus$ are replaced by different configurations, while (H1)–(H2) remain the same for their new counterparts and (H3) remains the same for the analogues of $\mathcal{P}$, $\mathcal{C}^\star$, $\mathcal{C}^\star_{\mathrm{bd}}$ and $\mathcal{C}^\star_{\mathrm{att}}$. The proof in Section 2.3 will show that Theorems 2.7–2.9 continue to hold under (H1)–(H3) in the new setting. For further reading we refer the reader to the monograph in progress by Bovier and den Hollander [BdH].

2.2.3 Consequences of the three hypotheses

Lemmas 2.15–2.19 below are immediate consequences of (H1)–(H3) and will be needed in the proof of Theorems 2.7–2.9 in Section 2.3.

Lemma 2.15 (H1)–(H2) *imply that* $V_\square = \Gamma^\star$.

Proof. By Definitions 2.2(c–f) and (H1), $\boxplus \in \mathcal{I}_\square$, which implies that $V_\square \le \Gamma^\star$. We show that (H2) implies $V_\square = \Gamma^\star$. The proof is by contradiction. Suppose that $V_\square < \Gamma^\star$. Then, by Definition 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 $\eta_0,\dots,\eta_m \in \mathcal{X}$ with $\eta_0 = \eta$ and $\eta_m = \boxplus$ such that $\eta_{i+1} \in \mathcal{I}_{\eta_i}$ and $\Phi(\eta_i,\eta_{i+1}) \le H(\eta_i) + V^\star$ for $i = 0,\dots,m-1$. Therefore

$$\Phi(\eta,\boxplus) \le \max_{i=0,\dots,m-1} \Phi(\eta_i,\eta_{i+1}) \le \max_{i=0,\dots,m-1} [H(\eta_i) + V^\star] = H(\eta) + V^\star < H(\square) + \Gamma^\star, \tag{2.21}$$

where in the first inequality we use that

$$\Phi(\eta,\sigma) \le \max\{\Phi(\eta,\xi),\Phi(\xi,\sigma)\} \qquad \forall\, \eta,\sigma,\xi \in \mathcal{X}, \tag{2.22}$$

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

$$\Gamma^\star = \Phi(\square, \boxplus) - H(\square) \le \max\{\Phi(\square, \eta), \Phi(\eta, \boxplus)\} - H(\square) < \Gamma^\star, \tag{2.23}$$

which is a contradiction. ★

Lemma 2.16 (H2) *implies that* $\Phi(\eta, \{\square, \boxplus\}) - H(\eta) \le V^\star$ *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 $\eta_0, \dots, \eta_m \in \mathcal{X}$ with $\eta_0 = \eta$ and $\eta_m \in \{\square, \boxplus\}$ such that $\eta_{i+1} \in \mathcal{I}_{\eta_i}$ and $\Phi(\eta_i, \eta_{i+1}) \le H(\eta_i) + V^\star$ for $i = 0, \dots, m-1$. Therefore, as in (2.21), we get $\Phi(\eta, \{\square, \boxplus\}) \le H(\eta) + V^\star$. ★

Lemma 2.17 (H1)–(H2) *imply that* $H(\eta) > H(\square)$ *for all* $\eta \in \mathcal{X}\backslash\square$ *such that* $\Phi(\eta, \square) \le \Phi(\eta, \boxplus)$.

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 $H(\eta) \le H(\square) = 0$. Then $\square \notin \mathcal{I}_\eta$. By (H2) and the finiteness of $\mathcal{X}$, there exist an $m \in \mathbb{N}$ and a sequence $\eta_0, \dots, \eta_m \in \mathcal{X}$ with $\eta_0 = \eta$ and $\eta_m = \boxplus$ such that $\eta_{i+1} \in \mathcal{I}_{\eta_i}$ and $\Phi(\eta_i, \eta_{i+1}) \le H(\eta_i) + V^\star$ for $i = 0, \dots, m-1$. Therefore, as in (2.21), we get $\Phi(\eta, \boxplus) \le H(\eta) + V^\star \le H(\square) + V^\star < H(\square) + \Gamma^\star$. Hence

$$\begin{aligned}\Gamma^\star &= \Phi(\square, \boxplus) - H(\square) \le \max\{\Phi(\square, \eta), \Phi(\eta, \boxplus)\} - H(\square) \\ &= \max\{\Phi(\eta, \square), \Phi(\eta, \boxplus)\} - H(\square) = \Phi(\eta, \boxplus) - H(\square) < \Gamma^\star,\end{aligned} \tag{2.24}$$

which is a contradiction. ★

Lemma 2.18 $\mathcal{C}^\star_{\mathrm{bd}}$ *is a minimal gate.*

Proof. Let $\mathcal{A} = \{\eta \in \mathcal{C}^\star_{\mathrm{bd}} \colon \exists\, \omega \in \Omega(\eta) \colon \omega \cap \mathcal{C}^\star_{\mathrm{bd}} = \{\eta\}\}$, and let $\tilde{\mathcal{A}} = \mathcal{C}^\star_{\mathrm{bd}}\backslash\mathcal{A}$. In words, for each $\eta \in \mathcal{A}$ there is a path in $(\square \to \boxplus)_{\mathrm{opt}}$ entering $\mathcal{G}(\square, \boxplus)$ via η and reaching $\boxplus$ without hitting $\mathcal{C}^\star_{\mathrm{bd}}$ again, while if a path in $(\square \to \boxplus)_{\mathrm{opt}}$ enters $\mathcal{C}^\star_{\mathrm{bd}}$ via a configuration in $\tilde{\mathcal{A}}$, then it must go back to $\mathcal{C}^\star_{\mathrm{bd}}$ before reaching $\boxplus$. We will show that $\tilde{\mathcal{A}}$ is empty. The proof is by contradiction.

Assume that $\eta \in \tilde{\mathcal{A}}$ and let $\omega \in \Omega(\eta)$. Let ζ be the last configuration in $\mathcal{C}^\star_{\mathrm{bd}}$ visited by ω before reaching $\boxplus$. Then there is an $\omega' \in (\square \to \boxplus)_{\mathrm{opt}}$ entering $\mathcal{G}(\square, \boxplus)$ via ζ. The path ω'' obtained by joining the part of ω' from $\square$ to ζ and the part of ω from ζ to $\boxplus$ belongs to $(\square \to \boxplus)_{\mathrm{opt}}$, and $\eta \notin \omega''$. Therefore η is unessential and, by Theorem 5.1 in [MNOS04] (Lemma 4.3 in this paper), it does not belong to $\mathcal{G}(\square, \boxplus)$. This contradicts the assumption $\eta \subset \mathcal{C}^\star_{\mathrm{bd}} \subset \mathcal{G}(\square, \boxplus)$. ★

Lemma 2.19 (H3a), (H3-c) *and Definition* 4.5(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. The proof is by contradicion. Let $\mathcal{C}^\star_{\rm att} \ni \eta = (\hat{\eta}, x)$, and assume that there is a path $\omega_1\colon \square \to \eta$ that does not visit $\mathcal{C}^\star_{\rm bd}$ and such that $H(\sigma) \leq \Gamma^\star$ for all $\sigma \in \omega_1$. By the definition of $\mathcal{C}^\star_{\rm att}$, there exists a configuration $\mathcal{C}^\star_{\rm bd} \ni \zeta = (\hat{\eta}, z)$ such that ζ is obtained from η by moving the particle of type 2 from x to z. Consequently, there exists a path ω_2 from η to ζ consisting of a sequence of configurations of the type $(\hat{\eta}, y_i)$ with $y_i \in \Lambda$ for all i. Note that, since $H(\zeta) = \Gamma^\star$, the particle of type 2 at site z in ζ has no active bond (it is in $\partial^-\Lambda$) and all configurations in ω_2 have the same number of particles of both types, we have $H(\sigma) \leq \Gamma^\star$ for all σ in ω_2. Since ζ belongs to the minimal gate $\mathcal{C}^\star_{\rm bd}$, there is a path $\omega_3\colon \zeta \to \boxplus$ such that $\omega_3 \cap \mathcal{C}^\star_{\rm bd} = \{\zeta\}$ and such that $H(\sigma) \leq \Gamma^\star$ for all $\sigma \in \omega_3$.

Now consider the following two cases.

(1) $\eta \in \omega_3$. Let ω_4 be the part of ω_3 from η to $\boxplus$. Then the path obtained by joining ω_1 and ω_4 is a path in $(\square \to \boxplus)_{\rm opt}$ that does not visit $\mathcal{C}^\star_{\rm bd}$. This contradicts the definition of $\mathcal{C}^\star_{\rm bd}$.

(2) $\eta \notin \omega_3$. Let $\omega = \omega_1 + \omega_2 + \omega_3$. Then, by construction, $\omega \in (\square \to \boxplus)_{\rm opt}$. Let $\pi = (\hat{\eta}, w)$ be the configuration in ω visited just before ζ. By definition, $\pi \in \mathcal{P}$. By (the first part of) (H3-a), π consists of a single droplet, and hence $w \notin \partial^-\Lambda$. Therefore ζ is obtained by "breaking" a droplet of a configuration in $\mathcal{P}$ and not by adding a particle of type 2 in $\partial^-\Lambda$ to a configuration in $\mathcal{P}$. This contradicts (the second part of) (H3-a).

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Note that Lemma 2.15 implies that $\mathcal{X}_{\rm meta} = \square$ and $\Gamma = \Gamma^\star$ (recall Definition 2.2(e–f).

2.3 Proof of main theorems

In this section we prove Theorems 2.7–2.9 subject to hypotheses (H1)–(H3). Sections 2.3.1–2.3.3 introduce the basic ingredients, while Sections 2.3.4–2.3.6 provide the proofs.

We will follow the *potential-theoretic* argument that was used in Bovier, den Hollander and Nardi [BdN06] for Kawasaki dynamics with one type of particle. In fact, we will see that (H1)–(H3) are the *minimal* assumptions needed to prove Theorems 2.7–2.9.

2.3.1 Dirichlet form and capacity

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

$$\mathcal{E}_\beta(h) = \tfrac{1}{2} \sum_{\eta,\eta' \in \mathcal{X}} \mu_\beta(\eta) c_\beta(\eta,\eta')[h(\eta) - h(\eta')]^2, \qquad h\colon\, \mathcal{X} \to [0,1], \tag{2.25}$$

where μ_β is the Gibbs measure defined in (2.4) and c_β is the kernel of transition rates defined in (2.5). 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

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) = \min_{\substack{h\colon\, \mathcal{X}\to[0,1] \\ h|_{\mathcal{A}}\equiv 1, h|_{\mathcal{B}}\equiv 0}} \mathcal{E}_\beta(h), \tag{2.26}$$

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 (2.26), called the *equilibrium potential* of the pair $\mathcal{A}, \mathcal{B}$, is given by

$$h^\star_{\mathcal{A},\mathcal{B}}(\eta) = P_\eta(\tau_{\mathcal{A}} < \tau_{\mathcal{B}}), \qquad \eta \in \mathcal{X}\backslash(\mathcal{A}\cup\mathcal{B}), \tag{2.27}$$

and is the solution of the equation

$$\begin{aligned} (c_\beta h)(\eta) &= 0, \qquad && \eta \in \mathcal{X}\backslash(\mathcal{A}\cup\mathcal{B}), \\ h(\eta) &= 1, && \eta \in \mathcal{A}, \\ h(\eta) &= 0, && \eta \in \mathcal{B}, \end{aligned} \tag{2.28}$$

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

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) = \sum_{\eta\in\mathcal{A}} \mu_\beta(\eta)\, c_\beta(\eta, \mathcal{X}\backslash\eta)\, \mathbb{P}_\eta(\tau_{\mathcal{B}} < \tau_{\mathcal{A}}) \tag{2.29}$$

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 2.1(f)). Note that the reversibility of the dynamics and (2.25–2.26) imply

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) = \mathrm{CAP}_\beta(\mathcal{B},\mathcal{A}). \tag{2.30}$$

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 2.20 *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*

$$C_1 \leq e^{\beta\Phi(\mathcal{A},\mathcal{B})} Z_\beta \mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) \leq C_2 \qquad \forall\, \beta \in (0,\infty). \tag{2.31}$$

Proof. The proof is given in [BdN06], 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 (2.26) by picking $h = 1_{K(\mathcal{A},\mathcal{B})}$ with

$$K(\mathcal{A},\mathcal{B}) = \{\eta \in \mathcal{X} \colon\ \Phi(\eta,\mathcal{A}) \leq \Phi(\eta,\mathcal{B})\}. \tag{2.32}$$

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

$$\begin{array}{ll} (1) & H(\eta') < H(\eta), \\ (2) & H(\eta) \geq \Phi(\mathcal{A},\mathcal{B}). \end{array} \tag{2.33}$$

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

$$H(\eta') \geq H(\eta) \qquad \Longleftrightarrow \qquad \Phi(\eta',\mathcal{F}) = \Phi(\eta,\mathcal{F}) \vee H(\eta')\ \ \forall\,\mathcal{F} \subset \mathcal{X}. \tag{2.34}$$

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 (2.34), and hence $\eta' \in K(\mathcal{A},\mathcal{B})$, which is a contradiction.

To see (2), note that (1) implies the reverse of (2.34):

$$H(\eta) \geq H(\eta') \qquad \Longleftrightarrow \qquad \Phi(\eta,\mathcal{F}) = \Phi(\eta',\mathcal{F}) \vee H(\eta)\ \ \forall\,\mathcal{F} \subset \mathcal{X}. \tag{2.35}$$

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

$$H(\eta) < \Phi(\eta,\mathcal{B}) = \Phi(\eta',\mathcal{B}) < \Phi(\eta',\mathcal{A}) = \Phi(\eta,\mathcal{A}), \tag{2.36}$$

where the equalities come from (2.35), 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 (2.33) with (2.4–2.5) and using reversibility, we find that

$$\mu_\beta(\eta) c_\beta(\eta,\eta') \leq \frac{1}{Z_\beta}\, e^{-\beta\Phi(\mathcal{A},\mathcal{B})} \qquad \forall\, \eta \in K(\mathcal{A},\mathcal{B}),\ \eta' \in \mathcal{X}\backslash K(\mathcal{A},\mathcal{B}),\ \eta \sim \eta'. \tag{2.37}$$

Hence

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) \le \mathcal{E}_\beta(1_{K(\mathcal{A},\mathcal{B})}) \le C_2 \frac{1}{Z_\beta}\, e^{-\beta\Phi(\mathcal{A},\mathcal{B})} \tag{2.38}$$

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.,

$$\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) \ge \min_{\substack{h\colon \omega\to[0,1] \\ h(\omega_0)=1, h(\omega_L)=0}} \mathcal{E}^\omega_\beta(h), \tag{2.39}$$

where the Dirichlet form $\mathcal{E}^\omega_\beta$ is defined as $\mathcal{E}_\beta$ in (2.25) 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

$$M = \left[\sum_{l=0}^{L-1} \frac{1}{\mu_\beta(\omega_l)c_\beta(\omega_l,\omega_{l+1})}\right]^{-1}, \tag{2.40}$$

and is uniquely attained at h given by

$$h(\omega_l) = M \sum_{k=0}^{l-1} \frac{1}{\mu_\beta(\omega_k)c_\beta(\omega_k,\omega_{k+1})}, \qquad l = 0,1,\dots,L. \tag{2.41}$$

We thus have

$$\begin{aligned}
\mathrm{CAP}_\beta(\mathcal{A},\mathcal{B}) &\ge M \\
&\ge \frac{1}{L} \min_{l=0,1,\dots,L-1} \mu_\beta(\omega_l)c_\beta(\omega_l,\omega_{l+1}) \\
&= \frac{1}{K}\frac{1}{Z_\beta} \min_{l=0,1,\dots,L-1} e^{-\beta[H(\omega_l)\vee H(\omega_{l+1})]} \\
&= C_1 \frac{1}{Z_\beta}\, e^{-\beta\Phi(\mathcal{A},\mathcal{B})}
\end{aligned} \tag{2.42}$$

with $C_1 = 1/L$. ★

2.3.2 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 2.21 *The sets $\mathcal{X}_\square$ and $\mathcal{X}_\boxplus$ are disjoint (and hence are disconnected in $\mathcal{X}^{\star\star}$), and*

$$\begin{aligned}\mathcal{X}_\square &= \{\eta \in \mathcal{X}\colon\ \Phi(\eta,\square) < \Phi(\eta,\boxplus) = \Gamma^\star\},\\ \mathcal{X}_\boxplus &= \{\eta \in \mathcal{X}\colon\ \Phi(\eta,\boxplus) < \Phi(\eta,\square) = \Gamma^\star\}.\end{aligned} \tag{2.43}$$

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 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 (2.22), $\Gamma^\star = \Phi(\square,\boxplus) \leq \max\{\varPhi(\eta,\square),\varPhi(\eta,\boxplus)\} \leq \Gamma^\star$, and hence either $\varPhi(\eta,\square) = \Gamma^\star$ or $\varPhi(\eta,\boxplus) = \Gamma^\star$ or both. To check the first line of (2.43) 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 (2.43) 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 all optimal paths from $\square$ to $\boxplus$ such that $\omega \cap \mathcal{C}^\star_{\mathrm{bd}} = \{\eta\}$ (note that this set is non-empty because $\mathcal{C}^\star_{\mathrm{bd}}$ is a minimal gate by Lemma 2.18). By Definition 2.5(b) and (H3-a), $\omega_i \in \Omega(\eta)$ 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 $\sigma^\star_i(\eta)$ be the last configuration $\sigma \in \omega_i\backslash S_i(\eta)$ such that $H(\sigma) = \Gamma^\star$, and put $\mathcal{L}(\eta) = \{\sigma^\star_1(\eta),\dots,\sigma^\star_{|\Omega(\eta)|}(\eta)\}$. Then the set $(\mathcal{C}^\star_{\mathrm{bd}}\backslash\eta) \cup \mathcal{L}(\eta)$ is a minimal gate. But ω_i hits $\sigma^\star_i(\eta)$ 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 2.7–2.9 along the lines of [BdN06], 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 [BdN06], Section 2. They are the *minimal hypotheses* that are necessary to carry out the proof below. Their verification for our specific model will be given in Chapter 3 and Chapter 4.

2.3.3 Metastable set, link between average nucleation time and capacity

Bovier, Eckhoff, Gayrard and Klein [BEGK02] define metastable sets in terms of capacities:

Definition 2.22 *$\mathcal{A} \subset \mathcal{X}$ with $\mathcal{A} \neq \emptyset$ is called a metastable set if*

$$\lim_{\beta\to\infty} \frac{\max_{\eta\notin\mathcal{A}} \mu_\beta(\eta)/\mathrm{CAP}_\beta(\eta,\mathcal{A})}{\min_{\eta\in\mathcal{A}} \mu_\beta(\eta)/\mathrm{CAP}_\beta(\eta,\mathcal{A}\backslash\eta)} = 0. \tag{2.44}$$

The following key lemma, relying on hypotheses (H1)–(H2) and Definition 2.2(d)–(e), allows us to apply the theory in [BEGK02].

Lemma 2.23 $\{\square, \boxplus\}$ *is a metastable set in the sense of Definition* 2.22.

Proof. By (2.4), Lemma 2.16 and the lower bound in (2.31), 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 (2.4), the definition of $\Gamma^\star$ and the upper bound in (2.31), the denominator is bounded from below by $e^{\Gamma^\star\beta}/C_2$ (with the minimum being attained at $\square$). ★

Lemma 2.23 has an important consequence:

Lemma 2.24 $\mathbb{E}_\square(\tau_\boxplus) = [Z_\beta \mathrm{CAP}_\beta(\square,\boxplus)]^{-1}\,[1+o(1)]$ *as* $\beta\to\infty$.

Proof. According to [BEGK02], Theorem 1.3(i), we have

$$\mathbb{E}_\square(\tau_\boxplus) = \frac{\mu_\beta(\mathcal{R}_\square)}{\mathrm{CAP}_\beta(\square,\boxplus)}\,[1+o(1)] \qquad \text{as } \beta\to\infty, \tag{2.45}$$

where

$$\mathcal{R}_\square = \big\{\eta\in\mathcal{X}\colon\ \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) \geq \mathbb{P}_\eta(\tau_\boxplus < \tau_\square)\big\}. \tag{2.46}$$

Recalling (2.27), we can rewrite (2.46) as $\mathcal{R}_\square = \{\eta \in \mathcal{X}\colon\ h^\star_{\square,\boxplus}(\eta) \geq \frac{1}{2}\}$. It follows from Lemma 2.25 below that

$$\lim_{\beta\to\infty} \min_{\eta\in\mathcal{X}_\square} h^\star_{\square,\boxplus}(\eta) = 1, \qquad \lim_{\beta\to\infty} \max_{\eta\in\mathcal{X}_\boxplus} h^\star_{\square,\boxplus}(\eta) = 0. \tag{2.47}$$

Hence, for β large enough,

$$\mathcal{X}_\square \subset \mathcal{R}_\square \subset \mathcal{X}\backslash\mathcal{X}_\boxplus. \tag{2.48}$$

By Lemma 2.21, the second inclusion implies that $\Phi(\eta,\square) \leq \Phi(\eta,\boxplus)$ for all $\eta \in \mathcal{R}_\square$. Therefore Lemma 2.17 yields

$$\min_{\eta\in\mathcal{R}_\square\backslash\square} H(\eta) > H(\square) = 0, \tag{2.49}$$

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 2.24 shows that the proof of Theorem 2.8 revolves around getting sharp bounds on $Z_\beta\mathrm{CAP}_\beta(\square,\boxplus)$. The a priori estimates in Lemma 2.20 serve as a jump board for the derivation of these bounds.

2.3.4 Proof of theorem on nucleation time

In this section we prove Theorem 2.8.

Our starting point is Lemma 2.24. Recalling (2.25–2.27), our task is to show that

$$\begin{aligned} Z_\beta\mathrm{CAP}_\beta(\square,\boxplus) &= \tfrac{1}{2}\sum_{\eta,\eta'\in\mathcal{X}} Z_\beta\mu_\beta(\eta)c_\beta(\eta,\eta')\,[h^\star_{\square,\boxplus}(\eta) - h^\star_{\square,\boxplus}(\eta')]^2 \\ &= [1+o(1)]\,\Theta\, e^{-\Gamma^\star\beta} \qquad \text{as } \beta\to\infty, \end{aligned} \tag{2.50}$$

and to identify the constant Θ, since (2.50) will imply (2.16) with $\Theta = 1/K$. This is done in four steps, organized in Sections 2.3.4–2.3.4.

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 (2.50) at the cost of a prefactor $1 + O(e^{-\delta\beta})$. Moreover, we have the following analogue of [BdN06], Lemma 3.3.1.

Lemma 2.25 *There exist $C < \infty$ and $\delta > 0$ such that*

$$\min_{\eta \in \mathcal{X}_\square} h^\star_{\square,\boxplus}(\eta) \geq 1 - Ce^{-\delta\beta}, \qquad \max_{\eta \in \mathcal{X}_\boxplus} h^\star_{\square,\boxplus}(\eta) \leq Ce^{-\delta\beta}, \qquad \forall\, \beta \in (0,\infty). \quad (2.51)$$

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

$$\mathbb{P}_\eta(\tau_\boxplus < \tau_\square) = \frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_{\square\cup\eta})}{1 - \mathbb{P}_\eta(\tau_{\square\cup\boxplus} > \tau_\eta)}, \qquad \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) = \frac{\mathbb{P}_\eta(\tau_\square < \tau_{\boxplus\cup\eta})}{1 - \mathbb{P}_\eta(\tau_{\square\cup\boxplus} > \tau_\eta)}. \quad (2.52)$$

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

$$h^\star_{\square,\boxplus}(\eta) = 1 - \mathbb{P}_\eta(\tau_\boxplus < \tau_\square) = 1 - \frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_{\square\cup\eta})}{\mathbb{P}_\eta(\tau_{\square\cup\boxplus} < \tau_\eta)} \geq 1 - \frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_\eta)}{\mathbb{P}_\eta(\tau_\square < \tau_\eta)} \quad (2.53)$$

and, with the help of (2.29) and Lemma 2.20,

$$\frac{\mathbb{P}_\eta(\tau_\boxplus < \tau_\eta)}{\mathbb{P}_\eta(\tau_\square < \tau_\eta)} = \frac{Z_\beta \,\mathrm{CAP}_\beta(\eta,\boxplus)}{Z_\beta \,\mathrm{CAP}_\beta(\eta,\square)} \leq C(\eta)\, e^{-[\Phi(\eta,\boxplus)-\Phi(\eta,\square)]\beta} \leq C(\eta)\, e^{-\delta\beta}, \quad (2.54)$$

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

$$h^\star_{\square,\boxplus}(\eta) = \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) = \frac{\mathbb{P}_\eta(\tau_\square < \tau_{\boxplus\cup\eta})}{\mathbb{P}_\eta(\tau_{\square\cup\boxplus} < \tau_\eta)} \leq \frac{\mathbb{P}_\eta(\tau_\square < \tau_\eta)}{\mathbb{P}_\eta(\tau_\boxplus < \tau_\eta)} \quad (2.55)$$

and, with the help of (2.29) and Lemma 2.20,

$$\frac{\mathbb{P}_\eta(\tau_\square < \tau_\eta)}{\mathbb{P}_\eta(\tau_\boxplus < \tau_\eta)} = \frac{Z_\beta \,\mathrm{CAP}_\beta(\eta,\square)}{Z_\beta \,\mathrm{CAP}_\beta(\eta,\boxplus)} \leq C(\eta)\, e^{-[\Phi(\eta,\square)-\Phi(\eta,\boxplus)]\beta} \leq C(\eta)\, e^{-\delta\beta}, \quad (2.56)$$

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

In view of Lemma 2.25, $h^\star_{\square,\boxplus}$ is trivial on the set $\mathcal{X}_\square \cup \mathcal{X}_\boxplus$, and its contribution to the sum in (2.50), 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

$$\mathcal{X}^\star \backslash (\mathcal{X}_\square \cup \mathcal{X}_\boxplus) = \{\eta \in \mathcal{X}^\star\colon\ \Phi(\eta,\square) = \Phi(\eta,\boxplus) = \Gamma^\star\}. \quad (2.57)$$

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

$$\mathcal{X}^{\star\star}\backslash(\mathcal{X}_\square \cup \mathcal{X}_\boxplus) = \bigcup_{i=1}^{I} \mathcal{X}_i, \tag{2.58}$$

which is a union of wells $\mathcal{X}_i$, $i = 1, \dots, I$, 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 [BdN06], Lemma 3.3.2.

Lemma 2.26 *There exist $C < \infty$ and $\delta > 0$ such that*

$$\max_{\eta,\eta' \in \mathcal{X}_i} |h^\star_{\square,\boxplus}(\eta) - h^\star_{\square,\boxplus}(\eta')| \leq Ce^{-\delta\beta} \qquad \forall\, i = 1, \dots, I,\ \beta \in (0, \infty). \tag{2.59}$$

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

$$h^\star_{\square,\boxplus}(\eta) = \mathbb{P}_\eta(\tau_\square < \tau_\boxplus) \leq \mathbb{P}_\eta(\tau_\square < \tau_{\eta'}) + \mathbb{P}_\eta(\tau_{\eta'} < \tau_\square < \tau_\boxplus). \tag{2.60}$$

First, as in the proof of Lemma 2.25, we have

$$\begin{aligned}\mathbb{P}_\eta(\tau_\square < \tau_{\eta'}) &= \frac{\mathbb{P}_\eta(\tau_\square < \tau_{\eta \cup \eta'})}{1 - \mathbb{P}_\eta(\tau_{\square \cup \eta'} > \tau_\eta)} \leq \frac{\mathbb{P}_\eta(\tau_\square < \tau_\eta)}{\mathbb{P}_\eta(\tau_{\eta'} < \tau_\eta)} \\ &= \frac{Z_\beta \mathrm{CAP}_\beta(\eta, \square)}{Z_\beta \mathrm{CAP}_\beta(\eta, \eta')} \leq C(\eta, \eta')\, e^{-[\Phi(\eta,\square) - \Phi(\eta,\eta')]\beta} \leq C(\eta, \eta')\, e^{-\delta\beta},\end{aligned} \tag{2.61}$$

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

$$\mathbb{P}_\eta(\tau_{\eta'} < \tau_\square < \tau_\boxplus) = \mathbb{P}_\eta(\tau_{\eta'} < \tau_{\square \cup \boxplus})\mathbb{P}_{\eta'}(\tau_\square < \tau_\boxplus) \leq \mathbb{P}_{\eta'}(\tau_\square < \tau_\boxplus) = h^\star_{\square,\boxplus}(\eta'). \tag{2.62}$$

Combining (2.60–2.62), we get

$$h^\star_{\square,\boxplus}(\eta) \leq C(\eta, \eta')\, e^{-\delta\beta} + h^\star_{\square,\boxplus}(\eta'). \tag{2.63}$$

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 2.26, the contribution to the sum in (2.50) 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.

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 [BdN06], Proposition 3.3.3.

Lemma 2.27 *$Z_\beta \mathrm{CAP}_\beta(\square, \boxplus) = [1 + o(1)]\, \Theta\, e^{-\Gamma^\star \beta}$ as $\beta \to \infty$ with*

$$\Theta = \min_{C_1 \dots, C_I} \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h|_{\mathcal{X}_\square} \equiv 1,\, h|_{\mathcal{X}_\boxplus} \equiv 0,\, h|_{\mathcal{X}_i} \equiv C_i\ \forall i=1,\dots,I}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^\star} 1_{\{\eta \sim \eta'\}}\, [h(\eta) - h(\eta')]^2. \tag{2.64}$$

Proof. First, recalling (2.4–2.5) and (2.25–2.26), we have

$$\begin{aligned} Z_\beta\, \mathrm{CAP}_\beta(\square, \boxplus) &= Z_\beta \min_{\substack{h:\ \mathcal{X} \to [0,1] \\ h(\square)=1,\, h(\boxplus)=0}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}} \mu_\beta(\eta) c_\beta(\eta, \eta') [h(\eta) - h(\eta')]^2 \\ &= O\left(e^{-(\Gamma^\star + \delta)\beta}\right) + Z_\beta \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h(\square)=1,\, h(\boxplus)=0}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta, \eta') [h(\eta) - h(\eta')]^2. \end{aligned} \tag{2.65}$$

Next, with the help of Lemmas 2.25–2.26, we get

$$\begin{aligned} &\min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h(\square)=1,\, h(\boxplus)=0}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta, \eta') [h(\eta) - h(\eta')]^2 \\ &= \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h = h^\star_{\square,\boxplus} \text{ on } \mathcal{X}_\square \cup \mathcal{X}_\boxplus \cup (\mathcal{X}_1, \dots, \mathcal{X}_I)}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta, \eta') [h(\eta) - h(\eta')]^2 \\ &= [1 + O(e^{-\delta\beta})] \min_{C_1, \dots, C_I} \min_{\substack{h:\ \mathcal{X}^\star \to [0,1] \\ h|_{\mathcal{X}_\square} \equiv 1,\, h|_{\mathcal{X}_\boxplus} \equiv 0,\, h|_{\mathcal{X}_i} \equiv C_i\ \forall i=1,\dots,I}} \frac{1}{2} \sum_{\eta, \eta' \in \mathcal{X}^\star} \mu_\beta(\eta) c_\beta(\eta, \eta') [h(\eta) - h(\eta')]^2, \end{aligned} \tag{2.66}$$

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

$$h = \begin{cases} 1 - O(e^{-\delta\beta}) & \text{on } \mathcal{X}_\square, \\ O(e^{-\delta\beta}) & \text{on } \mathcal{X}_\boxplus, \\ C_i + O(e^{-\delta\beta}) & \text{on } \mathcal{X}_i,\ i = 1, \dots, I, \end{cases} \tag{2.67}$$

by the *sharp* boundary conditions

$$h = \begin{cases} 1 & \text{on } \mathcal{X}_\square, \\ 0 & \text{on } \mathcal{X}_\boxplus, \\ C_i & \text{on } \mathcal{X}_i,\ i = 1, \dots, I. \end{cases} \tag{2.68}$$

Finally, by (2.4–2.5) and reversibility, we have

$$Z_\beta \mu_\beta(\eta) c_\beta(\eta,\eta') = 1_{\{\eta\sim\eta'\}}\, e^{-\Gamma^\star\beta} \text{ for all } \eta,\eta' \in \mathcal{X}^\star \text{ that are not either both in } \mathcal{X}_\square \text{ or both in } \mathcal{X}_\boxplus \text{ or both in } \mathcal{X}_i \text{ for some } i=1,\dots,I. \tag{2.69}$$

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 2.24 and 2.27, we see that we have completed the proof of (2.16) 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 $\mathcal{X}_i$, $i = 1,\dots,I$.

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 (2.17). The intuition behind (2.17) is the following. When the free particle attaches itself to the protocritial droplet, the dynamics enters the set $\mathcal{C}^\star_{\mathrm{att}}$. The entrance configurations of $\mathcal{C}^\star_{\mathrm{att}}$ 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 2.19, if the path exits an $\mathcal{X}_i$, then for it to return to $\mathcal{X}_\square$ it must pass through $\mathcal{C}^\star_{\mathrm{bd}}$, 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 [BdN06], 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 $\mathcal{C}^\star_{\mathrm{att}}$ 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 2.28 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 [BdN06], 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 2.29 *(a) For $F \subset \mathbb{Z}^2$, $\partial^+ F$ and $\partial^- F$ are the external, respectively, internal boundary of F.*
(b) For $\eta \in \mathcal{X}$, supp(η) 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 $i = 1, \ldots, I$.
(e) For $\hat{\eta} \in \mathcal{P}$, let

$$
\begin{aligned}
G(\hat{\eta}) &= \{x \in A(\hat{\eta}) \colon (\hat{\eta}, x) \in \mathcal{X}_\boxplus\}, \\
B(\hat{\eta}) &= \{x \in A(\hat{\eta}) \colon \exists\, i = 1, \ldots, I \colon (\hat{\eta}, x) \in \mathcal{X}_i\},
\end{aligned}
\tag{2.70}
$$

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

$$
I(\hat{\eta}) = \{i \in 1, \ldots, I \colon \exists\, x \in B(\hat{\eta}) \colon (\hat{\eta}, x) \in \mathcal{X}_i\}. \tag{2.71}
$$

Note that $B(\hat{\eta})$ can be partitioned into disjoint sets $B_1(\hat{\eta}), \ldots, B_{|I(\hat{\eta})|}(\hat{\eta})$ 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 $\mathrm{CS}^{++}(\hat{\eta}) = \partial^+ \mathrm{CS}^+(\hat{\eta}) \cap \Lambda^-$.

Note that Definitions 2.29(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 2.21. 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 [BdN06], Proposition 3.3.4.

Lemma 2.30 $\Theta \in [\Theta_1, \Theta_2]$ *with*

$$
\begin{aligned}
\Theta_1 &= [1 + o(1)] \sum_{\hat{\eta} \in \mathcal{P}} \mathrm{CAP}^{\Lambda^+}\left(\partial^+ \Lambda, \mathrm{CS}(\hat{\eta})\right), \\
\Theta_2 &= \sum_{\hat{\eta} \in \mathcal{P}} \mathrm{CAP}^{\Lambda^+}\left(\partial^+ \Lambda, \mathrm{CS}^{++}(\hat{\eta})\right),
\end{aligned}
\tag{2.72}
$$

where

$$
\mathrm{CAP}^{\Lambda^+}\left(\partial^+ \Lambda, F\right) = \min_{\substack{g \colon \Lambda^+ \to [0,1] \\ g|_{\partial^+ \Lambda} \equiv 1,\, g|_F \equiv 0}} \tfrac{1}{2} \sum_{(x,x') \in (\Lambda^+)^\star} [g(x) - g(x')]^2, \qquad F \subset \Lambda, \tag{2.73}
$$

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 (2.64) 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 (2.64) 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

$$\begin{aligned}\Theta \geq \sum_{\hat\eta \in \mathcal{P}'} \min_{C_i(\hat\eta),\, i \in I(\hat\eta)} \; &\min_{\substack{g\colon \Lambda^+ \to [0,1] \\ g|_{G(\hat\eta)} \equiv 0,\, g|_{B_i(\hat\eta)} \equiv C_i(\hat\eta),\, i \in I(\hat\eta),\, g|_{\partial^+\Lambda} \equiv 1}} \\ &\tfrac12 \sum_{(x,x') \in [\Lambda^+ \backslash \mathrm{supp}(\hat\eta)]^\star} [g(x) - g(x')]^2,\end{aligned} \tag{2.74}$$

where $\mathcal{P}' \subset \mathcal{P}$ is the set of protocritical configurations whose support has lattice distance at least two form $\partial^-\Lambda$. Note that for all $\hat\eta \in \mathcal{P}'$ there is a lattice path connecting every two points adjacent to $\mathrm{supp}(\hat\eta)$ and avoiding $\partial^+\Lambda$. To see how this bound arises from (2.64), pick h in (2.64) and g in (2.74) such that

$$h(\eta) = h(\hat\eta, x) = g(x), \qquad \hat\eta \in \mathcal{P},\ x \in \Lambda^+ \backslash \mathrm{supp}(\hat\eta), \tag{2.75}$$

and use that, by Definitions 2.29(c–f), for every $\hat\eta \in \mathcal{P}$ (recall Lemma 2.21)

$$\begin{array}{ll} (\hat\eta, x) \in \mathcal{X}_\boxplus, & x \in G(\hat\eta), \\ (\hat\eta, x) \in \mathcal{X}_i & x \in B_i(\hat\eta),\ i \in I(\hat\eta), \\ (\hat\eta, x) \in \mathcal{P} \subset \mathcal{X}_\square, & x \in \partial^+\Lambda. \end{array} \tag{2.76}$$

A further lower bound is obtained by removing from the right-hand side of (2.76) the boundary condition on the sets $B_i(\hat\eta)$, $i \in I(\hat\eta)$. This gives

$$\begin{aligned}\Theta &\geq \sum_{\hat\eta \in \mathcal{P}'} \min_{\substack{g\colon \Lambda^+ \to [0,1] \\ g|_{G(\hat\eta)} \equiv 0,\, g|_{\partial^+\Lambda} \equiv 1}} \tfrac12 \sum_{(x,x') \in [\Lambda^+ \backslash \mathrm{supp}(\hat\eta)]^\star} [g(x) - g(x')]^2 \\ &= \sum_{\hat\eta \in \mathcal{P}'} \mathrm{CAP}^{\Lambda^+ \backslash \mathrm{supp}(\hat\eta)} \left(\partial^+\Lambda, G(\hat\eta)\right),\end{aligned} \tag{2.77}$$

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 $\Lambda \to \mathbb{Z}^2$,

$$\begin{aligned}&\mathrm{CAP}^{\Lambda^+}\big(\partial^+\Lambda, \mathrm{supp}(\hat\eta) \cup G(\hat\eta)\big) \geq \mathrm{CAP}^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}\big(\partial^+\Lambda, G(\hat\eta)\big)\\ &\geq \mathrm{CAP}^{\Lambda^+}\big(\partial^+\Lambda, \mathrm{supp}(\hat\eta) \cup G(\hat\eta)\big) - O([1/\log|\Lambda|]^2).\end{aligned} \tag{2.78}$$

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 (2.78), note that the capacity in the right-hand side of (2.78) includes more transitions than the capacity in the left-hand side, namely, all transitions from $\mathrm{supp}(\hat\eta)$ to $B(\hat\eta)$. Let

$$g^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}_{\partial^+\Lambda, G(\hat\eta)}(x) = \text{ equilibrium potential for } \mathrm{CAP}^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}\big(\partial^+\Lambda, G(\hat\eta)\big) \text{ at } x. \tag{2.79}$$

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 (2.73) the equilibrium potential appears squared, the error made by adding to the capacity in the left-hand side of (2.78) 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 (2.78) 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 2.25, and recalling the probabilistic interpretation of the equilibrium potential in (2.27) and of the capacity in (2.29), we get

$$\begin{aligned}g^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}_{\partial^+\Lambda, G(\hat\eta)}(x) = \mathbb{P}^{\hat\eta}_x(\tau_{\partial^+\Lambda} < \tau_{G(\hat\eta)}) &= \frac{\mathbb{P}^{\hat\eta}_x(\tau_{\partial^+\Lambda} < \tau_{G(\hat\eta)\cup x})}{\mathbb{P}^{\hat\eta}_x(\tau_{G(\hat\eta)\cup\partial^+\Lambda} < \tau_x)}\\ &\leq \frac{\mathbb{P}^{\hat\eta}_x(\tau_{\partial^+\Lambda} < \tau_x)}{\mathbb{P}^{\hat\eta}_x(\tau_y < \tau_x)} = \frac{\mathrm{CAP}^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}(x, \partial^+\Lambda)}{\mathrm{CAP}^{\Lambda^+\backslash\mathrm{supp}(\hat\eta)}(x, y)}.\end{aligned} \tag{2.80}$$

The denominator of (2.80) 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 2.20. 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 2.31 below, we will see that $\mathrm{CAP}^{\Lambda^+}(\partial^+\Lambda, G(\hat\eta))$ decays like $C''/\log|\Lambda|$ for some $C'' < \infty$ (see (2.87–2.88) 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 (2.64) by picking $C_i = 0$, $i = 1, \dots, I$, and

$$h(\eta) = \begin{cases} 1 & \text{for } \eta \in \mathcal{X}_\square, \\ g(x) & \text{for } \eta = (\hat{\eta}, x) \in \mathcal{C}^{++}, \\ 0 & \text{for } \eta \in \mathcal{X}^\star \backslash [\mathcal{X}_\square \cup \mathcal{C}^{++}], \end{cases} \tag{2.81}$$

where

$$\mathcal{C}^{++} = \left\{ \eta = (\hat{\eta}, x)\colon\ \hat{\eta} \in \mathcal{P},\ x \in \Lambda \backslash \mathrm{CS}^{++}(\hat{\eta}) \right\} \tag{2.82}$$

consists of those configurations in $\mathcal{C}^\star$ for which the free particle is at distance ≥ 2 of the protocritical droplet. The choice in (2.81) gives

$$\Theta \leq \sum_{\hat{\eta} \in \mathcal{P}} \mathrm{CAP}^{\Lambda^+} \left(\partial^+ \Lambda, \mathrm{CS}^{++}(\hat{\eta}) \right). \tag{2.83}$$

To see how this upper bound arises, note that:

- The choice in (2.81) satisfies the boundary conditions in (2.64) because (recall (2.57–2.58))

$$\mathcal{C}^{++} \subset \mathcal{C}^\star,\ [\mathcal{X}_\square \cup \mathcal{C}^\star] \cap [\mathcal{X}_\boxplus \cup (\cup_{i=1}^I \mathcal{X}_i)] = \emptyset \Longrightarrow \mathcal{X}^\star \backslash [\mathcal{X}_\square \cup \mathcal{C}^{++}] \supset [\mathcal{X}_\boxplus \cup (\cup_{i=1}^I \mathcal{X}_i)]. \tag{2.84}$$

- By Lemma 2.21, $\mathcal{P} \subset \mathcal{X}_\square$. Therefore the first line of (2.81) 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 (2.73).

- The third line of (2.81) 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 (2.73) for $F = \mathrm{CS}^{++}(\hat{\eta})$.

Further note that:

- By Definitions 2.5–4.5 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 enters $\mathrm{CS}^{++}(\hat{\eta})$. 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 (2.73) includes all the transitions in (2.64). ★

Step 4: Sharp asymptotics for capacities of simple random walk

With Lemma 2.30 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 2.31 below, which is the analogue of [BdN06], 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. In the limit $M \to \infty$ we have $|\mathcal{P}| \sim N^\star|\Lambda| \sim |\mathcal{P}'|$. It is straightforward to extend the proof to other shapes of Λ (see van den Berg [vdB05] for relevant estimates).

Lemma 2.31 *For any $\varepsilon > 0$,*

$$\begin{aligned}
&\lim_{M\to\infty} \max_{\substack{\hat\eta\in\mathcal{P}' \\ d(\partial^+ B_M, supp(\hat\eta))\geq \varepsilon M}} \left| \frac{\log M}{2\pi}\,\mathrm{CAP}^{B_M^+}\big(\partial^+ B_M, \mathrm{CS}(\hat\eta)\big) - 1 \right| = 0,\\
&\lim_{M\to\infty} \max_{\substack{\hat\eta\in\mathcal{P} \\ d(\partial^+ B_M, supp(\hat\eta))\geq \varepsilon M}} \left| \frac{\log M}{2\pi}\,\mathrm{CAP}^{B_M^+}\big(\partial^+ B_M, \mathrm{CS}^{++}(\hat\eta)\big) - 1 \right| = 0,
\end{aligned} \tag{2.85}$$

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

Proof. We only prove the first line of (2.85). 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

$$\begin{aligned}
\mathrm{CAP}^{B_M^+}(\partial^+ B_M, \mathrm{CS}(\hat\eta)) &\geq \mathrm{CAP}^{B_M^+}(\partial^+ B_M, y)\\
&= \mathrm{CAP}^{(B_M-y)^+}(\partial^+(B_M-y), 0) \geq \mathrm{CAP}^{B_{2M}^+}(\partial^+ B_{2M}, 0),
\end{aligned} \tag{2.86}$$

where the last equality uses that $(B_M - y)^+ \subset B_{2M}^+$ because $y \in B_M$. By the analogue of (2.29–2.30) for simple random walk, we have (compare (2.73) with (2.25–2.26))

$$\mathrm{CAP}^{B_{2M}^+}(\partial^+ B_{2M}, 0) = \mathrm{CAP}^{B_{2M}^+}(0, \partial^+ B_{2M}) = 4\,\mathbb{P}_0(\tau_{\partial^+ B_{2M}} < \tau_0), \tag{2.87}$$

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 [RÝ0], Lemma 22.1, we have

$$\mathbb{P}_0(\tau_{\partial^+ B_{2M}} < \tau_0) \sim \frac{\pi}{2\log(2M)}, \qquad M \to \infty. \tag{2.88}$$

Combining (2.86–2.88), we get the desired lower bound.

Upper bound: As in (2.86), we have

$$\begin{aligned}
&\mathrm{CAP}^{B_M^+}(\partial^+ B_M, \mathrm{CS}(\hat\eta)) \le \mathrm{CAP}^{B_M^+}(\partial^+ B_M, S_y(\hat\eta)) \\
&\quad = \mathrm{CAP}^{(B_M-y)^+}(\partial^+(B_M - y), S_y(\hat\eta) - y) \le \mathrm{CAP}^{B_{\varepsilon M}^+}(\partial^+ B_{\varepsilon M}, S_y(\hat\eta) - y),
\end{aligned} \tag{2.89}$$

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 $d(\partial^+ B_M, \mathrm{supp}(\hat\eta)) \ge \varepsilon M$. By the recurrence of simple random walk, we have

$$\mathrm{CAP}^{B_{\varepsilon M}^+}(\partial^+ B_{\varepsilon M}, S_y(\hat\eta) - y) \sim \mathrm{CAP}^{B_{\varepsilon M}^+}(\partial^+ B_{\varepsilon M}, 0), \qquad M \to \infty. \tag{2.90}$$

Combining (2.88–2.90), we get the desired upper bound. ★

Combining Lemmas 2.30–2.31, we find that $\Theta \in [\Theta_1, \Theta_2]$ with

$$\begin{aligned}
\Theta_1 &= O(\varepsilon M) + \sum_{\substack{\hat\eta \in \mathcal{P} \\ d(\partial^+ B_M, \mathrm{supp}(\hat\eta)) \ge \varepsilon M}} \mathrm{CAP}^{B_M^+}(\partial^+ B_M, \mathrm{CS}(\hat\eta)) \\
&= O(\varepsilon M) + \frac{2\pi}{\log M} \left|\left\{\hat\eta \in \mathcal{P} \colon\ d(\partial^+ B_M, \mathrm{supp}(\hat\eta)) \ge \varepsilon M\right\}\right| [1 + o(1)] \\
&= O(\varepsilon M) + \frac{2\pi}{\log M} N^\star [2(1-\varepsilon)M]^2 [1 + o(1)],
\end{aligned} \tag{2.91}$$

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

$$\mathrm{CAP}^{B_M^+}\big(\partial^+ B_M, \mathrm{CS}(\hat\eta)\big) \le \mathrm{CAP}^{B_M^+}\big(B_M^+ \backslash \mathrm{CS}(\hat\eta), \mathrm{CS}(\hat\eta)\big) = \tfrac{1}{2}|\mathrm{CS}^+(\hat\eta)| \le \tfrac{1}{2}(L^\star + 2)^2, \tag{2.92}$$

and we recall from Definition 2.5(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 (2.17) in Theorem 2.8.

2.3.5 Proof of theorem on exponential distribution

In this section we prove Theorem 2.9.

Proof. The proof is immediate from Lemma 2.23 and Bovier, Eckhoff, Gayrard and Klein [BEGK02], Theorem 1.3(iv) and relies on (H1)–(H2) only. 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 (2.27) and (2.51))) and to "start from scratch". Thus, the dynamics manages to grow a critical droplet and go over the hill to $\boxplus$ 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. ★

2.3.6 Proof of theorem on critical configurations

In this section we prove Theorem 2.7.

Proof. (a) The proof relies on (H1)–(H2) only. We will show that there exist $C < \infty$ and $\delta > 0$ such that

$$\mathbb{P}_\square\left(\tau_{\mathcal{C}^\star} < \tau_\boxplus \mid \tau_\boxplus < \tau_\square\right) \geq 1 - Ce^{-\delta\beta}, \qquad \forall\, \beta \in (0,\infty), \tag{2.93}$$

which implies the claim.

By (2.29), $\mathrm{CAP}_\beta(\square,\boxplus) = \mu_\beta(\square)\, c_\beta(\square, \mathcal{X}\backslash\square)\mathbb{P}_\square(\tau_\boxplus < \tau_\square)$ with $\mu_\beta(\square) = 1/Z_\beta$. From the lower bound in Lemma 2.20 it therefore follows that

$$\mathbb{P}_\square(\tau_\boxplus < \tau_\square) \geq C_1 e^{-\Gamma^\star\beta}\,\frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)}. \tag{2.94}$$

We will show that

$$\mathbb{P}_\square\left(\{\tau_{\mathcal{C}^\star} < \tau_\boxplus\}^c,\, \tau_\boxplus < \tau_\square\right) \leq C_2 e^{-(\Gamma^\star+\delta)\beta}\,\frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)}. \tag{2.95}$$

Combining (2.94–2.95), we get (2.93) with $C = C_2/C_1$.

By Definitions 2.2(f) and 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

$$\mathbb{P}_\square\left(\{\tau_{\mathcal{C}^\star} < \tau_\boxplus\}^c,\, \tau_\boxplus < \tau_\square\right) \leq \mathbb{P}_\square\left(\tau_{\mathcal{S}} < \tau_\square\right). \tag{2.96}$$

Now estimate, with the help of reversibility,

$$\begin{aligned}
\mathbb{P}_\square\left(\tau_{\mathcal{S}} < \tau_\square\right) &\leq \sum_{\eta \in \mathcal{S}} \mathbb{P}_\square\left(\tau_\eta < \tau_\square\right) \\
&= \sum_{\eta \in \mathcal{S}} \frac{\mu_\beta(\eta) c_\beta(\eta, \mathcal{X}\backslash\eta)}{\mu_\beta(\square) c_\beta(\square, \mathcal{X}\backslash\square)}\, \mathbb{P}_\eta\left(\tau_\square < \tau_\eta\right) \\
&\leq \frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)} \sum_{\eta \in \mathcal{S}} |\{\eta' \in \mathcal{X}\backslash\eta\colon\ \eta \sim \eta'\}|\, e^{-\beta H(\eta)} \\
&\leq \frac{1}{c_\beta(\square, \mathcal{X}\backslash\square)}\, C_2\, e^{-(\Gamma^\star + \delta)\beta}
\end{aligned} \tag{2.97}$$

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 (2.96–2.97) to get the claim in (2.95).

(b) The proof relies on (H1) and (H3). Write

$$\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta \mid \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big) = \frac{\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta,\, \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big)}{\mathbb{P}_\square\big(\tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big)}, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.98}$$

By reversibility,

$$\begin{aligned}
\mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta,\, \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big) &= \frac{\mu_\beta(\eta) c_\beta(\eta, \mathcal{X}\backslash\eta)}{\mu_\beta(\square) c_\beta(\square, \mathcal{X}\backslash\square)}\, \mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) \\
&= e^{-\Gamma^\star\beta}\, \frac{c_\beta(\eta, \mathcal{X}\backslash\eta)}{c_\beta(\square, \mathcal{X}\backslash\square)}\, \mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big), \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}.
\end{aligned} \tag{2.99}$$

Moreover (recall (2.27–2.28)),

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) = \sum_{\substack{\eta' \in \mathcal{X}\backslash\mathcal{C}^\star_{\mathrm{bd}} \\ \eta \sim \eta'}} \frac{c_\beta(\eta, \eta')}{c_\beta(\eta, \mathcal{X}\backslash\eta)}\, h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta'), \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}, \tag{2.100}$$

where

$$h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') = \begin{cases} 0 & \text{if } \eta' \in \mathcal{C}^\star_{\mathrm{bd}}, \\ 1 & \text{if } \eta' = \square, \\ \mathbb{P}_{\eta'}(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}) & \text{otherwise.} \end{cases} \tag{2.101}$$

Because $\mathcal{P} \subset \mathcal{X}_\boxdot$ by Lemma 2.21 and $\mathcal{C}^\star_{\mathrm{bd}} \subset \mathcal{G}(\square, \boxplus)$ by Definition 2.5(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 2.25, it follows that

$$\min_{\eta' \in \mathcal{P}} h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') \geq 1 - Ce^{-\delta\beta}, \tag{2.102}$$

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

$$\max_{\eta' \in \bar{\mathcal{C}}^\star} h^\star_{\square, \mathcal{C}^\star_{\mathrm{bd}}}(\eta') \leq Ce^{-\delta\beta}. \tag{2.103}$$

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

$$\text{Any path from } \bar{\mathcal{C}}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}} \text{ to } \square \text{ that avoids } \mathcal{C}^\star_{\mathrm{bd}} \text{ must reach an energy level } > \Gamma^\star. \tag{2.104}$$

To obtain (2.103) from (2.104), we can do an estimate similar to (2.53–2.54) for $\eta' \in \bar{\mathcal{C}}^\star \backslash \mathcal{C}^\star_{\mathrm{bd}}$.

To prove (2.104) 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 2.19. 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 2.5–4.5, this implies that $\zeta \in \mathcal{P}$, which is impossible because $\mathcal{P} \cap \mathcal{C}^\star = \emptyset$.

The estimates in (2.102–2.103) can be used as follows. By restricting the sum in

(2.100) to $\eta' \in \mathcal{P}$ and inserting (2.102), we get

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) \geq (1 - Ce^{-\delta\beta})\, \frac{c_\beta(\eta, \mathcal{P})}{c_\beta(\eta, \mathcal{X}\backslash\eta)}, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.105}$$

On the other hand, by inserting (2.103), we get

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) \leq \frac{c_\beta(\eta, \mathcal{P})}{c_\beta(\eta, \mathcal{X}\backslash\eta)} + Ce^{-\delta\beta}|\bar{\mathcal{C}}^\star|, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.106}$$

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

$$c_\beta(\eta, \mathcal{P}) = \sum_{\eta' \in \mathcal{P}} c_\beta(\eta, \eta') = |\{\eta' \in \mathcal{P}\colon\ \eta \sim \eta'\}|, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}, \tag{2.107}$$

and, since $c_\beta(\eta, \mathcal{X}\backslash\eta) \leq |\mathcal{X}|$, 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 (2.105–2.106), to get

$$\mathbb{P}_\eta\big(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}}\big) = [1 + O(e^{-\delta\beta})]\, \frac{c_\beta(\eta, \mathcal{P})}{c_\beta(\eta, \mathcal{X}\backslash\eta)}, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \tag{2.108}$$

Combining this in turn with (2.98–2.99), we arrive at

$$\begin{aligned} \mathbb{P}_\square\big(\eta_{\tau_{\mathcal{C}^\star_{\mathrm{bd}}}} = \eta \mid \tau_{\mathcal{C}^\star_{\mathrm{bd}}} < \tau_\square\big) &= \frac{c_\beta(\eta, \mathcal{X}\backslash\eta)\, \mathbb{P}_\eta(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}})}{\sum_{\eta' \in \mathcal{C}^\star_{\mathrm{bd}}} c_\beta(\eta', \mathcal{X}\backslash\eta')\, \mathbb{P}_{\eta'}(\tau_\square < \tau_{\mathcal{C}^\star_{\mathrm{bd}}})} \\ &= [1 + O(e^{-\delta\beta})]\, \frac{c_\beta(\eta, \mathcal{P})}{\sum_{\eta' \in \mathcal{C}^\star_{\mathrm{bd}}} c_\beta(\eta', \mathcal{P})}, \qquad \eta \in \mathcal{C}^\star_{\mathrm{bd}}. \end{aligned} \tag{2.109}$$

Finally, each site in $\partial^-\Lambda$ has one edge towards $\partial^+\Lambda$ and hence, by (2.107), $\eta \mapsto c_\beta(\eta, \mathcal{P})$ is constant on $\mathcal{C}^\star_{\mathrm{bd}}$. Together with (2.109) this proves the claim. ★

3 Stable configurations, communication height and recurrence property

This chapter is based on:
F. den Hollander, F. R. Nardi, A. Troiani, *Kawasaki dynamics with two types of particles: Stable/metastable configurations and communication heights*, Journal of Statistical Physics, 145, 1423–1457, 2011.

3.1 Overview and main results

Section 3.1.1 defines the model, Section 3.1.2 introduces basic notation, Section 3.1.3 states the main theorems, while Section 3.1.4 discusses the main theorems and provides further perspectives.

3.1.1 Lattice gas subject to Kawasaki dynamics

Let $\Lambda \subset \mathbb{Z}^2$ be a large box centered at the origin (later it will be convenient to choose Λ rhombus-shaped). Let ($|\cdot|$ denotes the Euclidean norm)

$$\begin{aligned} \partial^-\Lambda &= \{x \in \Lambda\colon\ \exists\, y \notin \Lambda\colon\ |y-x| = 1\}, \\ \partial^+\Lambda &= \{x \notin \Lambda\colon\ \exists\, y \in \Lambda\colon\ |y-x| = 1\}, \end{aligned} \tag{3.1}$$

be the internal, respectively, 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, respectively. 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

$$H = -U \sum_{(x,y)\in\Lambda^{*,-}} 1_{\{\eta(x)\eta(y)=2\}} + \Delta_1 \sum_{x\in\Lambda} 1_{\{\eta(x)=1\}} + \Delta_2 \sum_{x\in\Lambda} 1_{\{\eta(x)=2\}}, \tag{3.2}$$

where $\Lambda^{*,-} = \{(x,y)\colon\ x,y \in \Lambda^-,\ |x-y| = 1\}$ 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, 2 inside Λ. Without loss of generality we will assume that

$$\Delta_1 \le \Delta_2. \tag{3.3}$$

The Gibbs measure associated with H is

$$\mu_\beta(\eta) = \frac{1}{Z_\beta}\, e^{-\beta H(\eta)}, \qquad \eta \in \mathcal{X}, \tag{3.4}$$

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, $(\eta_t)_{t\ge 0}$ with state space $\mathcal{X}$ whose transition rates are

$$c_\beta(\eta,\eta') = e^{-\beta[H(\eta')-H(\eta)]_+}, \qquad \eta,\eta' \in \mathcal{X},\ \eta \ne \eta',\ \eta \leftrightarrow \eta', \tag{3.5}$$

where $\eta \leftrightarrow \eta'$ means that η' can be obtained from η by one of the following moves:

- interchanging 0 and 1 or 0 and 2 between two neighboring sites in Λ ("hopping of particles in Λ"),
- changing 0 to 1 or 0 to 2 in $\partial^-\Lambda$ ("creation of particles in $\partial^-\Lambda$"),
- changing 1 to 0 or 2 to 0 in $\partial^-\Lambda$ ("annihilation of particles in $\partial^-\Lambda$"),

and $c_\beta(\eta,\eta') = 0$ otherwise. Note that this dynamics preserves particles in Λ^-, but allows particles to be created and annihilated in $\partial^-\Lambda$. Think of the latter as describing particles entering and exiting Λ along non-oriented bonds between $\partial^+\Lambda$ and $\partial^-\Lambda$ (the rates of these moves are associated with the bonds rather than with the sites). The pairs (η,η') with $\eta \leftrightarrow \eta'$ are called *communicating configurations*, the transitions between them are called *allowed moves*. Note that particles in $\partial^-\Lambda$ do not interact: the interaction only works in Λ^- (see (3.2)). Also note that the

Gibbs measure is the reversible equilibrium of the Kawasaki dynamics:

$$\mu_\beta(\eta)c_\beta(\eta,\eta') = \mu_\beta(\eta')c_\beta(\eta',\eta) \qquad \forall\, \eta,\eta' \in \mathcal{X}. \tag{3.6}$$

The dynamics defined by (3.2) and (3.5) 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 fixed at $\rho_1 = e^{-\beta\Delta_1}$ and $\rho_2 = e^{-\beta\Delta_2}$. In the above model this reservoir is replaced by an *open boundary* $\partial^-\Lambda$, where particles are created and annihilated at a rate that matches these densities. Thus, the dynamics is a *finite-state* Markov process, ergodic and reversible with respect to the Gibbs measure μ_β in (3.4).

Note that there is *no* binding energy between neighboring particles of the *same* type (including such an interaction would make the model much more complicated). Consequently, our dynamics has an “anti-ferromagnetic flavor”, and does *not* reduce to Kawasaki dynamics for one type of particle when $\Delta_1 = \Delta_2$. Also note that our dynamics does not allow swaps between particles, i.e., interchanging 1 and 1 or 2 and 2 or 1 and 2 between two neighboring sites in Λ. (The first two would not effect the dynamics, but the third would; for Kawasaki dynamics with one type of particle swaps between 1 and 1 have no effect.)

See Sections 3.1.3–3.1.4 for a further discussion on the choice of the parameters U, Δ_1, Δ_2.

3.1.2 Notation

To state our main theorems in Section 3.1.3, we need some notation.

Definition 3.1 *(a)* $\square$ *is the configuration where* Λ *is empty.*
(b) $\boxplus$ *is the set consisting of the two configurations where* Λ *is filled with the largest possible checkerboard droplet such that all particles of type* 2 *are surrounded by particles of type* 1.
(c) $\omega\colon\ \eta \to \eta'$ *is any path of allowed moves from* $\eta \in \mathcal{X}$ *to* $\eta' \in \mathcal{X}$.
(d) $\Phi(\eta,\eta')$ *is the communication height between* $\eta,\eta' \in \mathcal{X}$ *defined by*

$$\Phi(\eta,\eta') = \min_{\omega\colon\ \eta\to\eta'} \max_{\xi\in\omega} H(\xi), \tag{3.7}$$

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

$$\Phi(A,B) = \min_{\eta\in A,\eta'\in B} \Phi(\eta,\eta'). \tag{3.8}$$

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

$$V_\eta = \Phi(\eta, \mathcal{I}_\eta) - H(\eta), \tag{3.9}$$

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

In Chapter 2 we were interested in the transition of the Kawasaki dynamics from $\square$ to $\boxplus$ in the limit as $\beta \to \infty$. This transition, which is viewed as a crossover from a "gas phase" to a "liquid phase", is triggered by the appearance of a *critical droplet* somewhere in Λ. The critical droplets form a subset of the set of configurations realizing the energetic minimax of the paths of the Kawasaki dynamics from $\square$ to $\boxplus$, which all have energy $\Gamma^\star$ because $H(\square) = 0$.

In Chapter 2 we showed that the first entrance distribution on the set of critical droplets is uniform, computed the expected transition time up to and including a multiplicative factor of order one, and proved that the nucleation time divided by its expectation is exponentially distributed, all in the limit as $\beta \to \infty$. These results, which are typical for metastable behavior, were proved under *three hypotheses*:

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

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

(H3) A hypothesis about the shape of the configurations in and near the essential gate for the transition from $\square$ to $\boxplus$ (for details see Chapter 2).

As shown in Chapter 2, (H1–H3) are the *geometric input* that is needed to derive the metastability theorems in Chapter 2 with the help of the *potential-theoretic approach* to metastability outlined in Bovier [Bov09]. In this chapter we prove (H1–H2) and identify the energy $\Gamma^\star$ of critical droplets. In Chapter 4 we prove (H3) and identify the configurations that form the critical droplets.

Lemma 3.2 (H1–H2) *imply that $V_\square = \Gamma^\star$. Consequently, by Definition* 3.1(g–h), *$\Gamma = \Gamma^\star$ and $\mathcal{X}_{\mathrm{meta}} = \square$.*

Proof. By Definition 3.1(e–h) 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 3.1(h), there exists a $\eta_0 \in \mathcal{I}_{\square} \backslash \boxplus$ such that $\Phi(\square, \eta_0) - H(\square) < \Gamma^\star$. But (H2), together with the finiteness of $\mathcal{X}$, implies that there exist an $m \in \mathbb{N}$ and a sequence $\eta_1, \ldots, \eta_m \in \mathcal{X}$ with $\eta_m = \boxplus$ 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

$$\Phi(\eta_0, \boxplus) \leq \max_{i=0,\ldots,m-1} \Phi(\eta_i, \eta_{i+1}) \leq \max_{i=0,\ldots,m-1} [H(\eta_i) + V^\star] = H(\eta_0) + V^\star < H(\square) + \Gamma^\star, \tag{3.10}$$

where in the first inequality we use that $\Phi(\eta, \sigma) \leq \max\{\Phi(\eta, \xi), \Phi(\xi, \sigma)\}$ for all $\eta, \sigma, \xi \in \mathcal{X}$, and in the last inequality that $\eta_0 \in \mathcal{I}_{\square}$ and $V^\star < \Gamma^\star$. It follows that

$$\Phi(\square, \boxplus) - H(\square) \leq \max\{\Phi(\square, \eta_0) - H(\square), \Phi(\eta_0, \boxplus) - H(\square)\} < \Gamma^\star, \tag{3.11}$$

which contradicts Definition 3.1(h).

The claim that $\Gamma = \Gamma^\star$ follows from Definition 3.1(g–h). To see why $\mathcal{X}_{\mathrm{meta}} = \square$, suppose that there exists a configuration $\eta_m \in \mathcal{X}_{\mathrm{meta}} \backslash \square$. Then, by Definition 3.1(h), $V_{\eta_m} = V_{\square} = \Gamma^\star$, which contradicts H2.

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Hypotheses (H1–H2) imply that $(\mathcal{X}_{\mathrm{meta}}, \mathcal{X}_{\mathrm{stab}}) = (\square, \boxplus)$, and that the highest energy barrier between any two configurations in $\mathcal{X}$ is the one separating $\square$ and $\boxplus$, i.e., $(\square, \boxplus)$ is the unique *metastable pair*. Hypothesis (H3) is needed only to find the asymptotics of the prefactor of the expected transition time in the limit as $\Lambda \to \mathbb{Z}^2$. The main theorems in Chapter 2 involve *three model-dependent quantities*: the energy, the shape and the number of critical droplets.

3.1.3 Main theorems

In Chapter 2 it was shown that $0 < \Delta_1 + \Delta_2 < 4U$ is the *metastable region*, i.e., the region of parameters for which $\square$ is a local minimum but not a global minimum of H. Moreover, it was argued that within this region the subregion where $\Delta_1, \Delta_2 < U$ is of no interest because the critical droplet consists of two free particles, one of type 1 and one of type 2. Therefore the *proper metastable region* is

$$0 < \Delta_1 \leq \Delta_2, \quad \Delta_1 + \Delta_2 < 4U, \quad \Delta_2 \geq U, \tag{3.12}$$

as indicated in Fig. 3.1.

In this chapter, the analysis will be carried out for the subregion of the proper

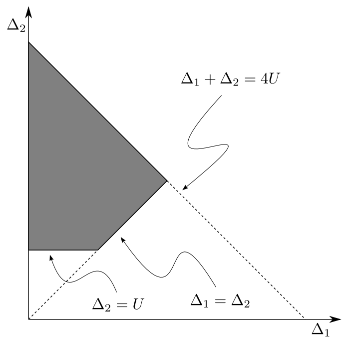


Figure 3.1: Proper metastable region.

metastable region where

$$\Delta_1 < U, \quad \Delta_2 - \Delta_1 > 2U, \quad \Delta_1 + \Delta_2 < 4U, \tag{3.13}$$

as indicated in Fig. 3.2. *Note*: The second and third restriction imply the first restriction. Nevertheless, we write all three because each plays an important role in the sequel.

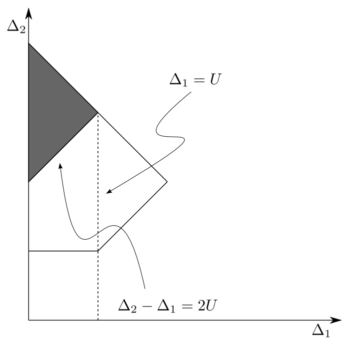


Figure 3.2: Subregion of the proper metastable region given by (3.13).

The following three theorems are the main result of the present chapter and are valid subject to (3.13). We write $\lceil\cdot\rceil$ to denote the upper integer part.

Theorem 3.3 $\mathcal{X}_{\mathrm{stab}} = \boxplus$.

Theorem 3.4 *There exists a* $V^\star \leq 10U - \Delta_1$ *such that* $V_\eta \leq V^\star$ *for all* $\eta \in \mathcal{X}\backslash\{\square, \boxplus\}$. *Consequently, if* $\Gamma^\star > 10U - \Delta_1$, *then* (H1–H2) *hold and, by Lemma* 3.2, $\mathcal{X}_{\mathrm{meta}} = \square$ *and* $\Gamma = \Gamma^\star$.

Theorem 3.5 $\Gamma^\star = -[\ell^\star(\ell^\star-1)+1](4U-\Delta_1-\Delta_2)+(2\ell^\star+1)\Delta_1+\Delta_2$ *with*

$$\ell^\star = \left\lceil \frac{\Delta_1}{4U-\Delta_1-\Delta_2} \right\rceil \in \mathbb{N}. \tag{3.14}$$

Theorem 3.3 settles hypothesis (H1) , Theorem 3.4 settles hypothesis (H2) when $\Gamma^\star > 10U - \Delta_1$, while Theorem 3.5 identifies $\Gamma^\star$, which is the energy of the critical droplets.

As soon as $V^\star < \Gamma^\star$, the energy landscape does not contain wells deeper than those surrounding $\square$ and $\boxplus$. Theorems 3.3 and 3.4 imply that this occurs at least when $\Gamma^\star > 10U - \Delta_1$, while Theorem 3.5 identifies $\Gamma^\star$ and allows us to exhibit a further subregion of (3.13) where the latter inequality is satisfied. This further subregion contains the shaded region in Fig. 3.3.

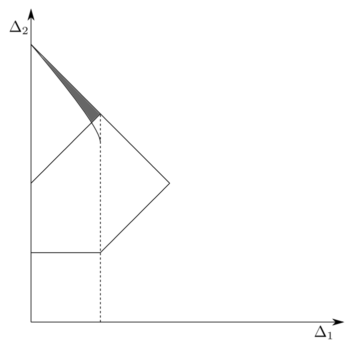


Figure 3.3: The parameter region where $\Gamma^\star > 10U - \Delta_1$ contains the shaded region.

3.1.4 Discussion

1. In Section 3.4 we will see that the *critical droplets* for the crossover from $\square$ to $\boxplus$ consist of a *rhombus-shaped checkerboard with a protuberance plus a free particle*, as indicated in Fig. 3.4. The fact that the free particle is of type 2 is due to the fact that $\Delta_2 > \Delta_1$. A more detailed description will be given in Chapter 4.

2. Abbreviate

$$\varepsilon = 4U - \Delta_1 - \Delta_2 \tag{3.15}$$

and write $\ell^\star = (\Delta_1/\varepsilon) + \iota$ with $\iota \in [0,1)$. Then an easy computation shows that

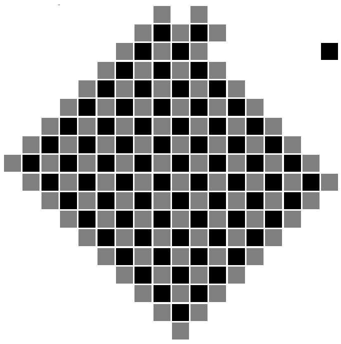


Figure 3.4: A critical droplet. Light-shaded squares are particles of type 1, dark-shaded squares are particles of type 2. The particles of type 2 form an $\ell^\star \times (\ell^\star - 1)$ quasi-square with a protuberance attached to one of its longest sides, and are all surrounded by particles of type 1. In addition, there is a free particle of type 2. As soon as this free particle attaches itself "properly" to a particle of type 1 the dynamics is "over the hill".

$\Gamma^\star = (\Delta_1)^2/\varepsilon + \Delta_1 + 4U + \varepsilon\iota(1-\iota)$. From this we see that

$$\ell^\star \sim \Delta_1/\varepsilon, \qquad \Gamma^\star \sim (\Delta_1)^2/\varepsilon, \qquad \varepsilon \downarrow 0. \tag{3.16}$$

The limit $\varepsilon \downarrow 0$ corresponds to the *weakly supersaturated* regime, where the lattice gas wants to condensate but the energetic threshold to do so is high (because the critical droplet is large). From the viewpoint of metastability this regime is the most interesting. The shaded region in Fig. 3.3 captures this regime for all $0 < \Delta_1 < U$. This region contains the set of parameters where $(\Delta_1)^2/\varepsilon+\Delta_1+4U > 10U - \Delta_1$, i.e., $\varepsilon/U < (\Delta_1/U)^2/[6-2(\Delta_1/U)]$.

3. The simplifying features of (3.13) over (3.12) 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 a 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. In Chapter 2 we conjectured that the metastability results presented there actually hold throughout the region given by (3.12), even though the critical droplets will be *different* when $\Delta_1 \geq U$.

As will become clear in Section 3.3, the constraint $\Delta_1 < U$ has the effect that in all configurations that are local minima of H all particles on the boundary of a droplet are of type 1. It will turn out that such configurations consist of a single *rhombus-shaped checkerboard droplet*. We expect that as Δ_1 increases from U to $2U$ there is a gradual transition from a rhombus-shaped checkerboard critical droplet to a square-shaped checkerboard critical droplet. This is one of the reasons why it is difficult to go beyond (3.13).

4. What makes Theorem 3.4 hard to prove is that the estimate on V_η has to be uniform in $\eta \notin \{\square, \boxplus\}$. In configurations containing several droplets and/or droplets close to $\partial^-\Lambda$ there may be a lack of free space making the motion of particles inside Λ difficult. The mechanisms developed in Section 3.5 allow us to realize an *energy reduction* to a configuration that lies on a suitable *reference path for the nucleation* within an energy barrier $10U - \Delta_1$ also in the absence of free space around each droplet.

We will see in Section 3.5 that for droplets sufficiently far away from other droplets and from $\partial^-\Lambda$ a reduction within an energy barrier $\leq 4U + \Delta_1$ is possible. Thus, if we would be able to control the configurations that fail to have this property, then we would have $V^\star \leq 4U + \Delta_1$ and, consequently, would have $\mathcal{X}_{\mathrm{meta}} = \square$ and $\Gamma = \Gamma^\star$ throughout the subregion given by (3.13) because $\Gamma^\star > 4U + \Delta_1$.

Another way of phrasing the last observation is the following. We view the "liquid phase" as the configuration filling the entire box Λ. If, instead, we would let the liquid phase correspond to the set of configurations filling most of Λ but staying away from $\partial^-\Lambda$, then the metastability results derived in Chapter 2 would apply throughout the subregion given by (3.13).

5. Theorems 3.3 and 3.5 can actually be proved *without* the restriction $\Delta_2 - \Delta_1 > 2U$. However, removal of this restriction makes the task of showing that in droplets with minimal energy all particles of type 2 are surrounded by particles of type 1 more involved than what is done in Section 3.3. We omit this extension, since the restriction $\Delta_2 - \Delta_1 > 2U$ is needed for Theorem 3.4 anyway.

6. In Chapter 2 we describe four classes of models that have a flavor similar to our model of Kawasaki dynamics with two types of particles: (1) Glauber dynamics of spins taking values $\{-1, 0, +1\}$ (Blume-Capel model); (2) Glauber dynamics of Ising spins with an anisotropic interaction or in a staggered magnetic field; (3) Kawasaki dynamics of one type of particle with an anisotropic interaction; (4) probabilistic cellular automata. In each of these models the geometry of the energy landscape is highly complex, like in our model of Kawasaki dynamics with two types of particles, and considerable work is needed to arrive at a full description of the metastable behavior.

Outline. Section 3.2 contains preparations. Theorems 3.3–3.5 are proved in Sections 3.3–3.5, respectively. The proofs are *purely combinatorial*, and are rather involved due to the presence of two types of particles rather than one. Sections 3.3–3.4 deal with *statics* and Section 3.5 with *dynamics*. Section 3.5 is technically the hardest and takes up about half of the chapter. More detailed outlines are given at the beginning of each section.

3.2 Coordinates, definitions and polyominoes

Section 3.2.1 introduces two coordinate systems that are used to describe the particle configurations: standard and dual. Section 3.2.2 lists the main geometric definitions that are needed in the rest of the chapter. Section 3.2.3 proves a lemma about polyominoes (finite unions of unit squares) and Section 3.2.4 a lemma about 2–tiled clusters (checkerboard configurations where all particles of type 2 are surrounded by particles of type 1). These lemmas are needed in Section 3.3 to identify the droplets of minimal energy given the number of particles of type 2 in Λ.

3.2.1 Coordinates

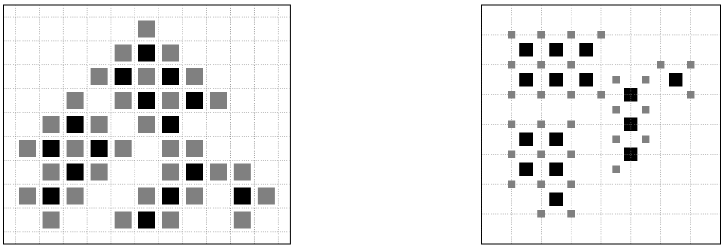
1. A site $i \in \Lambda$ is identified by its *standard coordinates* $x(i) = (x_1(i), x_2(i))$, and is called odd when $x_1(i) + x_2(i)$ is odd and even when $x_1(i) + x_2(i)$ is even. The standard coordinates of a particle p in a configuration η are denoted by $x(p) = (x_1(p), x_2(p))$. The *parity* of a particle p is defined as $x_1(p) + x_2(p) + \eta(x(p))$ modulo 2, and p is said to be odd when the parity is 1 and even when the parity is 0.

2. A site $i \in \Lambda$ is also identified by its *dual coordinates*

$$u_1(i) = \frac{x_1(i) - x_2(i)}{2}, \qquad u_2(i) = \frac{x_1(i) + x_2(i)}{2}. \tag{3.17}$$

Two sites i and j are said to be *adjacent*, written $i \sim j$, when $|x_1(i) - x_1(j)| + |x_2(i) - x_2(j)| = 1$ or, equivalently, $|u_1(i) - u_1(j)| = |u_2(i) - u_2(j)| = \frac{1}{2}$ (see Fig. 3.5).

3. For convenience, we take Λ to be the $(L+\frac{3}{2}) \times (L+\frac{3}{2})$ dual square with bottom-left corner at site with dual coordinates $(-\frac{L+1}{2}, -\frac{L+1}{2})$ for some $L \in \mathbb{N}$ with $L > 2\ell^\star$ (to allow for $H(\boxplus) < H(\square)$; see Section 3.3.1). Particles interact only inside Λ^-, which is a $(L+\frac{1}{2}) \times (L+\frac{1}{2})$ dual square. This dual square, a *rhombus* in standard coordinates, is convenient because the local minima of H are rhombus-shaped as well (see Section 3.3).



(a) (b)

Figure 3.5: A configuration represented in: (a) standard coordinates; (b) dual coordinates. Light-shaded squares are particles of type 1, dark-shaded squares are particles of type 2. In dual coordinates, particles of type 2 are represented by larger squares than particles of type 1 to exhibit the "tiled structure" of the configuration.

3.2.2 Definitions

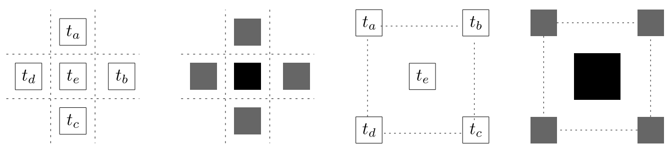
1. A site $i \in \Lambda$ is said to be *lattice-connecting* in the configuration η if there exists a lattice path λ from i to $\partial^- \Lambda$ such that $\eta(j) = 0$ for all $j \in \lambda$ with $j \neq i$. We say that a particle p is lattice-connecting if $x(p)$ is a lattice-connecting site.

2. Two particles in η at sites i and j are called *connected* if $i \sim j$ and $\eta(i)\eta(j) = 2$. If two particles p_1 and p_2 are connected, then we say that there is an *active bond* b between them. The bond b is said to be *incident* to p_1 and p_2. A particle p is said to be *saturated* if it is connected to four other particles, i.e., there are four active bonds incident to p. The support of the configuration η, i.e., the union of the unit squares centered at the occupied sites of η, is denoted by $\mathrm{supp}(\eta)$. For a configuration η, $n_1(\eta)$ and $n_2(\eta)$ denote the number of particles of type 1 and 2 in η, and $B(\eta)$ denotes the number of active bonds. The energy of η equals $H(\eta) = \Delta_1 n_1(\eta) + \Delta_2 n_2(\eta) - UB(\eta)$.

3. Let $G(\eta)$ be the *graph* associated with η, i.e., $G(\eta) = (V(\eta), E(\eta))$, where $V(\eta)$ is the set of sites $i \in \Lambda$ such that $\eta(i) \neq 0$, and $E(\eta)$ is the set of the pairs $\{i, j\}$, $i, j \in V(\eta)$, such that the particles at sites i and j are connected. A configuration η' is called a *subconfiguration* of η, written $\eta' \prec \eta$, if $\eta'(i) = \eta(i)$ for all $i \in \Lambda$ such that $\eta'(i) > 0$. A subconfigu ration $c \prec \eta$ is a *cluster* if the graph $G(c)$ is a maximal connected component of $G(\eta)$. The set of non-saturated particles in c is called the *boundary* of c, and is denoted by ∂c. Clearly, all particles in the same cluster have the same parity. Therefore the concept of parity extends from particles to clusters.

4. For a site $i \in \Lambda$, the *tile* centered at i, denoted by $\mathrm{t}(i)$, is the set of five sites consisting of i and the four sites adjacent to i. If i is an even site, then the tile is said to be even, otherwise the tile is said to be odd. The five sites of a tile are labeled a, b, c, d, e as in Fig. 3.6. The sites labeled a, b, c, d are called *junction sites.* If a particle p sits at site i, then $\mathrm{t}(i)$ is also denoted by $\mathrm{t}(p)$ and is called the tile associated with p. In standard coordinates, a tile is a square of size $\sqrt{2}$. In dual coordinates, it is a unit square.

5. A tile whose central site is occupied by a particle of type 2 and whose junction sites are occupied by particles of type 1 is called a 2*–tile* (see Fig. 3.6). Two 2–tiles are said to be adjacent if their particles of type 2 have dual distance 1. A horizontal (vertical) 12*–bar* is a maximal sequence of adjacent 2–tiles all having the same horizontal (vertical) coordinate. If the sequence has length 1, then the 12–bar is called a 2*–tiled protuberance.* A cluster containing at least one particle of type 2 such that all particles of type 2 are saturated is said to be 2–tiled. A 2–tiled configuration is a configuration consisting of 2–tiled clusters only.



(a) (b) (c) (d)

Figure 3.6: Tiles: (a) standard representation of the labels of a tile; (b) standard representation of a 2–tile; (c) dual representation of the labels of a tile; (d) dual representation of a 2–tile.

6. The *tile support* of a configuration η is defined as

$$[\eta] = \bigcup_{p \in \varpi_2(\eta)} \mathrm{t}(p), \tag{3.18}$$

where $\varpi_2(\eta)$ is the set of particles of type 2 in η. Obviously, $[\eta]$ is the union of the tile supports of the clusters making up η. For a standard cluster c the *dual perimeter*, denoted by $P(c)$, is the length of the Euclidean boundary of its tile support $[c]$ (which includes an inner boundary when c contains holes). The dual perimeter $P(\eta)$ of a 2–tiled configuration η is the sum of the dual perimeters of the clusters making up η.

7. $\mathcal{V}_{\star,n_2}$ is the set of configurations such that in $(\Lambda^-)^-$ the number of particles of type 2 is n_2. $\mathcal{V}_{\star,n_2}^{4n_2}$ is the set of configurations such that in $(\Lambda^-)^-$ the number of particles of type 2 is n_2, the number of active bonds is $4n_2$, and there are no non-interacting particles of type 1. In other words, $\mathcal{V}_{\star,n_2}^{4n_2}$ is the set of 2–tiled configurations with n_2 particles of type 2. A configuration η is called *standard* if $\eta \in \mathcal{V}^{4n_2}_{\star,n_2}$, and its tile support is a standard polyomino in dual coordinates (see Definition 3.6 below for the definition of a standard polyomino).

8. A *unit hole* is an empty site such that all four of its neighbors are occupied by particles of the same type (either all of type 1 or all of type 2). An empty site with three neighboring sites occupied by a particle of type 1 is called a *good dual corner*. In the dual representation a good dual corner is a concave corner (see Fig. 3.7).

3.2.3 A lemma on polyominoes

The tile support of a collection of clusters c can be represented by polyominoes, i.e., finite unions of unit squares, with each polyomino representing a cluster on the dual lattice. The following notation is used:

$\ell_1(c)$ = width of c (= number of columns).

$\ell_2(c)$ = height of c (= number of rows).

$v_i(c)$ = number of vertical edges in the i-th non-empty row of c.

$h_j(c)$ = number of horizontal edges in the j-th non-empty column of c.

$C(c)$ = number of clusters in c.

$P(c)$ = length of the perimeter of c.

$Q(c)$ = number of holes in c.

$\psi(c)$ = number of convex corners of c.

$\phi(c)$ = number of concave corners of c.

Note that $\psi(c) = \sum_{i=1}^{N(c)} \psi(i)$ and $\phi(c) = \sum_{i=1}^{N(c)} \phi(i)$, where $N(c)$ is the number of vertices along the perimeter of the polyomino representing c. If two edges e_1 and e_2 are incident to vertex i at a right angle with a unit square inside and no unit squares outside, then $\psi(i) = 1$ and $\phi(i) = 0$ (Fig. 3.7(a)). On the other hand, if there is no unit square inside and three unit squares outside, then $\psi(i) = 0$ and $\phi(i) = 1$ (Fig. 3.7(b)). If four edges e_1, e_2, e_3, e_4 are incident to vertex i, with two unit squares in opposite angles, then $\psi(i) = 0$ and $\phi(i) = 2$ (Fig. 3.7(c)).

Definition 3.6 [Alonso and Cerf [AC96].] *A polyomino is called monotone if its perimeter is equal to the perimeter of its circumscribing rectangle. A polyomino whose support is a quasi-square (i.e., a rectangle whose side lengths differ by at most one), with possibly a bar attached to one of its longest sides, is called a standard polyomino.*

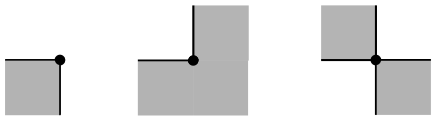


Figure 3.7: Corners of polyominoes: (a) one convex corner; (b) one concave corner; (c) two concave corners. Shaded mean occupied by a unit square.

In the sequel, a key role will be played by the quantity

$$\mathcal{T}(c) = 2P(c) + [\psi(c) - \phi(c)]. \tag{3.19}$$

The geometric meaning of $\mathcal{T}(c)$ will be discussed at the beginning of the proof of Lemma 3.8. Note that

$$\psi(c) - \phi(c) = 4[C(c) - Q(c)]. \tag{3.20}$$

Lemma 3.7 *(i) All polyominoes c with a fixed number of monominoes minimizing $\mathcal{T}(c)$ are single-component monotone polyominoes of minimal perimeter, which include the standard polyominoes.*
(ii) If the number of monominoes is ℓ^2, $\ell^2 - 1$, $\ell(\ell-1)$ or $\ell(\ell-1) - 1$ for some $\ell \in \mathbb{N}\backslash\{1\}$, then the standard polyominoes are the only minimizers of $\mathcal{T}(c)$.

Proof. In the proof we assume without loss of generality that the polyomino consists of a single cluster c.

(i) The proof uses projection. Pick any non-monotone cluster c. Let

$$\tilde{c} = (\pi_2 \circ \pi_1)(c), \tag{3.21}$$

where π_2 and π_1 denote the vertical, respectively, the horizontal projection of c. The effect of vertical and horizontal projection is illustrated in Fig. 3.8. By construction, $\tilde{c}$ is a monotone polyomino (see e.g. the statement on Ferrers diagrams in the proof of Alonso and Cerf [AC96], Theorem 2.2).

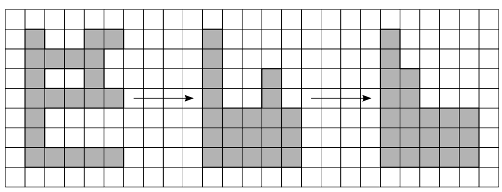


Figure 3.8: Effect of vertical and horizontal projection.

Suppose first that $Q(c) = 0$. Then $\mathcal{T}(c) = 2P(c) + 4$. Since c is not monotone, we have $P(\tilde{c}) < P(c)$, and so c is not a minimizer of $\mathcal{T}(c)$.

Suppose next that $Q(c) \geq 1$. Since

$$P(c) = \sum_{i=1}^{\ell_2(c)} v_i(c) + \sum_{j=1}^{\ell_1(c)} h_j(c) \tag{3.22}$$

and every hole belongs to at least one row and one column, we have

$$P(c) \geq 2[\ell_1(c) + \ell_2(c)] + 4Q(c). \tag{3.23}$$

On the other hand, since $\tilde{c}$ is a monotone polyomino, we have $v_i(\tilde{c}) = h_j(\tilde{c}) = 2$ for all i and j, and so

$$P(\tilde{c}) = 2[\ell_1(\tilde{c}) + \ell_2(\tilde{c})]. \tag{3.24}$$

Moreover, since $\ell_1(\tilde{c}) \leq \ell_1(c)$ and $\ell_2(\tilde{c}) \leq \ell_2(c)$, we can combine (3.23–3.24) to get

$$P(\tilde{c}) - P(c) \leq -4Q(c), \tag{3.25}$$

Using (3.25), we obtain

$$\begin{aligned} \mathcal{T}(\tilde{c}) - \mathcal{T}(c) &= [2P(\tilde{c}) + 4] - [2P(c) + 4 - 4Q(c)] \\ &= 2[P(\tilde{c}) - P(c)] + 4Q(c) \leq -4Q(c) \leq -4 < 0, \end{aligned} \tag{3.26}$$

and so c is not a minimizer of $\mathcal{T}(c)$.

(ii) We saw in the proof of (i) that if c is a minimizer of $\mathcal{T}(c)$, then c is monotone, and hence does not contain holes and minimizes $P(c)$. The claim therefore follows from Alonso and Cerf [AC96], Corollary 3.7, which states that if the number of monominoes is ℓ^2, $\ell^2 - 1$, $\ell(\ell-1)$ or $\ell(\ell-1) - 1$ for some $\ell \in \mathbb{N}\backslash\{1\}$, then the standard polyominoes are the only minimizers of $P(c)$. ★

3.2.4 Number of bonds in 2–tiled clusters

In this section we consider 2–tiled clusters and link the number of particles of type 1 and type 2 to the number of active bonds and the geometric quantity $\mathcal{T}$ considered in Section 3.2.3. Recall from Section 3.2.2, item 2, that $B(c)$ is the number of active bonds in c.

Lemma 3.8 *For any 2–tiled cluster c (i.e., $c \in \mathcal{V}^{4n_2}_{\star,n_2}$ for some n_2), $4n_1(c) = B(c) + \mathcal{T}(c)$ and $4n_2(c) = B(c)$.*

Proof. The claim of the lemma is equivalent to the affirmation that $\mathcal{T}(c) = M(c)$ with $M(c)$ the number of missing bonds in c. Indeed, informally, for every unit perimeter two bonds are lost with respect to the four bonds that would be incident to each particle of type 1 if it were saturated, while one bond is lost at each convex corner and one bond is gained at each concave corner. Hence (3.19) yields the claim.

Formally, let p be a particle of type 1, $B(p)$ the number of bonds incident to p, and $M(p) = 4 - B(p)$ the number of missing bonds of p. Consider the set of particles of type 1 at the boundary of a 2–tiled cluster, i.e., the set of non-saturated particles of type 1. Each of these particles belongs to one of four classes (see Fig. 3.9, and recall the definition of 12–bar in Section 3.2.2, item 5):

class 1: p has two neighboring particles of type 2 belonging to the same 12–bar.

class 2: p has two neighboring particles of type 2 belonging to different 12–bars.

class 3: p has three neighboring particles of type 2.

class 4: p has one neighboring particle of type 2.

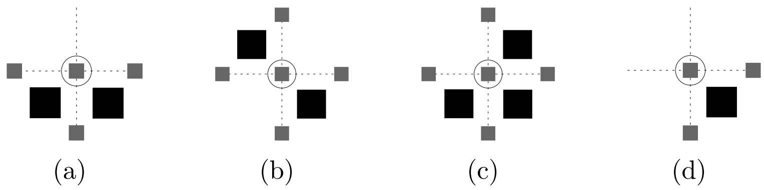


Figure 3.9: The circled boundary particle of type 1 belongs to: (a) class 1; (b) class 2; (c) class 3; (d) class 4.

Let $M_k(c)$ be the number of missing bonds of particles of class k in cluster c, and $A_k(c)$ the number of edges incident to particles of class k in cluster c. Then

$$\begin{aligned} M_1(c) = 2,\ A_1(c) = 2; \quad M_2(c) = 2,\ A_2(c) = 4; \\ M_3(c) = 1,\ A_3(c) = 2; \quad M_4(c) = 3,\ A_4(c) = 2. \end{aligned} \tag{3.27}$$

Let $N_k(c)$ be the number of particles of class k of type 1 in cluster c. Observing that a cluster has two concave corners per particle of class 2, one concave corner per particle of class 3 and one convex corner per particle of class 4, we can write

$$\mathcal{T}(c) = 2P(c) - 2N_2(c) - N_3(c) + N_4(c). \tag{3.28}$$

Since the dual perimeter of a cluster is equal to its total number of dual edges, we have

$$2P(c) = \sum_{k=1}^{4} A_k(c)N_k(c) = 2N_1(c) + 4N_2(c) + 2N_3(c) + 2N_4(c) \tag{3.29}$$

(the sum counts each edge of the 2–tile twice). The total number of missing bonds, on the other hand, is

$$M(c) = \sum_{k=1}^{4} M_k(c)N_k(c) = 2N_1(c) + 2N_2(c) + N_3(c) + 3N_4(c). \tag{3.30}$$

Combining (3.28–3.30), we arrive at $\mathcal{T}(c) = M(c)$. ★

3.3 Identification of $\mathcal{X}_{\text{stab}}$

In this section we prove Theorem 3.3.

Recall that Λ^- (the part of Λ where particles interact) is an $(L+\frac{1}{2}) \times (L+\frac{1}{2})$ dual square with $L > 2\ell^\star$. Let $\eta_{\text{stab}}, \eta'_{\text{stab}}$ be the configurations consisting of a 2–tiled dual square of size L with even parity, respectively, odd parity. (*Note:* Of the four corners of the $(L+\frac{1}{2}) \times (L+\frac{1}{2})$ dual square two diagonally opposite corners are empty since they do not correspond to a site of $\mathbb{Z}^2$.) These two configurations have the same energy. Theorem 3.3 says that $\mathcal{X}_{\text{stab}} = \{\eta_{\text{stab}}, \eta'_{\text{stab}}\} = \boxplus$. Section 3.3.1 contains two lemmas about 2–tiled configurations with minimal energy. Section 3.3.2 uses these two lemmas to prove Theorem 3.3.

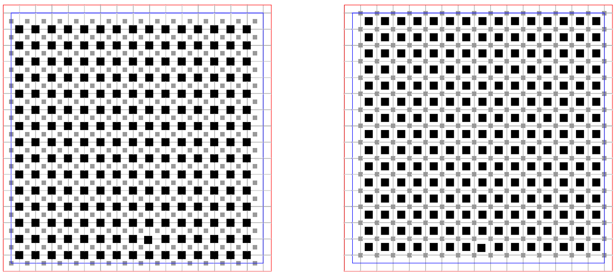
3.3.1 Standard configurations are minimizers among 2–tiled configurations

Lemma 3.9 *Within $\mathcal{V}^{4n_2}_{\star,n_2}$, the standard configurations achieve the minimal energy.*

Proof. Recall from item 2 in Section 3.2.2 that

$$H(\eta) = \Delta_1 n_1(\eta) + \Delta_2 n_2(\eta) - UB(\eta). \tag{3.31}$$

In $\mathcal{V}^{4n_2}_{\star,n_2}$ both n_2 and $B = 4n_2$ are fixed, and hence $\min_{\eta\in\mathcal{V}^{4n_2}_{\star,n_2}} H(\eta)$ is attained at



(a) (b)

Figure 3.10: Representation of Λ and Λ^- in dual coordinates, and the two possible ground states for $L = 15$ when the cluster is: (a) even; (b) odd. Note that sites in $\partial^-\Lambda$ are empty because there is no interaction in $\partial^-\Lambda$. Also note that the top-left and bottom-right corners of Λ and Λ^- in dual coordinates do not correspond to a site of $\mathbb{Z}^2$.

a configuration minimizing n_1. By Lemma 3.8, if $\eta \in \mathcal{V}^{4n_2}_{\star,n_2}$, then

$$n_1(\eta) = \tfrac{1}{4}[B(\eta) + \mathcal{T}(\eta)], \qquad n_2(\eta) = \tfrac{1}{4}B(\eta). \tag{3.32}$$

Hence, to minimize $n_1(\eta)$ we must minimize $\mathcal{T}(\eta)$. The claim therefore follows from Lemma 3.7(i). ★

For a standard configuration the computation of the energy is straightforward. For $\ell \in \mathbb{N}$, $\zeta \in \{0, 1\}$ and $k \in \mathbb{N}_0$ with $k \leq \ell + \zeta$, let $\eta^{\ell,\zeta,k}$ denote the standard configuration consisting of an $\ell \times (\ell + \zeta)$ (quasi-)square with a bar of length k attached to one of its longest sides (see Fig. 3.11).

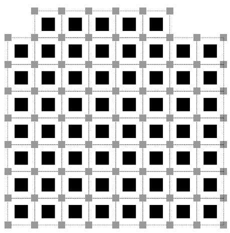


Figure 3.11: A standard configuration with $\ell = 7, \zeta = 1$ and $k = 5$.

Lemma 3.10 *The energy of $\eta^{\ell,\zeta,k}$ is (recall* (3.15)*)*

$$H(\eta^{\ell,\zeta,k}) = -\varepsilon[\ell(\ell + \zeta) + k] + \Delta_1[\ell + (\ell + \zeta) + 1 + 1_{\{k>0\}}]. \tag{3.33}$$

Proof. Note that $P(\eta^{\ell,\zeta,k}) = 2[\ell + (\ell+\zeta) + 1_{\{k>0\}}]$ and $Q(\eta^{\ell,\zeta,k}) = 0$, so that

$$\mathcal{T}(\eta^{\ell,\zeta,k}) = 4[\ell + (\ell+\zeta) + 1 + 1_{\{k>0\}}]. \tag{3.34}$$

Also note that

$$B(\eta^{\ell,\zeta,k}) = 4[\ell + (\ell+\zeta) + k], \tag{3.35}$$

because all particles of type 2 are saturated. However, by (3.31–3.32), we have

$$H(\eta^{\ell,\zeta,k}) = -\tfrac{1}{4}\varepsilon B(\eta^{\ell,\zeta,k}) + \tfrac{1}{4}\mathcal{T}(\eta^{\ell,\zeta,k})\Delta_1, \tag{3.36}$$

and so the claim follows by combining (3.34–3.36). ★

Note that the energy increases by $\Delta_1 - \varepsilon$ (which is > 0 if and only if $\ell^\star \geq 2$ by (3.14)) when a bar of length $k = 1$ is added, and decreases by ε each time the bar is extended. Note further that

$$H(\eta^{\ell,1,0}) - H(\eta^{\ell,0,0}) = \Delta_1 - \ell\varepsilon, \qquad H(\eta^{\ell+1,0,0}) - H(\eta^{\ell,1,0}) = \Delta_1 - (\ell+1)\varepsilon, \tag{3.37}$$

which show that the energy of a growing sequence of standard configurations goes up when $\ell < \ell^\star$ and goes down when $\ell \geq \ell^\star$. The highest energy is attained at $\eta^{\ell^\star-1,1,1}$, which is the critical droplet in Fig. 3.4.

It is worth noting that $H(\eta_s^{2\ell^\star,0,0}) < 0$, i.e., the energy of a dual square of side length $2\ell^\star$ is lower than the energy of $\square$. This is why we assumed $L > 2\ell^\star$, to allow for $H(\boxplus) < H(\square)$.

3.3.2 Stable configurations

In this section we use Lemmas 3.9–3.10 to prove Theorem 3.3.

Proof. Let η denote any configuration in $\mathcal{X}_{\text{stab}}$. Below we will show that:

(A) η does not contain any particle in $\partial^-\Lambda$.

(B) η is a 2–tiled configuration, i.e., $\eta \in \mathcal{V}_{\star,n_2}^{4n_2}$ for some n_2 $(= n_2(\eta))$.

Once we have (A) and (B), we observe that η cannot contain a number of 2–tiles larger than L^2. Indeed, consider the tile support of η. Since Λ^- is an $(L+\frac{1}{2}) \times (L+\frac{1}{2})$ dual square, if the tile support of η fits inside Λ^-, then so does the dual circumscribing rectangle of η. But any rectangle of area $\geq L^2$ has at least one side of length $L+1$. Hence $n_2(\eta) \leq L^2$, and therefore the number of 2–tiles in η is at most L^2. By Lemmas 3.9–3.10, the global minimum of the energy is attained at the largest dual quasi-square that fits inside Λ^-, since $L > 2\ell^\star$. We therefore conclude that $\eta \in \{\eta_{\rm stab}, \eta'_{\rm stab}\}$, which proves the claim.

Proof of (A). Since in $\partial^-\Lambda$ particles do not feel any interaction but have a positive energy cost, removal of a particle from $\partial^-\Lambda$ always lowers the energy.

Proof of (B). We note the following three facts:

(1) η does not contain isolated particles of type 1.

(2) $\partial^-\Lambda^-$ does not contain any particle of type 2.

(3) All particles of type 2 in η have all their neighboring sites occupied by a particle.

For (1), simply note that the configuration obtained from η by removing isolated particles has lower energy. For (2), note that particles in $\partial^-\Lambda^-$ have at most two active bonds. Therefore, if η would have a particle of type 2 in $\partial^-\Lambda^-$, then the removal of that particle would lower the energy, because $\Delta_2 - \Delta_1 > 2U$ and $\Delta_1 > 0$ (recall (3.13)) imply $\Delta_2 > 2U$. For (3), note that if a particle of type 2 has an empty neighboring site, then the addition of a particle of type 1 at this site lowers the energy, because $\Delta_1 < U$ (recall (3.13)).

We can now complete the proof of (B) as follows. The constraint $\Delta_2 - \Delta_1 > 2U$ implies that any particle of type 2 in η must have at least three neighboring sites occupied by a particle of type 1. Indeed, the removal of a particle of type 2 with at most two active bonds lowers the energy. But the fourth neighboring site must also be occupied by a particle of type 1. Indeed, suppose that this site would be occupied by a particle of type 2. Then this particle would have at most three active bonds. Consider the configuration $\tilde\eta$ obtained from η after replacing this particle by a particle of type 1. Then $B(\tilde\eta) - B(\eta) \geq -2$, $n_1(\tilde\eta) - n_1(\eta) = 1$ and $n_2(\tilde\eta) - n_2(\eta) = -1$. Consequently, $H(\tilde\eta) - H(\eta) \leq \Delta_1 - \Delta_2 + 2U < 0$. Hence, any particle of type 2 in η must be saturated. ★

3.4 Identification of $\Gamma^\star = \Phi(\square, \boxplus)$

In Section 3.4.1 we prove Theorem 3.5 subject to the following lemma.

Lemma 3.11 *For any $n_2 \leq L^2$, the configurations of minimal energy with n_2 particles of type 2 belong to $\mathcal{V}^{4n_2}_{\star,n_2}$, i.e., are 2–tiled configurations.*

The proof of this lemma is given in Section 3.4.2.

3.4.1 Saddle configurations

Proof. For $\mathcal{Y} \subset \mathcal{X}$, define the *external boundary* of $\mathcal{Y}$ by $\partial\mathcal{Y} = \{\eta \in \mathcal{X}\backslash\mathcal{Y}\colon \exists\eta' \in \mathcal{Y},\, \eta \leftrightarrow \eta'\}$ and the *bottom* of $\mathcal{Y}$ by $\mathcal{F}(\mathcal{Y}) = \arg\min_{\eta\in\mathcal{Y}} H(\eta)$. According to Manzo, Nardi, Olivieri and Scoppola [MNOS04], Section 4.2, $\Phi(\square, \boxplus) = \min_{\eta\in\partial\mathcal{B}} H(\eta)$ for $\mathcal{B} \subset \mathcal{X}$ any (!) set with the following properties:

(I) $\mathcal{B}$ is connected via allowed moves, $\square \in \mathcal{B}$ and $\boxplus \notin \mathcal{B}$.

(II) There is a path $\omega^\star\colon \square \to \boxplus$ such that $\{\arg\max_{\eta\in\omega^\star} H(\eta)\} \cap \mathcal{F}(\partial\mathcal{B}) \neq \emptyset$.

Thus, our task is to find such a $\mathcal{B}$ and compute the lowest energy of $\partial\mathcal{B}$.

For (I), choose $\mathcal{B}$ to be the set of all configurations η such that $n_2(\eta) \leq \ell^\star(\ell^\star-1)+1$. Clearly this set is connected, contains $\square$ and does not contain $\boxplus$.

For (II), choose $\omega^\star$ as follows. A particle of type 2 is brought inside Λ ($\Delta H = \Delta_2$), moved to the origin and is saturated by four times bringing a particle of type 1 ($\Delta H = \Delta_1$) and attaching it to the particle of type 2 ($\Delta H = -U$). After this first 2–tile has been completed, $\omega^\star$ follows a sequence of increasing 2–tiled dual quasi-squares. The passage from one quasi–square to the next is obtained by *adding* a 12–bar to one of the longest sides, as follows. First a particle of type 2 is brought inside Λ ($\Delta H = \Delta_2$) and is attached to one of the longest sides of the quasi-square ($\Delta H = -2U$). Next, twice a particle of type 1 is brought inside the box ($\Delta H = \Delta_1$) and is attached to the (not yet saturated) particle of type 2 ($\Delta H = -U$) in order to complete a 2–tiled protuberance. Finally, the 12–bar is completed by bringing a particle of type 2 inside Λ ($\Delta H = \Delta_2$), moving it to a concave corner ($\Delta H = -3U$), and saturating it with a particle of type 1 ($\Delta H = \Delta_1$, respectively, $\Delta H = -U$). It is obvious that $\omega^\star$ eventually hits $\boxplus$. The path $\omega^\star$ is referred to as the *reference path for the nucleation.*

Call $\eta^\star$ the configuration in $\omega^\star$ consisting of an $\ell^\star \times (\ell^\star - 1)$ quasi-square, a 2–tiled protuberance attached to one of its longest sides, and a free particle of type 2 (see Fig. 3.12; there are many choices for $\omega^\star$ depending on where the 2–tiled protuberances are added; all these choices are equivalent). Note that, in the notation of Lemma 3.10, $\eta^\star = \eta^{\ell^\star-1,1,1} + \mathrm{fp}[2]$, where $+\mathrm{fp}[2]$ denotes the addition of a free particle of type 2 in $\partial^-\Lambda$. Observe that:

(a) $\omega^\star$ exits $\mathcal{B}$ via the configuration $\eta^\star$;

(b) $\eta^\star \in \mathcal{F}(\partial\mathcal{B})$;

(c) $\eta^\star \in \{\arg\max_{\eta\in\omega^\star} H(\eta)\}$.

Observation (a) is obvious, while (b) follows from Lemmas 3.9 and 3.11. To see (c), note the following: (1) The total energy difference obtained by adding a 12–bar of length ℓ on the side of a 2–tiled cluster is ΔH(adding a 12–bar) $= \Delta_1 - \varepsilon\ell$, which changes sign at $\ell = \ell^\star$ (recall (3.37)); (2) The configurations of maximal energy in a sequence of growing quasi-squares are those where a free particle of type 2 enters the box after the 2–tiled protuberance has been completed. Thus, within energy barrier $2\Delta_1 + 2\Delta_2 - 4U = 4U - \varepsilon$ the 12–bar is completed downwards in energy. This means that, after configuration $\eta^\star$ is hit, the dynamics can reach the 2–tiled dual square of $\ell^\star \times \ell^\star$ while staying below the energy level $H(\eta^\star)$. Since all 2–tiled dual quasi-squares larger than $\ell^\star \times (\ell^\star - 1)$ have an energy smaller than that of the 2–tiled dual quasi-square $\ell^\star \times (\ell^\star - 1)$ itself, the path $\omega^\star$ does not again reach the energy level $H(\eta^\star)$.

Because of (a–c), we have $\Phi(\square, \boxplus) = H(\eta^\star)$. To complete the proof, use Lemma 3.10 to compute

$$H(\eta^\star) = H(\eta^{\ell^\star - 1,1,1} + \mathrm{fp}[2]) = -\varepsilon[\ell^\star(\ell^\star - 1) + 1] + \Delta_1(2\ell^\star + 1) + \Delta_2. \qquad (3.38)$$

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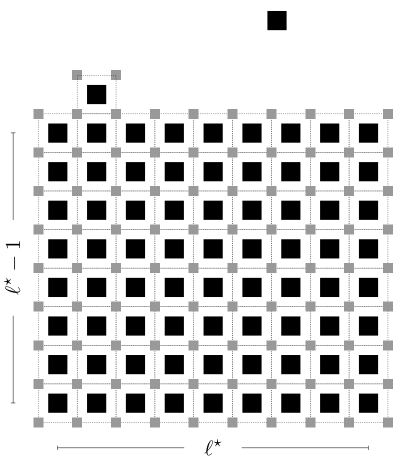


Figure 3.12: A critical configuration $\eta^\star$. This is the dual version of the critical droplet in Fig. 3.4.

3.4.2 Configurations of minimal energy

Here we prove Lemma 3.11. The proof is carried out in two steps. In Section 3.4.2 we show that the claim holds for single-cluster configurations with a fixed number of particles of type 2. In Section 3.4.2 we extend the claim to general configurations with a fixed number of particles of type 2.

Single clusters of minimal energy are 2–tiled clusters

Lemma 3.12 *For any single-cluster configuration $\eta \in \mathcal{V}_{\star,n_2} \backslash \mathcal{V}_{\star,n_2}^{4n_2}$ there exists a configuration $\tilde{\eta} \in \mathcal{V}_{\star,n_2}^{4n_2}$ such that $H(\tilde{\eta}) < H(\eta)$.*

Proof. Pick any $\eta \in \mathcal{V}_{\star,n_2} \backslash \mathcal{V}_{\star,n_2}^{4n_2}$. Every neighboring site of a particle of type 2 in the cluster is either empty or occupied by a particle of type 1, and there is at least one non-saturated particle of type 2. Since η consists of a single cluster, $\tilde{\eta}$ can be constructed in the following way:

- $\tilde{\eta}(i) = \eta(i)$ for all $i \in \mathrm{supp}(\eta)$.
- $\tilde{\eta}(j) = 1$ for all $j \notin \mathrm{supp}(\eta)$ such that there exists an $i \sim j$ with $\eta(i) = 2$.

Since

$$\begin{aligned} H(\eta) &= \Delta_1 n_1(\eta) + \Delta_2 n_2(\eta) - UB(\eta), \\ H(\tilde{\eta}) &= \Delta_1 n_1(\tilde{\eta}) + \Delta_2 n_2(\tilde{\eta}) - UB(\tilde{\eta}), \end{aligned} \tag{3.39}$$

and $n_2(\eta) = n_2(\tilde{\eta})$, we have

$$H(\tilde{\eta}) - H(\eta) = \Delta_1[n_1(\tilde{\eta}) - n_1(\eta)] - U[B(\tilde{\eta}) - B(\eta)]. \tag{3.40}$$

By construction, $B(\tilde{\eta}) - B(\eta) \geq n_1(\tilde{\eta}) - n_1(\eta) > 0$. Since $0 < \Delta_1 < U$ (recall (3.13)), it follows from (3.40) that $H(\tilde{\eta}) < H(\eta)$. ★

Configurations of minimal energy with fixed number of particles of type 2

Lemma 3.13 *For any n_2 and any configuration $\eta \in \mathcal{V}_{\star,n_2}$ consisting of at least two clusters, any configuration $\eta^\star$ such that $\eta^\star$ is a single cluster, $\eta^\star \in \mathcal{V}_{\star,n_2}^{4n_2}$ and $\eta^\star$ is a standard configuration satisfies $H(\eta^\star) < H(\eta)$.*

Proof. Let $\eta \in \mathcal{V}_{\star,n_2}$ be a configuration consisting of $k > 1$ clusters, labeled $c_1, \ldots, c_k$. Let $\eta^{n_2(c_i)}$ denote any standard configuration with $n_2(c_i)$ particles of type 2. By Lemmas 3.9 and 3.12, we have

$$H(\eta) = \sum_{i=1}^{k} H(c_i) \geq \sum_{i=1}^{k} H(\eta^{n_2(c_i)}). \tag{3.41}$$

By Lemma 3.8, we have (recall (3.15))

$$\begin{aligned}\sum_{i=1}^{k} H(\eta^{n_2(c_i)}) &= \sum_{i=1}^{k} \big[\Delta_1 n_1(\eta^{n_2(c_i)}) + \Delta_2 n_2(\eta^{n_2(c_i)}) - UB(\eta^{n_2(c_i)})\big] \\ &= \sum_{i=1}^{k} \big[\Delta_1\big\{n_2(\eta^{n_2(c_i)}) + \tfrac{1}{4}\mathcal{T}(\eta^{n_2(c_i)})\big\} + \Delta_2 n_2(\eta^{n_2(c_i)}) - U4n_2(\eta^{n_2(c_i)})\big] \\ &= \sum_{i=1}^{k} \big[-\varepsilon n_2(\eta^{n_2(c_i)}) + \tfrac{1}{4}\Delta_1\mathcal{T}(\eta^{n_2(c_i)})\big].\end{aligned} \tag{3.42}$$

But from Lemma 3.7 it follows that

$$\sum_{i=1}^{k} \mathcal{T}(\eta^{n_2(c_i)}) > \mathcal{T}\big(\eta^{\sum_{i=1}^{k} n_2(c_i)}\big), \tag{3.43}$$

where $\eta^{\sum_{i=1}^{k} n_2(c_i)}$ denotes any standard configuration with $\sum_{i=1}^{k} n_2(c_i) = n_2(\eta)$ particles of type 2. Combining (3.41–3.43), we arrive at

$$H(\eta) > -\varepsilon n_2(\eta) + \tfrac{1}{4}\Delta_1\mathcal{T}(\eta^{n_2(\eta)}) = H(\eta^{n_2(\eta)}). \tag{3.44}$$

★

3.5 Upper bound on V_η for $\eta \notin \{\square, \boxplus\}$

In this section we prove of Theorem 3.4.

In this section we show that for any configuration $\eta \notin \{\square, \boxplus\}$ it is possible to find a path $\omega\colon \eta \to \eta'$ with $\eta' \in \{\square, \boxplus\}$ such that $\max_{\xi\in\omega} H(\xi) \leq H(\eta) + V^\star$ with $V^\star \leq 10U - \Delta_1$ and $\eta' \in I_\eta$. By Definition 3.1(c–e), this implies that $V_\eta \leq V^\star$ for all $\eta \notin \{\square, \boxplus\}$ and therefore settles Theorem 3.4.

Section 3.5.3 describes an *energy reduction algorithm* to find ω. Roughly, the idea is that if η contains only "subcritical clusters", then these clusters can be removed one by one to reach $\square$, while if η contains some "supercritical cluster", then this cluster can be taken as a stepping stone to construct a path to $\boxplus$ that goes via a sequence of increasing rectangles. In particular, the supercritical cluster is first extended to a 2–tiled rectangle touching the north-boundary of Λ, after that it is extended to a 2–tiled rectangle touching the west-boundary and the east-boundary of Λ, and finally it is extended to $\boxplus$.

To carry out this task, six *energy reduction mechanisms* are needed, which are introduced and explained in Section 3.5.2:

- Moving unit holes inside 2–tiled clusters (Section 3.5.2).
- Adding and removing 12–bars from lattice-connecting rectangles (Section 3.5.2).
- Changing bridges into 12–bars (Section 3.5.2).
- Maximally expanding 2–tiled rectangles (Section 3.5.2).
- Merging adjacent 2–tiled rectangles (Section 3.5.2).
- Removing subcritical clusters (Section 3.5.2).

Each of Sections 3.5.2–3.5.2 states a definition and a lemma, and uses these to prove a proposition about the relevant energy reduction mechanism. The six propositions thus obtained will be crucial for the energy reduction algorithm in Section 3.5.3.

In Section 3.5.1 we begin by defining beams and pillars, which are needed throughout Section 3.5.2.

3.5.1 Beams and pillars

Lemma 3.14 *Let η be a configuration containing a tile t that has at least three junction sites occupied by a particle of type* 1*. Then the configuration η' obtained from η by turning t into a 2–tile satisfies $H(\eta') \leq H(\eta)$.*

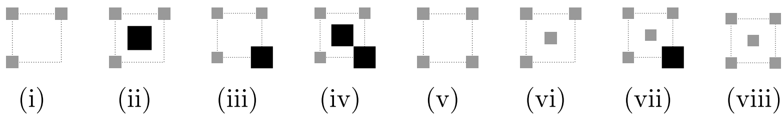


Figure 3.13: Possible tiles with at least three junction sites occupied by a particle of type 1.

Proof. Without loss of generality we may assume that $\eta(t_a) = \eta(t_b) = \eta(t_d) = 1$, and that η' is the configuration in Fig. 3.6(d), i.e., $\eta'(t_a) = \eta'(t_b) = \eta'(t_c) = \eta'(t_d) = 1$, $\eta'(t_e) = 2$. The following eight cases are possible (see Fig. 3.13 and recall (3.13)):

(i) $(\eta(t_c), \eta(t_e)) = (0, 0)$. One particle of type 1 and one particle of type 2 are added, and at least four new bonds are activated: $\Delta H \leq \Delta_1 + \Delta_2 - 4U < 0$.

(ii) $(\eta(t_c), \eta(t_e)) = (0, 2)$. One particle of type 1 is added, and one new bond is activated: $\Delta H = \Delta_1 - U < 0$.

(iii) $(\eta(t_c), \eta(t_e)) = (2, 0)$. One particle of type 2 is moved to another site without deactivating any bonds, after which case (ii) applies.

(iv) $(\eta(t_c), \eta(t_e)) = (2, 2)$. One particle of type 2 with at most three active bonds is replaced by one particle of type 1 with at least one active bond: $\Delta H \leq \Delta_1 - \Delta_2 + 2U < 0$.

(v) $(\eta(t_c), \eta(t_e)) = (1, 0)$. One particle of type 2 is added, and four new bonds are activated: $\Delta H = \Delta_2 - 4U < 0$.

(vi) $(\eta(t_c), \eta(t_e)) = (0, 1)$. One particle of type 1 is moved to another site without deactivating any active bond, one particle of type 2 is added, and at least four new bonds are activated: $\Delta H \leq \Delta_2 - 4U < 0$.

(vii) $(\eta(t_c), \eta(t_e)) = (2, 1)$. Two particles are exchanged without deactivating any bonds: $\Delta H \leq 0$.

(viii) $(\eta(t_c), \eta(t_e)) = (1, 1)$. One particle of type 1 is replaced by a particle of type 2, and four new bonds are activated: $\Delta H = \Delta_2 - \Delta_1 - 4U < 0$.

★

Definition 3.15 *A beam of length ℓ is a row (or column) of $\ell+1$ particles of type 1 at dual distance 1 of each other. A pillar is a particle of type 1 at dual distance 1 of the beam not located at one of the two ends of the beam. The particle in the beam sitting next to the pillar divides the beam into two sections. The lengths of these two sections are ≥ 0 and sum up to ℓ. The support of a pillared beam is the union of all the tile supports. The support consists of three rows (or columns) of sites – an upper, middle and lower row (or column) – which are referred to as roof, center and basement (*see Fig. 3.14*).*

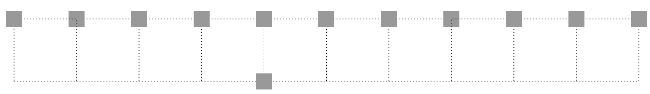


Figure 3.14: A south-pillared horizontal beam of length 10 with a west-section of length 4 and an east-section of length 6.

Note that a beam can have more than one pillar. Lemma 3.14 implies the following.

Corollary 3.16 *Let η be a configuration containing a pillared beam $\tilde{b}$ such that supp$(\tilde{b})$ is not 2–tiled. Then the configuration η' obtained from η by 2–tiling supp$(\tilde{b})$ satisfies $H(\eta') \leq H(\eta)$.*

3.5.2 Six energy reduction mechanisms

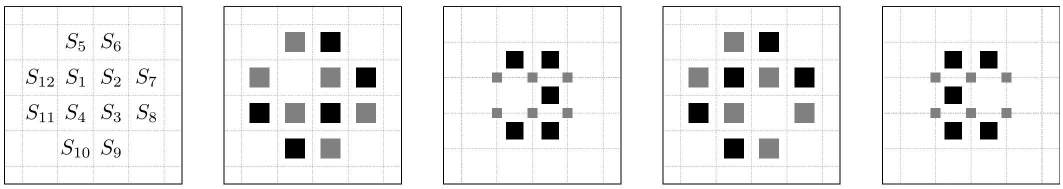
Moving unit holes inside 2–tiled clusters

In this section we show how a unit hole can move inside a 2–tiled cluster. In particular, we show that such motion is possible within an energy barrier $6U$ by changing the configuration only locally.

Definition 3.17 *A set of sites S inside Λ obtained from a 4×4 square after removing the four corner sites is called a slot.*

Given a slot S, we assign a label to each of the 12 sites in S as in Fig. 3.15 (a): first clockwise in the center of S and then clockwise on the boundary of S. We call the pairs (S_1, S_3) and (S_2, S_4) slot-conjugate sites.

Lemma 3.18 *Let S be a slot, and let η_0 be any configuration such that all particles in S have the same parity. Without loss of generality this parity may be taken to be even, so that $\eta(S_1) = 0$ and $\eta(S_3) = 2$. Let η_1 be the configuration obtained from η by interchanging the states of S_1 and S_3. Then $H(\eta_0) = H(\eta_1)$, and there exists a path $\omega\colon \eta_0 \to \eta_1$ that never exceeds the energy level $H(\eta_0) + 6U$.*



(a) (b) (c) (d) (e)

Figure 3.15: (a) labelling of the sites in the slot (standard representation); (b) example of η_0 in the slot (standard representation); (c) example of η_0 in the slot (dual representation). (d) η_1 in the slot (standard representation); (e) of η_1 in the slot (dual representation).

Proof. Without loss of generality we take η_0 as in Fig. 3.15(b–c). Let $a \to b$ denote the motion of a particle from site a to site b. For the path ω we choose the following sequence of moves: $S_4 \to S_1$; $S_3 \to S_4$; $S_2 \to S_3$; $S_1 \to S_2$; $S_4 \to S_1$; $S_3 \to S_4$. The first three moves and the second three moves each are a rotation by $\frac{\pi}{2}$ of the subconfiguration at the sites S_1, S_2, S_3, S_4. Note that all configurations in ω have the same number of particles of each type and hence the changes in energy only depend on the change in the number of active bonds. Let M_{RF} be the loss of the number of active bonds between the rotating particles and the fixed particles, and M_R the loss of the number of active bonds between the rotating particles.

We must show that $M_{RF} + M_R \leq 6$ during the six moves. To that end, we first observe that $M_{RF} \leq 6$, since the total number of active bonds between the rotating particles and the fixed particles is at most 6 (see Fig. 3.15(b)), and that $M_{RF} = 6$ only after the first three moves are completed, i.e., when the configuration is such that all the rotating particles have a different parity with respect to the parity they had in configuration η_0 (recall that particles with different parity cannot share a bond). Next we observe that, by the choice of ω, the value of M_R can only be 0 or 1, and that $M_R = 0$ after the first three moves are completed. ★

Lemma 3.18 implies the following.

Proposition 3.19 *Let η be a 2–tiled configuration with a unit hole. Then the configuration η' obtained from η by moving the unit hole elsewhere satisfies $H(\eta') = H(\eta)$ and $\Phi(\eta, \eta') \leq H(\eta) + 6U$.*

A possible $6U$-path for a unit hole inside a 2–tiled cluster is given in Fig. 3.16. This path is obtained through an iteration of local moves as explained in Fig. 3.15.

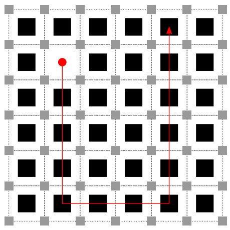


Figure 3.16: Motion of a unit hole inside a 2–tiled cluster.

Adding and removing 12–bars from lattice-connecting rectangles

Lemma 3.20 *Let η be a configuration consisting of a single 2–tiled lattice-connecting rectangle. Then the configuration η' obtained from η by, respectively,*

1. *adding a 12–bar of length $\ell \geq \ell^\star$,*
2. *adding a 12–bar of length $\ell < \ell^\star$,*
3. *removing a 12–bar of length $\ell \geq \ell^\star$,*
4. *removing a 12–bar of length $\ell < \ell^\star$,*

satisfies, respectively,

1. *$H(\eta') < H(\eta)$ and $\Phi(\eta, \eta') \leq H(\eta) + 2\Delta_1 + 2\Delta_2 - 4U$,*
2. *$H(\eta') > H(\eta)$ and $\Phi(\eta, \eta') \leq H(\eta) + 2\Delta_1 + 2\Delta_2 - 4U$,*

3. $H(\eta') > H(\eta)$ *and* $\Phi(\eta,\eta') \leq H(\eta) + (\ell-2)\varepsilon + 4U - \Delta_1$,

4. $H(\eta') < H(\eta)$ *and* $\Phi(\eta,\eta') \leq H(\eta) + (\ell-2)\varepsilon + 4U - \Delta_1$.

Proof. Recall the computations in Sections 3.3.1 and 3.4.1.

Adding a 12–bar. Adding a 12–bar of length ℓ on a lattice-connecting side of a 2–tiled rectangle (i.e., a side such that all the particles of type 1 on that side are lattice-connecting) can be done in two steps: (i) initiate the 12–bar by adding a 2–tiled protuberance (see Fig. 3.17); (ii) complete the 12–bar by adding a 2–tile (in a "corner") $\ell-1$ times (see Fig. 3.18). This can be achieved within energy barrier $\Delta H = 2\Delta_1 + 2\Delta_2 - 4U$ by following the same moves as the reference path $\omega^\star$ described in Section 3.4.1. The energy difference due to the extra 12–bar of length ℓ is $\Delta H(\ell) = \Delta_1 - \ell\varepsilon$, which changes sign at $\ell = \ell^\star$.

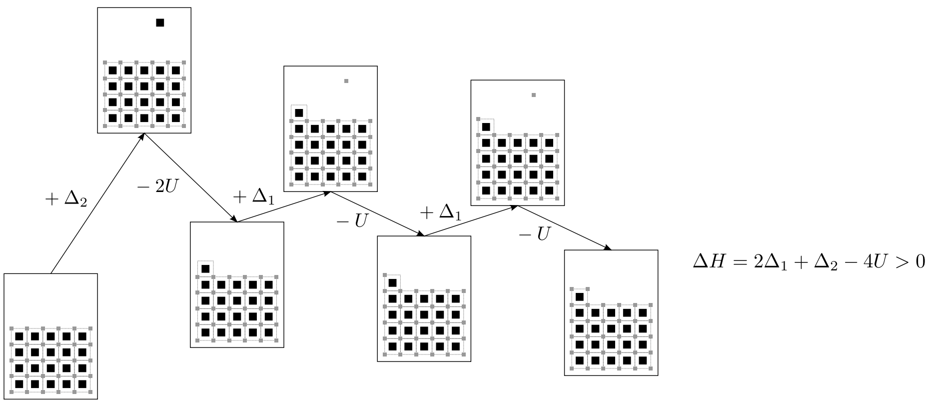


Figure 3.17: A 2–tiled protuberance is added to a side of a dual rectangle within energy barrier Δ_2.

Removing a 12–bar. Removing a 12–bar of length ℓ from a lattice-connecting rectangle can be done by following the reverse of the path used to add a 12–bar: (i) remove $\ell-1$ times a 2–tile from a bar; (ii) remove the last 2–tiled protuberance. This can be achieved within energy barrier $\Delta H(\ell) = (\ell-2)\varepsilon + 4U - \Delta_1$. If the cluster consists of one 12–bar only, then the path just described leaves $\ell+1$ free particles of type 1 inside Λ, which can be removed (free of energy cost) afterwards. ★

We use Lemma 3.20 to build a *northern rectangle* on top of a 12–bar as follows.

Definition 3.21 *Let b denote the vertical coordinate of the sites lying on the north-side of $\partial^-\Lambda^-$. For a given 2–tiled rectangle r in Λ^-, let b_r denote the vertical coordinate of the northern-most particles of type* 1*in r. Then r is said to be touching the north-side of $\partial^-\Lambda^-$ if $b_r = b$ or $b_r = b - \frac{1}{2}$.*

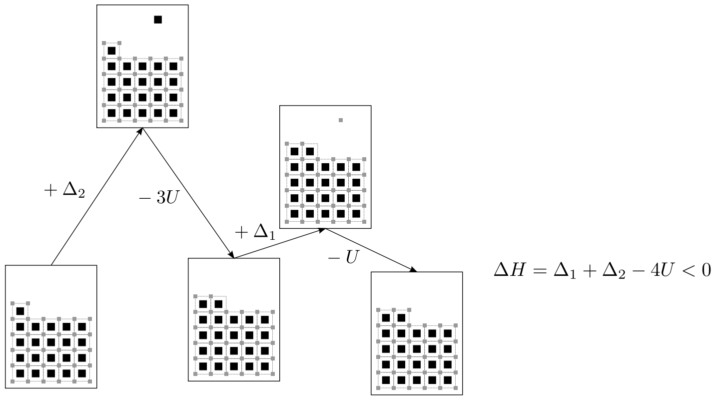


Figure 3.18: A 2–tile is added in a corner between 2–tiles within a energy barrier Δ_2.

In words, a 2–tiled rectangle is said to be touching the north-side of $\partial^-\Lambda^-$ if it is not possible to add a 12–bar on the north-side within Λ^-. Rectangles touching the south-, east- or west-side of Λ^- are defined similarly.

Let $\bar{b}$ be a horizontal 12–bar of length ℓ, i.e., a 2–tiled $\ell \times 1$ rectangle. Suppose that all sites above $\bar{b}$ are vacant. Then it is possible to successively add horizontal 12–bars, say m in total, on top of $\bar{b}$ until the north side of the rectangle grown in this way touches the north-side of Λ^-. The 2–tiled rectangle with $m+1$ rows and ℓ columns such that $\bar{b}$ is its lower-most horizontal 12–bar is denoted by $\sqcap\left(\bar{b}\right)$ and is called the northern rectangle of $\bar{b}$.

Lemma 3.20 implies the following.

Proposition 3.22 *Let η be a configuration containing a horizontal 12–bar $\bar{b}$ of length $\ell \geq \ell^\star$. Then the configuration η' obtained from η by building $\sqcap\left(\bar{b}\right)$ satisfies $H(\eta') < H(\eta)$ and $\Phi(\eta,\eta') \leq H(\eta) + 2\Delta_1 + 2\Delta_2 - 4U$.*

Changing bridges into 12–bars

Definition 3.23 *A (south-)bridge b consists of a beam $\tilde{b}$ and two (south-)pillars at the outer-most sites of the (south-)basement of $\tilde{b}$. The (south-)support of b coincides with the (south-)support of $\tilde{b}$. If each of the central sites of the tiles of the (south-)support of the bridge is occupied by a particle of type 2, then the bridge is said to be stable (see* Fig. 3.19*).*

Clearly, a 12–bar is a stable bridge. North-, east- and west-bridges are defined in a similar way.

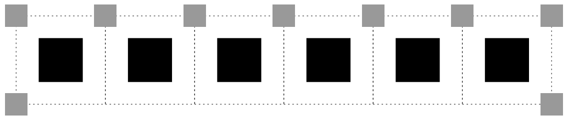


Figure 3.19: A stable bridge of length 6.

Given a bridge b, let $\bar{b}$ denote the 12–bar obtained by 2–tiling b. Lemma 3.14 implies the following.

Lemma 3.24 *Let η be a configuration containing a bridge b whose support is not 2–tiled. Then the configuration η' obtained from η by changing b to $\bar{b}$ satisfies $H(\eta') < H(\eta)$.*

Lemma 3.24 leads us to the following.

Proposition 3.25 *Let η be a configuration containing a (south-)bridge b whose (south-)support is not 2–tiled such that the particles of its beam are lattice-connecting. Then the configuration η' obtained from η by 2–tiling supp(b) satisfies $H(\eta') < H(\eta)$ and $\Phi(\eta, \eta') \leq H(\eta) + 4U + \Delta_1$.*

Proof. Let the (south-)bridge b have length ℓ. Label the $\ell + 1$ sites of its (south-)basement as $s_0, s_1, \ldots, s_\ell$, from the left to the right. In order to show that supp(b) can be 2–tiled within energy barrier $4U + \Delta_1$, it is enough to show that within the same energy barrier a particle of type 1 can be brought to a site of the basement of b (from the left) that is empty or is occupied by a particle of type 2. Without loss of generality s_1 may be assumed to be such a site. The configuration thus obtained has an energy that is at most the energy of the original configuration (see Lemma 3.14). The claim follows by noting that the particles of type 1 at the extremal sites s_1 and s_ℓ are the two pillars of a (south-)bridge of length $\ell - 1$ whose basement consists of the sites $s_1, s_2, \ldots, s_\ell$.

It remains to show how a particle of type 1 can be brought to site s_1. Label the site north-west of s_1 by v_1 , and the site north-east of v_1 by as v_2. Two cases need to be distinguished:

(1) If $\eta(s_1) = 0$, then, by the same argument as in the proof of Lemma 3.18, it is easy to show that the particle of type 1 at v_2 can be moved to s_1 (to obtain a configuration $\bar{\eta}$ with $H(\bar{\eta}) \leq H(\eta)$) without exceeding energy level $H(\eta) + 4U$. The configuration η' is reached within an energy barrier Δ_1 by bringing a particle of type 1 inside Λ and moving it to v_2.

(2) If $\eta(s_1) = 2$, then consider the following path. First detach ($\Delta H = 2U$) and remove ($\Delta H = -\Delta_1$) the particle of type 1 at v_2, and afterwards detach

($\Delta H = 2U$) and remove ($\Delta H = -\Delta_2$) the particle of type 2 at v_3. Next, move the particle of type 2 at site s_1 to site v_1 ($\Delta H \leq 0$; this particle has at most 2 active bonds when it sits at s_1), and finally bring a particle of type 1 ($\Delta H = \Delta_1$) to site v_2 ($\Delta H = -2U$). Call this configuration $\bar{\eta}$. Note that $H(\bar{\eta}) < H(\eta)$, since effectively a particle of type 2 with at most two active bonds has been removed, and $\Phi(\eta, \eta') = H(\eta) + 4U + \Delta_1$. Finally, observe that η' is the same configuration as η in Case (1). ★

Maximally expanding 2–tiled rectangles

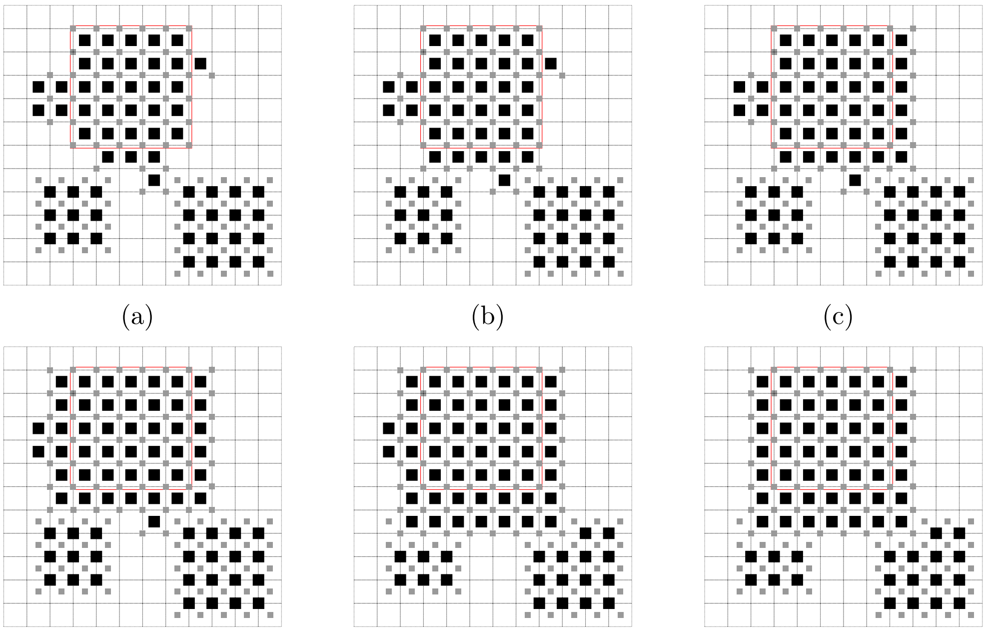
The mechanism presented in this section, which is called *north maximal expansion* of a 2–tiled rectangle, is such that it can be applied to a 2–tiled rectangle whose north-side is lattice-connecting (even though this condition is not restrictive). South, east and west maximal expansion of a 2–tiled cluster are analogous.

Definition 3.26 *The north maximal expansion comes in two phases: a growing phase and a smoothing phase.*
(i) The growing phase consists of the following three steps repeated cyclically:

1. *If the particles of type* 1 *on the south-side of the rectangle, either at the beginning or obtained after step 3, constitute a south-pillared beam* $\tilde{b}_s$*, then change* $supp(\tilde{b}_s)$ *into a* 12*–bar.*
2. *If the particles of type* 1 *on the east-side of the rectangle, obtained after step 1, constitute an east-pillared beam* $\tilde{b}_e$*, then change* $supp(\tilde{b}_e)$ *into a* 12*–bar.*
3. *If the particles of type* 1 *on the west -side of the rectangle, obtained after step 2, constitute a west-pillared beam* $\tilde{b}_w$*, then change* $supp(\tilde{b}_w)$ *into a* 12*–bar.*

The growing phase ends after three consecutive steps leave the configuration unchanged.
(ii) The smoothing phase consists of removing all the particles of type 2 *that are adjacent to the ones on the sides of the rectangle that is built during the growing phase. Note that these particles have at most two active bonds (otherwise it would be possible to identify another pillared beam), and therefore removal of these particles lowers the energy.*

The outcome of the north maximal expansion (see Fig. 3.20) of a 2–tiled rectangle is again a 2–tiled rectangle, containing the old rectangle and such that the northernmost 12–bar of the new rectangle has the same vertical coordinate.



(a) (b) (c)

(d) (e) (f)

Figure 3.20: Example of north maximal expansion of a 2–tiled rectangle. The outcome of the steps of the growing phase are represented in pictures (b–e), while the outcome of the smoothing phase is represented in picture (f).

Given a 2–tiled rectangle r, let $\mathcal{R}^{\top}(r)$ denote the north maximal expansion of r. Corollary 3.16 implies the following.

Lemma 3.27 *Let η be a configuration containing a 2–tiled rectangle. Then the configuration η' obtained from η via (north) maximal expansion of this 2–tiled rectangle satisfies then $H(\eta') \leq H(\eta)$.*

Lemma 3.27 leads us to the following.

Proposition 3.28 *Let η be a configuration containing a 2–tiled rectangle r whose north-side is lattice-connecting. Then the configuration η' obtained from η after replacing r by $\mathcal{R}^{\top}(r)$ satisfies $H(\eta') \leq H(\eta)$ and $\Phi(\eta, \eta') \leq H(\eta) + 10U - \Delta_1$.*

Proof. If $\mathcal{R}^{\top}(r) = r$, then there is nothing to prove. Therefore suppose that r is such that one its sides is a pillared beam. Without loss of generality we may assume that the south-side of r is a beam $\tilde{b}$ with a south-pillar. We must show that the south-support of $\tilde{b}$ can be turned into a 12–bar within energy barrier $10U - \Delta_1$.

Since $\text{supp}(\tilde{b})$ is not a 12–bar, a pillar can be chosen in such a way that at least one of the 2–tiles of the support the pillar belongs to (i.e., the first tile of each section of the support, counting from the pillar) is not a 2–tile. Without loss of generality we let this tile be the first tile of the right-section and call it t. Let v denote the tile adjacent to the right site of v. In the following, the term *superficial* refers to tiles that are in the top tile-bar of the rectangle. In analogy with the proof of Lemma 3.14, several cases need to be considered (we stick to the order in Fig. 3.13).

(i) $(\eta(t_c), \eta(t_e)) = (0, 0)$. A particle of type 2 has to be brought to site t_e and a particle of type 1 to site t_c. First bring a particle of type 2 to site t_e, to reach a configuration $\hat{\eta}$, and then proceed as in Case (ii). As we will see in Case (ii), since $H(\hat{\eta}) = H(\eta) - 3U + \Delta_2$, the second part of the path can be completed without exceeding energy level $H(\eta) + 6U + \Delta_2$. To reach configuration $\hat{\eta}$, move the particle of type 2 of the 2–tile above t to site t_e to reach a configuration called η'. This can be done without exceeding energy level $H(\eta) + 6U$. Note that $H(\eta') = H(\eta) + U$. The unit hole that has been created at the central site of the tile above t has to be filled. This can be done (see Lemma 3.18) by first moving the unit hole until it becomes superficial (configuration $\tilde{\eta}$ with energy $H(\tilde{\eta}) = H(\eta')$) without exceeding energy level $H(\eta') + 6U$, and then filling this unit hole with a particle of type 2 within energy level $H(\eta') + U - \Delta_1 + \Delta_2 = H(\eta) + 2U - \Delta_1 + \Delta_2$. Thus, η' can be reached without exceeding energy barrier $6U + \Delta_2$.

(ii) $(\eta(t_c), \eta(t_e)) = (0, 2)$. A particle of type 1 has to be brought to site t_c. Depending on the state of site v_e, there are three cases.

a) Site v_e is occupied by a particle of type 2. Move the particle of type 1 at site t_b to site t_c, to reach a configuration η' with energy $H(\eta') \leq H(\eta)+2U$ within an energy barrier of $6U$. The vacancy at site t_b can be moved (again by Lemma 3.18) to the north-side of the rectangle within energy barrier $6U$, to reach a configuration $\hat{\eta}$ with $H(\hat{\eta}) \leq H(\eta)$, and then filled with an extra particle of type 1. Thus, η' can be reached without exceeding energy level $H(\eta) + 8U$.

b) Site v_e is empty. Move the particle of type 1 at site t_b to site v_e ($\Delta H \leq 3U$), and then to site t_d ($\Delta H = 0$). Call this configuration η', and note that $H(\eta') \leq H(\eta) + 2U$. Arguing as above, we see that the vacancy at site t_b can be filled without exceeding the energy level $H(\eta) + 9U$.

c) Site v_e is occupied by a particle of type 1. Observe that the particle of type 1 at t_b has $k \leq 3$ active bonds and the particle of type 2 at v_e has $m \leq 2$ active bonds. It is possible to move the particle at site v_e to site t_c ($\Delta H = (m-k)U$), and then the particle at site t_b to site v_c ($\Delta H = (k-m)U$). The configuration η', reached within energy barrier $(k-m)U$, has energy $H(\eta') \leq H(\eta) + kU$. Again, the vacancy at site t_b has to be filled with a particle of type 1. This can be done without exceeding the energy level $H(\eta) + (6+k)U \leq H(\eta) + 9U$.

(iii) $(\eta(t_c), \eta(t_e)) = (2, 0)$. The particle of type 2 at site t_c is moved to site t_e without increasing the energy. Then argue as in Case (ii).

(iv) $(\eta(t_c), \eta(t_e)) = (2, 2)$. The particle of type 2 at site t_c has to be replaced by a particle of type 1. Remove the particle of type 2 at t_e. To do this, first create a superficial unit hole (which can be done within energy barrier $4U - \Delta_1$ by creating a hole in a corner tile of the rectangle) and move this vacancy to site t_e. By Lemma 3.18, this can be achieved without exceeding energy level $H(\eta_0) + 10U - \Delta_2$. Then move the particle of type 2 at site t_c to site t_e ($\Delta H \leq 0$). Call η' the configuration that is reached in this way. Note that $H(\eta') \leq H(\eta) - \Delta_2 + 3U$. To bring a particle of type 1 to site t_c, argue as in Case (ii), to arrive at $H(\hat{\eta}) \leq H(\eta) + 12U - \Delta_2$.

(v) $(\eta(t_c), \eta(t_e)) = (1, 0)$. A particle of type 2 has to be brought to site t_e. Move the unit hole at t_e to the top tile–bar of the rectangle. This does not change the energy of the configuration and can be done within energy barrier $6U$ by Proposition 3.19. The task reduces to filling a superficial unit hole on the surface of the cluster with a particle of type 2. This can be achieved within energy barrier $U + \Delta_2 - \Delta_1$. Therefore the maximal energy level reached in this case is $H(\eta) + 6U$.

(vi) $(\eta(t_c), \eta(t_e)) = (0, 1)$. Move the particle of type 2 from site t_e to site t_c. This move does not increase the energy of the configuration. Then proceed as in Case (v).

(vii) $(\eta(t_c), \eta(t_e)) = (2, 1)$. The occupation numbers of sites t_c and t_e have to be exchanged. To do this, first remove the particle of type 1 at site t_b to obtain a configuration η' with energy $H(\eta') \leq H(\eta) + 3U$ without exceeding the energy level $H(\eta) + 10U - \Delta_1$ (again use Lemma 3.18). Move the particle of type 1 from t_e to t_b ($\Delta H < 0$) and the particle of type 2 from t_c to t_e ($\Delta H = 0$). Call $\hat{\eta}$ the configuration that is reached in this way. Note that $H(\hat{\eta}) \leq H(\eta) + U - \Delta_1$. Proceed as in Case (ii) to conclude within energy barrier of $10U - \Delta_1$.

(viii) $(\eta(t_c), \eta(t_e)) = (1, 1)$. The particle of type 1 at site t_e has to be replaced by a particle of type 2. This can be done as follows. First the particle of type 1 sitting a site t_b is removed. To achieve this, first remove a particle of type 1 at the north-side of the rectangle and then (use Lemma 3.18) move the vacancy to site t_b. The configuration that is reached, which we call η', is such that $H(\eta') \leq H(\eta) + 3U - \Delta_1$. Next, move the particle of type 1 at t_e to site t_b ($\Delta H = 0$), to reach a configuration $\hat{\eta}$ whose energy is $H(\hat{\eta}) = H(\eta) - \Delta_1$. Finally, argue as in Case (v), to arrive at $H(\hat{\eta}) \leq H(\eta) + 3U - \Delta_1$.

Finally, note that (3.13) implies $\max\{6U + \Delta_2, 10U - \Delta_1, 12U - \Delta_2\} = 10U - \Delta_1$.

By Lemma 3.14, $H(\eta') \leq H(\eta)$, and therefore the same argument can be used to show that all the right-sections of the support can be 2–tiled within the same energy barrier. The left-section can be 2–tiled analogously.

To conclude, it remains to be shown how particles of type 2, possibly adjacent to one side of the rectangle, can be removed from Λ. Call t the tile associated with the particle p of type 2 that has to be removed (p sits at site t_e) and v the tile adjacent to t belonging to the rectangle. First bring a vacancy to site v_e within energy barrier $10U - \Delta_2$ (one way to achieve this has been described in Case (iv) above) and then move p to site v_e (see Lemma 3.18). ★

Merging adjacent 2–tiled rectangles

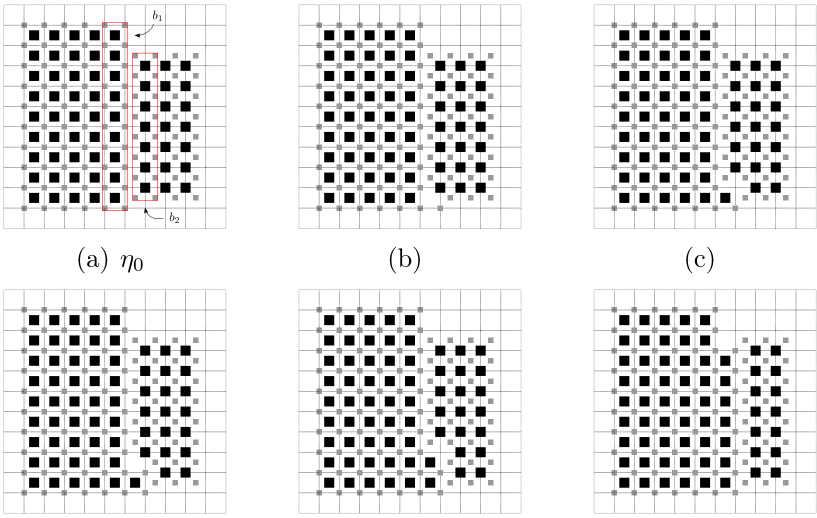
Definition 3.29 *A 12–bar b_1 of length ℓ of a cluster c_1 is said to be adjacent to a 12–bar b_2 of length $m \leq \ell$ of a cluster c_2 if there exist m mutually disjoint pairs (q_1^i, q_2^i) of particles of type 1 with $q_1^i \in b_1$ and $q_2^i \in b_2$ such that $u(q_1^i) - u(q_2^i) = v$ with $\|v\| = \frac{1}{2}\sqrt{2}$ for $i = 1, \ldots, m$. The vector v is called the offset of b_2 with respect to b_1. The tiles in b_1 have a different parity than the tiles in b_2. The* *particles* $q_1^i \in b_1$, $i = 1, \dots m$, *are called the external particles of* b_1 *with respect to* b_2, *and the particles* $q_2^i \in b_2$, $i = 1, \dots, m$, *are called the external particles of* b_2 *with respect to* b_1.

Proposition 3.30 *Let* η *be a configuration that contains two adjacent* 2*–tiled rectangles. Then the configuration* η' *obtained by "merging" these two rectangles satisfies* $H(\eta') = H(\eta)$ *and* $\Phi(\eta, \eta') \leq H(\eta) + 2U - \Delta_1$.

Proof. Given two adjacent bars b_1 and b_2 with offset $v = (v_1, v_2)$ in a configuration η, we want to define the sliding of b_2 onto b_1 along v. The resulting configuration η' is such that all the particles of type 2 originally in b_2 are slid by (v_1, v_2) with respect to their position in η, and all the external particles of type 1 of b_2 with respect to b_1 are slid by $(v_1, -v_2)$ when the two bars are horizontal and by$(-v_1, v_2)$ when the two bars are vertical. Via the sliding, the m 2–tiles in b_2 are turned into m 2–tiles with the same parity as the tiles in b_1. It is easy to see that $H(\eta') = H(\eta)$, since neither the total number of active bonds of the configuration nor the number of particles of each type is changed.

To describe the sliding of a bar onto another bar along a vector v, we may assume without loss of generality that the two bars are vertical and that the vector v is equal to $(-\frac{1}{2}, -\frac{1}{2})$ (Fig. 3.21(a)). Start by moving the lower-most external particle of type 1 in b_2 over the vector $v' = (\frac{1}{2}, -\frac{1}{2})$ (Fig. 3.21(b)). This leads to an increase by U in energy. Then move the lower-most particle of type 2 over the vector v (Fig. 3.21(c)). Since the number of deactivated bonds is equal to the number of new bonds activated, this move does not change the energy. Proceed by moving over the vector v' the second particle of type 1 from the bottom of the bar (Fig. 3.21(d)). This also is a move that does not change the energy. Afterwards, the second particle of type 2 from the top is moved over the vector v (Fig. 3.21(e)). This sequence of moves proceeds iteratively (without a change in energy) until the m-th particle of type 2 has been moved over the vector v. Finally, the $(m+1)$-st external particle of type 1 is moved over the vector v' (Fig. 3.21(f)). This move decreases the energy by U. Thus, U is the energy barrier that must be overcome in order to realize the sliding of a 12–bar onto another 12–bar over the vector v.

It is clear that, given a configuration η containing two 2–tiled rectangles c_1 (with vertical side length ℓ) and c_2 (with vertical side length $m \leq \ell$) with offset v, it is possible to reduce η to a configuration η' such that c_1 and c_2 are merged into of a single cluster by sliding one bar after another, without exceeding energy barrier $\Delta H = U$, provided the other clusters of η do not interfere with this procedure. Sliding the last bar of c_2 we get an excess of free particles of type 1, which can be removed from Λ, lowering the energy. In particular, the configuration η' obtained via the sliding of c_2 onto c_1 along v without exceeding energy level $H(\eta) + U$ has



(a) η_0 (b) (c)

(d) (e) (f) η_1

Figure 3.21: The sliding of b_2 onto b_1.

energy $H(\eta') = H(\eta) - (m+1)\Delta_1$, since the two configurations consist of the same number of 2–tiles, and η' contains $m+1$ particles of type 1 less than η. Moreover, $\Phi(\eta, \eta') = H(\eta) + U$.

In the argument above, the first move consisted of moving down-right a particle of type 1 of b_2 to an empty site (say, site i). If in configuration η site i is occupied by a particle of type 1, then the sliding of the vertical 12–bar can be realized by modifying the procedure as follows. First remove from the box the top-left particle of type 1 of b_2 sitting at site j to reach a configuration with energy $H(\eta) + U - \Delta_1$ (which can be done without exceeding energy level $H(\eta) + U$). Then move to j the particle of type 1 sitting at site $k = j + v = j + (-\frac{1}{2}, -\frac{1}{2})$ in η, which increases the energy up to level $H(\eta) + 2U - \Delta_1$. Then site k is filled with the particle of type 1 originally at site $k + (\frac{1}{2}, -\frac{1}{2})$ without an increase in energy. It is possible to continue in this way until the configuration obtained after the first step of the above case is reached. This configuration has energy $H(\eta) + U - \Delta_1$. Then proceed as in the above case until b_2 is slid onto b_1. This leads to a configuration with energy $H(\eta) - \Delta_1 < H(\eta)$. In order to perform the (modified) sliding procedure, it is sufficient to assume that the north-side of rectangle c_2 is lattice-connecting. ★

Removing subcritical clusters

The *cleaning mechanism* defined in this section produces a configuration for which we have a certain control on the geometry of the constituent clusters. In particular, these clusters will be suitable for the application of the previous five energy reduction mechanisms. We begin by looking at pending dimers (see Fig. 3.22).

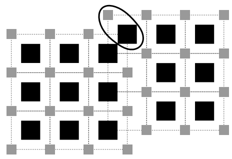


Figure 3.22: A pending dimer is the pair of particles circled in the picture.

Definition 3.31 *A pending dimer consists of two adjacent particles of different type such that the particle of type* 1 *is lattice-connecting and has only one active bond and the particle of type* 2 *has at most three active bonds.*

Proposition 3.32 *Let* η *be a configuration containing pending dimers. Then there exists a configuration* η' *not containing pending dimers that satisfies* $H(\eta') < H(\eta)$ *and* $\Phi(\eta, \eta') \leq H(\eta) + 3U + \Delta_2$.

Proof. If the particle of type 2 has at most two active bonds, then simply remove the pending dimer. This reduces the energy, since two bonds are deactivated and a particle of each type is removed from Λ ($\Delta H \leq 2U - \Delta_1 - \Delta_2 < 0$), and can be achieved within an energy barrier $2U - \Delta_1$ along the following path: first detach ($\Delta H = U$) and remove ($\Delta H = -\Delta_1$) the particle of type 1, then detach ($\Delta H \leq U$) and remove ($\Delta H = -\Delta_2$) the particle of type 2.

If the particle of type 2 has three active bonds we have two cases:

(i) The fourth neighbor of the particle of type 2 of the pending dimer is empty. In this case η' is obtained by filling this empty site with a particle of type 1 in order to obtain a 2–tile, which lowers the energy since $\Delta_1 < U$. To do this, temporarily remove the pending dimer as described above. This leads to a configuration $\tilde{\eta}$ with energy $H(\tilde{\eta}) = H(\eta) + 3U - \Delta_1 - \Delta_2$ reached within energy barrier $3U - \Delta_1$. Then bring a particle of type 1 to the designated site ($\Delta H \leq \Delta_1$) and finally put back the dimer. The whole path is realized within energy barrier $3U + \Delta_2$.

(ii) The fourth neighbor of the particle of type 2 is occupied by a particle of type 2. In this case η' is the configuration such that the dimer is removed and the site originally occupied by the particle of type 2 of the dimer is occupied by a particle of type 1. To obtain η' from η, remove the pending dimer (again, as above, within energy barrier $3U-\Delta_1$), to reach a configuration $\tilde{\eta}$ with energy $H(\tilde{\eta} = H(\eta) + 3U - \Delta_1 - \Delta_2$, and bring a particle of type 1 within energy barrier Δ_1. To conclude, observe that $H(\eta') = H(\eta) + 2U - \Delta_2 < H(\eta)$.

★

The cleaning mechanism works as follows:

1. Remove all the lattice-connecting free particles from the configuration.

After that repeat cyclically the following two steps:

2. Iteratively remove/transform all the lattice-connecting pending dimers.
3. Bring a particle of type 1 to any of the free sites adjacent to the lattice-connecting particles of type 2.

Repeat the cleaning mechanism until the configuration is not affected anymore. Each of the three steps can be performed within energy barrier $3U+\Delta_2$. Moreover, each step reduces the energy.

Lemma 3.33 *The outcome of the cleaning mechanism is either a configuration such that the first particle encountered while scanning Λ in the lexicographic order is a particle of type* 1 *belonging to a horizontal stable (south-)bridge, or the configuration* $\square$.

Proof. Call q the first particle of Λ in the lexicographic order. Recall that the dual coordinates of q are denoted by $u(q) = (u_1(q), u_2(q))$. Step 3 of the cleaning mechanism guarantees that q is a particle of type 1. The fact that q is the first particle in the lexicographic order implies that: (i) all the sites above $u(q)$ are empty; (ii) all the sites with the same vertical coordinate as q lying on the left of q are empty as well. As a consequence of (ii), all the sites on the left of q with vertical coordinate $u_2(q) - \frac{1}{2}$ are lattice-connecting and therefore cannot be occupied by a particle of type 2. Since q cannot be a free particle, the site with coordinates $(u_1(q) + \frac{1}{2}, u_2(q) - \frac{1}{2})$ must be occupied by a particle p of type 2. Let $s(p)$ be the longest sequence of tiles adjacent to $t(p)$ such that the central site is occupied by a particle of type 2. Obviously, p is the left-most particle of type 2 in $s(p)$. Call $\tilde{p}$ the last particle of type 2 in $s(p)$ and $\tilde{q}$ the particle of type 1 with coordinates $(u_1(p) + \frac{1}{2}, u_2(p) + \frac{1}{2})$. (Note that p and $\tilde{p}$ may coincide.) All the sites on the north-side of $s(p)$ are lattice-connecting and hence are occupied by a particle of type 1. To conclude, observe that both p and $\tilde{p}$ must be saturated, otherwise at least one of the pairs (q, p) and $(\tilde{q}, \tilde{p})$ constitutes a pending dimer. ★

3.5.3 Energy reduction of a general configuration

In this section we complete the proof of Theorem 3.4.

Fix any $\eta \notin \{\square, \boxplus\}$. In this section we will give a general procedure, called *energy reduction algorithm*, that allows us to construct a path $\omega\colon\ \eta \to \eta_r$ with $\eta_r \in \{\square, \boxplus\}$ such that $\max_{\xi\in\omega} H(\xi) \le H(\eta) + V^\star$ with $V^\star \le 10U - \Delta_1$ and $H(\eta_r) < H(\eta)$. Note that if $\eta_r = \boxplus$, then $H(\eta_r) < H(\eta)$ because $\mathcal{X}_{\mathrm{stab}} = \boxplus$. The construction uses the six energy reduction mechanisms described in Sections 3.5.2–3.5.2 and relies on Propositions 3.19, 3.22, 3.25, 3.28, 3.30, 3.32, which are the key results of these sections. The maximal energy barrier in these propositions is $10U - \Delta_1$. *Note*: The energy reduction mechanisms in Sections 3.5.2 and 3.5.2 concern single droplets far away from $\partial^-\Lambda$ and have an energy barrier not exceeding $4U + \Delta_1 < \Gamma^\star$ (see below (3.15)). For such configurations, the energy can be essentially reduced by saturating particles of type 2 and by adding and removing 12–bars. This explains the remark made in Section 3.1.4, item 4.

In the remainder of this section we call *supercritical* a 12–bar of length $\ge \ell^\star$. Similarly, we call *supercritical* a dual rectangle with both side lengths $\ge \ell^\star$.

Proof. As a preliminary step, perform the cleaning mechanism. If the outcome is $\square$, then the claim is proven. Otherwise, let b_1 be the first bridge encountered in the lexicographic order (which exists by Lemma 3.33). This bridge can be turned into an 12–bar $\bar{b}_1$ (see Section 3.5.2). If the length of b_1 is $< \ell^\star$, then the 12–bar $\bar{b}_1$ can be removed, which lowers the energy (see Section 3.5.2). In this case, go back to performing the cleaning mechanism. Without loss of generality we may therefore assume that the length of b_1 is $> \ell^\star$.

By construction, all sites above $\bar{b}_1$ are empty, and therefore it is possible first to construct the 2–tiled rectangle $r_1 = \sqcap\left(\bar{b}_1\right)$ within energy barrier $2\Delta_1 + 2\Delta_2 - 4U$ (again lowering the energy), and then expand r_1 to the rectangle $R_1 = \mathcal{R}^\top(r_1)$ (see Section 3.5.2). If the vertical side length of R_1 is $< \ell^\star$, then R_1 can be removed (lowering the energy), and it is possible to perform again the cleaning mechanism.

Therefore suppose that R_1 has both its side lengths $\ge \ell^\star$. In the remainder of the section we will show how to reach within energy barrier $10U - \Delta_1$ a configuration containing a rectangle R_{NW} touching both the north-side and the west-side of Λ^- whose support contains the support of R_1. Once this has been achieved, it is possible to argue for R_{NW} in the same way as for R_1 in order to reach a configuration containing a rectangle R_{NWE} touching the north-side, the east-side and the west-side of Λ^- whose support contains the support of R_{NW}. Repeating the same argument for R_{NWE}, it is possible to reach $\boxplus$.

The construction of R_{NW} is obtained by using an algorithm called *invasion* of R_1, which is constructed with the help of techniques similar to the ones that were used to build R_1.

(A) Invasion of R_1. See Fig. 3.23. Let (a_1, b_1) be, respectively, the horizontal and the vertical coordinate of the left lower-most particle of R_1 (which is of type 1). Define $\Lambda(R_1) \subset \Lambda$ to be the set consisting of the sites whose vertical coordinate is $\geq b_1$ and horizontal coordinate is $< a_1$. In words, $\Lambda(R_1)$ contains the sites of Λ on the left of R_1. Perform the cleaning mechanism (see Section 3.5.2) and scan $\Lambda(R_1)$ in the lexicographic order. Three cases are possible.

1. $\Lambda(R_1)$ is empty. Add, if possible (R_1 might already be touching the west-boundary of Λ^-), 12–bars onto the left side of R_1 until the resulting cluster touches the west-boundary of Λ^-.
2. The first horizontal bridge b_2 encountered in $\Lambda(R_1)$ has length $< \ell^\star$. Remove the particles of the (south)-support of the bridge, lowering the energy of the configuration, and restart the covering of $\Lambda(R_1)$.
3. The first horizontal bridge b_2 encountered in $\Lambda(R_1)$ has length $\geq \ell^\star$. As for b_1, first turn b_2 into the 12–bar $\bar{b}_2$, then build the 2–tiled rectangle $r_2 = \sqcap\left(\bar{b}_2\right)$, after that expand r_2 to $R_2 = \mathcal{R}^\top(r_2)$, and finally perform the cleaning mechanism. Note that the support of R_2 may cover (part or possibly all of) the support of R_1. This means that during the maximal expansion, some of the sites of $\mathrm{supp}(R_1)$ were in the support of the pillared beam that is going to be 2–tiled. Each time this happens, R_2 absorbs an entire vertical supercritical 12–bar of R_1 (see Section 3.5.2). Call $\tilde{R}_1$ what is left of R_1 after the maximal expansion of R_2. The following three cases are possible: (i) $\tilde{R}_1$ does not contain any particle ($\tilde{R}_1 = \emptyset$); (ii) $\tilde{R}_1 \prec R_1$ (in the proper sense); (iii) $\tilde{R}_1 = R_1$. In Case (ii), the rectangles R_2 and $\tilde{R}_1$ are necessarily adjacent (more precisely, the right-most 12–bar of R_2 is adjacent to the left-most 12–bar of R_1), whereas in Case (iii) the two rectangles may or may not be adjacent. Note that this implies that if $\tilde{R}_1 \prec R_1$, then R_2 is necessarily supercritical. Obviously, if $\tilde{R}_1 \neq \emptyset$, then it is again a 2–tiled rectangle, and there are several possibilities.
   (a) R_2 is not supercritical. This implies that $\tilde{R}_1 = R_1$. Remove R_2 from Λ, put $R_1 = \tilde{R}_1$ and restart the invasion of R_1.
   (b) R_2 is supercritical and $\tilde{R}_1 = \emptyset$. Change the name of R_2 to R_1 and restart the covering of $\Lambda(R_1)$.
   (c) R_2 is supercritical and is adjacent to $\tilde{R}_1$. Note that both rectangles touch the north-side of Λ^-. Call $R^{\max}$ the rectangle with the largest vertical length (in case of a tie, without loss of generality choose R_1) and call $R^{\min}$

the other rectangle. Slide $R^{\min}$ onto $R^{\max}$. This is possible because the smoothing phase of the maximal expansion (see Section 3.5.2) removes all the particles of type 2 that may interfere with the sliding of the 12–bars. Then perform again the maximal expansion of $R^{\max}$, i.e., the rectangle that has not been moved during the sliding. These steps bring the configuration to a rectangle whose support contains $\mathrm{supp}(R_2) \cup \mathrm{supp}(R_1) \cup \Lambda(R_1)$. Call this rectangle R_1 and restart the invasion of R_1.

(d) R_2 is supercritical and is not adjacent to $\tilde{R}_1$. This implies $\tilde{R}_1 = R_1$. Start the invasion of R_2 (see below).

In order to complete the proof, it remains to show how the invasion of R_2 carries over. To that end, we introduce the following *recursive algorithm* realizing the *invasion of* R_i for $i = 2, 3, \ldots$, etc.

(B) Invasion of R_i. Call $\bar{R}_{i-1}$ what is left of R_{i-1} after the invasion of R_{i+1}. There are three cases:

I. $\bar{R}_{i-1} = \emptyset$ (i.e., the support of R_{i-1} is completely covered by R_i). Put $R_{i-1} = R_i$ and restart the invasion of R_{i-1}.

II. $\bar{R}_{i-1} \neq \emptyset$ and R_i and $\bar{R}_{i-1}$ are adjacent. Call $R^{\max}$ the rectangle with the largest vertical side between R_i and $\bar{R}_{i-1}$ (in case of a tie, without loss of generality choose $R^{\max} = R_i$) and call $R^{\min}$ the other rectangle. Slide $R^{\min}$ onto $R^{\max}$ and perform the maximal expansion of $R^{\max}$. Call R_{i-1} the outcome of the maximal expansion of $R^{\max}$ and restart the invasion of R_{i-1}.

III. $\bar{R}_{i-1} \neq \emptyset$ and R_i and $\bar{R}_{i-1}$ are not adjacent. If R_i is on the left of R_{i-1}, then let (a_i, b_i) denote, respectively, the horizontal and the vertical coordinate of the lower right-most particle (which is of type 1) of R_i, and call $\Lambda(R_i)$ the subset of $\Lambda(R_{i-1})$ consisting of those sites whose vertical coordinates are $\geq b_i$ and whose horizontal coordinates are $> a_i$. If R_i is on the right of R_{i-1}, then let (a_i, b_i) denote, respectively, the horizontal and the vertical coordinate of the lower left-most particle (which is of type 1) of R_i, and call $\Lambda(R_i)$ the subset of $\Lambda(R_{i-1})$ consisting of those sites whose vertical coordinates are $\geq b_i$ and whose horizontal coordinates are $< a_i$. In words, $\Lambda(R_i)$ consists of those sites of $\Lambda(R_{i-1})$ between R_{i-1} and R_i. Perform the cleaning mechanism and scan $\Lambda(R_i)$ in the lexicographic order. There are again several cases.

1. $\Lambda(R_i)$ is empty. Call $R^{\max}$ the rectangle with the largest vertical side between R_i and $\bar{R}_{i-1}$ (in case of tie, without loss of generality choose $R^{\max} = R_i$) and call $R^{\min}$ the other rectangle. Add vertical 12–bars on the side of $R^{\min}$ facing $R^{\max}$ until (depending on the parity of the rectangles) it becomes adjacent (different parity) to $R^{\max}$ or it is at distance 1

(same parity) from $R^{\max}$. In the first case, slide the extended $R^{\min}$ onto $R^{\max}$. Perform the maximal expansion of $R^{\max}$, and call R_{i-1} the rectangle obtained in this way, whose support contains $\text{supp}(R_i) \cup R_{i-1} \cup \Lambda(R_{i-1})$. Restart the invasion of R_{i-1}.

2. The first horizontal bridge b_{i+1} encountered in $\Lambda(R_i)$ has length $< \ell^\star$. Remove the particles of the (south)-support of the bridge, lowering the energy of the configuration, and restart the invasion of R_i.
3. The first horizontal bridge b_{i+1} encountered in $\Lambda(R_i)$ has length $\geq \ell^\star$. First turn b_{i+1} into the 12–bar $\bar{b}_{i+1}$, then build the 2–tiled rectangle $r_{i+1} = \sqcap\left(\bar{b}_{i+1}\right)$, after that expand r_i to $R_{i+1} = \mathcal{R}^\top(r_{i+1})$, and finally perform the cleaning mechanism. Call $\tilde{R}_i$ what is left of R_i after the maximal expansion of R_{i+1}. The following cases are possible.
   (a) R_{i+1} is not supercritical. This implies $\tilde{R}_i = R_i$. Remove R_{i+1} from Λ, put $R_i = \tilde{R}_i$, and restart the invasion of R_i.
   (b) R_{i+1} is supercritical and $\tilde{R}_i = \emptyset$. Change the name of R_{i+1} to R_i, and restart the invasion of R_i.
   (c) R_{i+1} is supercritical and is adjacent to $\tilde{R}_i$. Note that both rectangles touch the north-side of Λ^-. Slide the rectangle with the shorter vertical length onto the other rectangle and perform again the maximal expansion of the rectangle that has not been moved during the sliding. These steps bring the configuration to a rectangle whose support contains $\text{supp}(R_{i+1}) \cup \text{supp}(R_i) \cup \Lambda(R_i)$. Call this rectangle R_i and restart the invasion of R_i.
   (d) R_{i+1} is supercritical and is not adjacent to $\tilde{R}_i$. This implies $\tilde{R}_i = R_i$. Start the invasion of R_{i+1}.

The finiteness of Λ ensures that the algorithm eventually terminates. ★

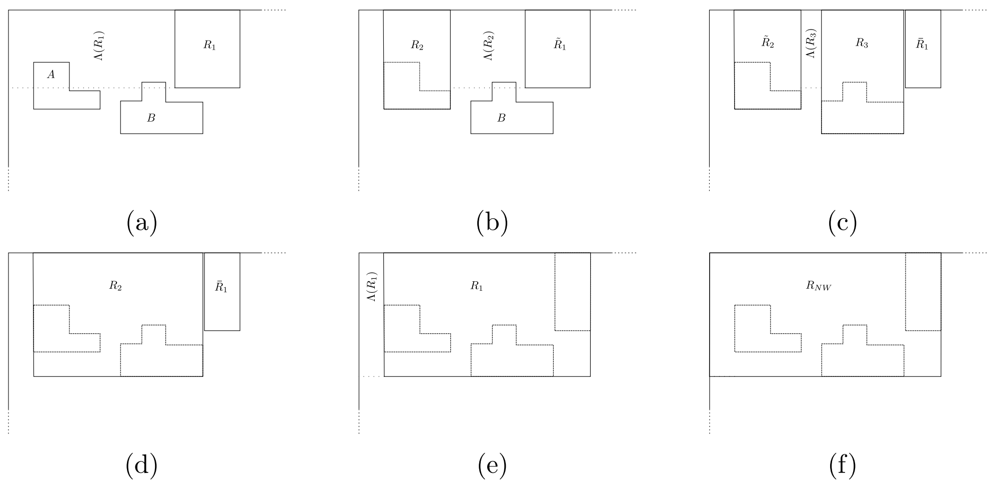


Figure 3.23: Example of invasion of the dual rectangle R_1. Only the support of the relevant clusters are drawn and the parity of different clusters is not indicated. The set $\Lambda(R_1)$ contains a supercritical bridge belonging to cluster A (Fig. 3.23(a)). Growing this bridge via the construction of its northern rectangle and its subsequent maximal expansion leads to the supercritical rectangle R_2 (Fig. 3.23(b)). Next, the invasion of $\Lambda(R_2)$ has to be performed in order to complete the invasion of R_1. The set $\Lambda(R_2)$ contains a supercritical bridge belonging to cluster B, which is grown into the supercritical rectangle R_3 (Fig. 3.23(c)). Note that R_3 partly covers the support of $\tilde{R}_1$ and that R_3 and $\bar{R}_1$ are adjacent. The invasion of R_2 proceeds via the invasion of R_3. Since $\Lambda(R_3)$ is empty, the invasion of R_3 is carried out by adding 12–bars to the left-side of R_3 until $\tilde{R}_2$ is at dual distance 1. After that a maximal expansion produces a dual rectangle that covers the support of $\tilde{R}_2$ (Fig. 3.23(d)). The new dual rectangle R_2 is adjacent to $\bar{R}_1$. The two rectangles are merged and a maximal expansion gives a new rectangle R_1 (Fig.3.23(e)). Now $\Lambda(R_1)$ is empty and can be filled by adding 12–bars to the left-side of R_1 until the rectangle R_{NW} is obtained (Fig. 3.23(f)).

4 Critical configurations

This chapter is based on:
F. den Hollander, F. R. Nardi, A. Troiani, *Kawasaki dynamics with two types of particles: critical droplets*, Submitted to Journal of Statistical Physics.

4.1 Overview and main results

Section 4.1.1 defines the model, Section 4.1.2 introduces basic notation and key definitions, Section 4.1.3 states the main theorems, while Section 4.1.4 discusses these theorems.

4.1.1 Lattice gas subject to Kawasaki dynamics

Let $\Lambda \subset \mathbb{Z}^2$ be a large box centered at the origin (later it will be convenient to choose Λ rhombus-shaped). Let $|\cdot|$ denote the Euclidean norm, let

$$\begin{aligned} \partial^-\Lambda &= \{x \in \Lambda\colon\ \exists\, y \notin \Lambda\colon\ |y-x| = 1\}, \\ \partial^+\Lambda &= \{x \notin \Lambda\colon\ \exists\, y \in \Lambda\colon\ |y-x| = 1\}, \end{aligned} \tag{4.1}$$

be the internal, respectively, 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, respectively. 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

$$H = -U \sum_{(x,y)\in\Lambda^{*,-}} 1_{\{\eta(x)\eta(y)=2\}} + \Delta_1 \sum_{x\in\Lambda} 1_{\{\eta(x)=1\}} + \Delta_2 \sum_{x\in\Lambda} 1_{\{\eta(x)=2\}}, \tag{4.2}$$

where $\Lambda^{*,-} = \{(x,y)\colon\ x,y \in \Lambda^-,\ |x-y| = 1;\ |x-z| > 2,\ |y-z| > 2\ \forall\, z \in \partial^-\Lambda\}$ is the set of non-oriented bonds in Λ at distance at least 3 from $\partial^-\Lambda$, $-U < 0$ is the *binding energy* between neighboring particles of *different* types in Λ^-, and $\Delta_1 > 0$

and $\Delta_2 > 0$ are the *activation energies* of particles of type 1, respectively, 2 in Λ. Without loss of generality we will assume that

$$\Delta_1 \leq \Delta_2. \tag{4.3}$$

The Gibbs measure associated with H is

$$\mu_\beta(\eta) = \frac{1}{Z_\beta}\, e^{-\beta H(\eta)}, \qquad \eta \in \mathcal{X}, \tag{4.4}$$

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

$$c_\beta(\eta,\eta') = \begin{cases} e^{-\beta[H(\eta')-H(\eta)]_+}, & \eta,\eta' \in \mathcal{X},\ \eta \neq \eta',\ \eta \leftrightarrow \eta', \\ 0, & \text{otherwise}, \end{cases} \tag{4.5}$$

where $\eta \leftrightarrow \eta'$ means that η' can be obtained from η by one of the following moves:

- interchanging 0 and 1 or 0 and 2 between two neighboring sites in Λ ("hopping of particles in Λ"),
- changing 0 to 1 or 0 to 2 in $\partial^-\Lambda$ ("creation of particles in $\partial^-\Lambda$"),
- changing 1 to 0 or 2 to 0 in $\partial^-\Lambda$ ("annihilation of particles in $\partial^-\Lambda$").

Note that this dynamics preserves particles in Λ^-, but allows particles to be created and annihilated in $\partial^-\Lambda$. Think of the latter as describing particles entering and exiting Λ along non-oriented bonds between $\partial^+\Lambda$ and $\partial^-\Lambda$ (the rates of these moves are associated with the bonds rather than with the sites). The pairs (η,η') with $\eta \leftrightarrow \eta'$ are called *communicating configurations*, the transitions between them are called *allowed moves*. Note that particles in $\partial^-\Lambda$ do not interact: the interaction only works in Λ^- (see (4.2)). Also note that the Gibbs measure is the reversible equilibrium of the Kawasaki dynamics:

$$\mu_\beta(\eta)c_\beta(\eta,\eta') = \mu_\beta(\eta')c_\beta(\eta',\eta) \qquad \forall\, \eta,\eta' \in \mathcal{X}. \tag{4.6}$$

The dynamics defined by (4.2) and (4.5) models the behavior in Λ of a lattice gas in $\mathbb{Z}^2$, consisting of two types of particles subject to random hopping, hard-core repulsion, and nearest-neigbor attraction between different types. We may think of

$\mathbb{Z}^2\backslash\Lambda$ as an *infinite reservoir* that keeps the particle densities fixed at $\rho_1 = e^{-\beta\Delta_1}$, respectively, $\rho_2 = e^{-\beta\Delta_2}$. In the above model this reservoir is replaced by an *open boundary* $\partial^-\Lambda$, where particles are created and annihilated at a rate that matches these densities. Thus, the dynamics is a *finite-state* Markov process, ergodic and reversible with respect to the Gibbs measure μ_β in (4.4).

Note that there is *no* binding energy between neighboring particles of the *same* type (including such an interaction would make the model much more complicated). Consequently, our dynamics has an "anti-ferromagnetic flavor", and does *not* reduce to Kawasaki dynamics with one type of particle when $\Delta_1 = \Delta_2$. Also note that our dynamics does not allow swaps between particles, i.e., interchanging 1 and 1, or 2 and 2, or 1 and 2, between two neighboring sites in Λ. (The first two swaps would not effect the dynamics, but the third would; for Kawasaki dynamics with one type of particle swaps have no effect.)

4.1.2 Basic notation and key definitions

To state our main theorems in Section 4.1.3, we need some notation.

Definition 4.1 (a) $\square$ *is the configuration where* Λ *is empty.*
(b) $\boxplus$ *is the set consisting of the two configurations where* Λ *is filled with the largest possible checkerboard droplet such that all particles of type* 2 *are surrounded by particles of type* 1.
(c) $\omega\colon \eta \to \eta'$ *is any (self-avoiding) path of allowed moves from* $\eta \in \mathcal{X}$ *to* $\eta' \in \mathcal{X}$.
(d) $\Phi(\eta, \eta')$ *is the communication height between* $\eta, \eta' \in \mathcal{X}$ *defined by*

$$\Phi(\eta, \eta') = \min_{\omega\colon\, \eta\to\eta'} \max_{\xi\in\omega} H(\xi), \tag{4.7}$$

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

$$\Phi(A, B) = \min_{\eta\in A, \eta'\in B} \Phi(\eta, \eta'). \tag{4.8}$$

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

$$\mathcal{S}(\eta, \eta') = \left\{ \zeta \in \mathcal{X}\colon\, \exists\, \omega\colon\, \eta \to \eta',\, \omega \ni \zeta\colon\, \max_{\xi\in\omega} H(\xi) = H(\zeta) = \Phi(\eta, \eta') \right\}. \tag{4.9}$$

A configuration $\zeta \in \mathcal{S}(\eta, \eta')$ *is called a saddle for* (η, η').
(f) V_η *is the stability level of* $\eta \in \mathcal{X}$ *defined by*

$$V_\eta = \Phi(\eta, \mathcal{I}_\eta) - H(\eta), \tag{4.10}$$

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

Definition 4.2 (a) $(\eta \to \eta')_{\mathrm{opt}}$ *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* $\omega \in (\eta \to \eta')_{\mathrm{opt}}$.
(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* $\omega' \in (\eta \to \eta')_{\mathrm{opt}}$ *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* $(\eta \to \eta')_{\mathrm{opt}}$. *The configurations in* $\mathcal{S}(\eta, \eta')\backslash\mathcal{G}(\eta, \eta')$ *are called dead-ends.*
(e) *Let* $S(\omega) = \{\arg\max_{\xi\in\omega} H(\xi)\}$. *A saddle* $\zeta \in \mathcal{S}(\eta, \eta')$ *is called unessential if, for all* $\omega \in (\eta \to \eta')_{\mathrm{opt}}$ *such that* $\omega \ni \zeta$ *the following holds:* $S(\omega)\backslash\{\zeta\} \neq \emptyset$ *and there exists an* $\omega' \in (\eta \to \eta')_{\mathrm{opt}}$ *such that* $S(\omega') \subseteq S(\omega)\backslash\{\zeta\}$.
(f) *A saddle* $\zeta \in \mathcal{S}(\eta, \eta')$ *is called essential if it is not unessential, i.e., if either of the following occurs:*

(f1) *There exists an* $\omega \in (\eta \to \eta')_{\mathrm{opt}}$ *such that* $S(\omega) = \{\zeta\}$.
(f2) *There exists an* $\omega \in (\eta \to \eta')_{\mathrm{opt}}$ *such that* $S(\omega) \supseteq \{\zeta\}$ *and* $S(\omega') \nsubseteq S(\omega)\backslash\{\zeta\}$ *for all* $\omega' \in (\eta \to \eta')_{\mathrm{opt}}$.

Lemma 4.3 [Manzo, Nardi, Olivieri and Scoppola [MNOS04], Theorem 5.1]
A saddle $\zeta \in \mathcal{S}(\eta, \eta')$ *is essential if and only if* $\zeta \in \mathcal{G}(\eta, \eta')$.

In Chapter 2 we were interested in the transition of the Kawasaki dynamics from $\square$ to $\boxplus$ in the limit as $\beta \to \infty$. This transition, which is viewed as a crossover from a "gas phase" to a "liquid phase", is triggered by the appearance of a *critical droplet* somewhere in Λ. The critical droplets form a subset $\mathcal{C}^\star$ of the essential gate $\mathcal{G}(\square, \boxplus)$, and all have energy $\Gamma^\star$ (because $H(\square) = 0$).

In Chapter 2 we showed that the first entrance distribution on the set of critical droplets is uniform, computed the expected transition time up to and including a multiplicative factor of order one, and proved that the nucleation time divided by its expectation is exponentially distributed, all in the limit as $\beta \to \infty$. These results, which are typical for metastable behavior, were proved under *three hypotheses*:

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

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

(H3) See (H3-a,b,c) and Fig. 4.1 below.

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

Definition 4.4 (a) $\mathcal{C}^\star_{\text{bd}}$ *is the minimal set of configurations in* $\mathcal{G}(\square, \boxplus)$ *such that all paths in* $(\square \to \boxplus)_{\text{opt}}$ *enter* $\mathcal{G}(\square, \boxplus)$ *through* $\mathcal{C}^\star_{\text{bd}}$.
(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 $\eta \in \mathcal{C}^\star_{\text{bd}}$ consists of a single droplet $\hat{\eta} \in \mathcal{P}$ and one *additional free particle* of type 2 somewhere in $\partial^-\Lambda$.

Definition 4.5 (a) $\mathcal{C}^\star_{\text{att}}$ *is the set of configurations obtained from* $\mathcal{C}^\star_{\text{bd}}$ *by moving the free particle of type* 2 *along a path of empty sites in* Λ *and attaching it to the single droplet (i.e., creating at least one additional active bond). This set decomposes as* $\mathcal{C}^\star_{\text{att}} = \cup_{\hat{\eta}\in\mathcal{P}}\mathcal{C}^\star_{\text{att}}(\hat{\eta})$.
(b) $\mathcal{C}^\star$ *is the set of configurations obtained from* $\mathcal{C}^\star_{\text{bd}}$ *by moving the free particle of type* 2 *along a path of empty sites in* Λ. *This set decomposes as* $\mathcal{C}^\star = \cup_{\hat{\eta}\in\mathcal{P}}\mathcal{C}^\star(\hat{\eta})$.

Note that $\Gamma^\star = H(\mathcal{C}^\star) = H(\mathcal{P}) + \Delta_2$, and that $\mathcal{C}^\star$ consists of precisely those configurations "interpolating" between $\mathcal{P}$ and $\mathcal{C}^\star_{\text{att}}$: a free particle of type 2 enters $\partial^-\Lambda$ and moves to the single droplet where it attaches itself via an active bond, i.e., a bond between particles of type 1 and 2. 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 4.5; see also Chapter 2, Section 2.3.4). The sets $\mathcal{P}$ and $\mathcal{C}^\star$ are referred to as the *protocritical droplets*, respectively, the *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 $\omega \in (\mathcal{C}^\star_{\text{bd}} \to \boxplus)_{\text{opt}}$ pass through $\mathcal{C}^\star_{\text{att}}$. For every $\hat{\eta} \in \mathcal{P}$ there exists a $\zeta \in \mathcal{C}^\star_{\text{att}}(\hat{\eta})$ such that $\Phi(\zeta, \boxplus) < \Gamma^\star$.

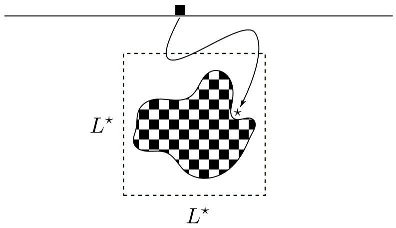


Figure 4.1: A qualitative representation of a configuration in $\mathcal{C}^\star_{\mathrm{bd}}$. If the free particle of type 2 reaches the site marked as $\star$, then the dynamics has entered the "basin of attraction" $\boxplus$.

As shown in Chapter 2, (H1–H3) constitute the *geometric input* needed to derive the metastability theorems in Chapter 2 with the help of the *potential-theoretic approach* to metastability outlined in Bovier [Bov09]. In Chapter 3 we proved (H1–H2) and identified the energy $\Gamma^\star$ of critical droplets. In this Chapter (H3), identify the set $\mathcal{C}^\star$ of critical droplets, and compute the cardinality $N^\star$ of the set $\mathcal{P}$ of protocritical droplets modulo shifts, thereby completing our analysis.

Hypotheses (H1–H2) imply that $(\mathcal{X}_{\mathrm{meta}}, \mathcal{X}_{\mathrm{stab}}) = (\square, \boxplus)$, and that the highest energy barrier between a configuration and the set of configurations with lower energy is the one separating $\square$ and $\boxplus$, i.e., $(\square, \boxplus)$ is the unique *metastable pair*. Hypothesis (H3) is needed to find the asymptotics of the prefactor of the expected transition time in the limit as $\Lambda \to \mathbb{Z}^2$ and will be proved in Theorem 4.7 below. The main theorems in Chapter 2 involve *three model-dependent quantities*: the energy, the shape and the number of critical droplets. The first ($\Gamma^\star$) was identified in Chapter 3, the second ($\mathcal{C}^\star$) and the third ($N^\star$) will be identified in Theorems 4.8–4.10 below.

4.1.3 Main theorems

In Chapter 2 it was shown that $0 < \Delta_1 + \Delta_2 < 4U$ is the *metastable region*, i.e., the region of parameters for which $\square$ is a local minimum but not a global minimum of H. Moreover, it was argued that within this region the subregion where $\Delta_1, \Delta_2 < U$ is of little interest because the critical droplet consists of two free particles, one of type 1 and one of type 2. Therefore the *proper metastable region* is

$$0 < \Delta_1 \leq \Delta_2, \quad \Delta_1 + \Delta_2 < 4U, \quad \Delta_2 \geq U, \tag{4.11}$$

as indicated in Fig. 4.2.

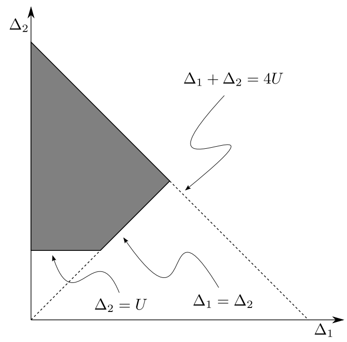


Figure 4.2: Proper metastable region.

In this Chapter, as in Chapter 3, the analysis will be carried out for the subregion of the proper metastable region defined by

$$\Delta_1 < U, \quad \Delta_2 - \Delta_1 > 2U, \quad \Delta_1 + \Delta_2 < 4U, \tag{4.12}$$

as indicated in Fig. 4.3. (*Note*: The second and third restriction imply the first restriction. Nevertheless, we write all three because each plays an important role in the sequel.)

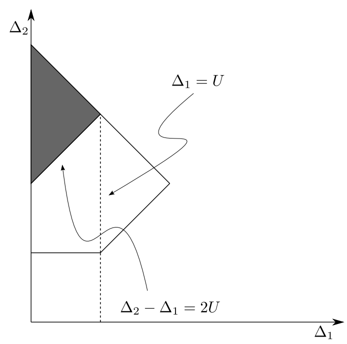


Figure 4.3: Subregion of the proper metastable region given by (4.12).

Hypothesis (H3) involves additional characterizations of the sets $\mathcal{P}$ and $\mathcal{C}^\star$. It turns out that these sets vary over the region defined in (4.12). The subregion where $\Delta_2 \leq 4U - 2\Delta_1$ is trivial: the configurations in $\mathcal{P}$ consist of a single droplet, with one particle of type 2 surrounded by four particles of type 1, located anywhere in Λ^-. For this case, $\Gamma^\star = 4\Delta_1 + 2\Delta_2 - 4U$ and $N^\star = 1$. We will split the subregion where $\Delta_2 > 4U - 2\Delta_1$ into four further subregions (see Fig. 4.4).

For three of these subregions we will indentify $\mathcal{P}$, $\mathcal{C}^\star$ and $\mathcal{C}^\star_{\mathrm{bd}}$, prove (H3), and compute $N^\star$, namely,

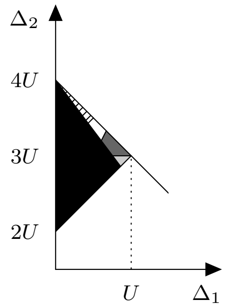


Figure 4.4: Subregions of the parameter space. In the black region $\ell^\star \le 3$; **RA**, **RB** and **RC** are, respectively, the light gray, the dark grey and the dashed region.

RA: $\Delta_1 < 3U$;

RB: $3U < \Delta_2 < 2U + 2\Delta_1$;

RC: $\Delta_2 > 3U + \Delta_1$.

The fourth subregion is more subtle and is not analyzed in detail (see Section 4.1.4 for comments). All subregions are open sets. This is done to avoid parity problems. We also require that

$$\Delta_1/\varepsilon \notin \mathbb{N} \quad \text{with} \quad \varepsilon = 4U - \Delta_1 - \Delta_2 \tag{4.13}$$

and put

$$\ell^\star = \left\lceil \frac{\Delta_1}{\varepsilon} \right\rceil \in \mathbb{N} \setminus \{1\}. \tag{4.14}$$

To state our main theorem we need the following definitions. A 2–tile is a particle of type 2 surrounded by four particles of type 1. Dual coordinates map the support of a 2–tile to a unit square. A monotone polyomino is a polyomino whose perimeter has the same length as that of its circumscribing rectangle. Given a set of configurations $\mathcal{D}$, we write $\mathcal{D}^{\mathrm{bd2}}$ to denote the configurations obtained from $\mathcal{D}$ by adding a particle of type 2 to a site in $\partial^-\Lambda$. (For precise definitions see Sections 4.2.1–4.2.2.)

Definition 4.6 *(a) $\mathcal{D}_A$ is the set of 2–tiled configurations with $\ell^\star(\ell^\star - 1) + 1$ particles of type 2 whose dual tile support is a rectangle of side lengths $\ell^\star, \ell^\star - 1$ plus a protuberance on one of the four side of the rectangle (see Fig. 4.14).*
(b) $\mathcal{D}_B$ is the set of 2–tiled configurations with $\ell^\star(\ell^\star - 1) + 1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing rectangle has side lengths either $\ell^\star, \ell^\star$ or $\ell^\star + 1, \ell^\star - 1$ (see Fig. 4.20).

(c) $\mathcal{D}_C$ *is the set of* 2*–tiled configurations with* $\ell^\star(\ell^\star-1)+1$ *particles of type* 2 *whose dual tile support is a monotone polyomino and whose circumscribing rectangle has perimeter* $4\ell^\star$ *(see Fig.* 4.27*).*
Note that $\mathcal{D}_A \subseteq \mathcal{D}_B \subseteq \mathcal{D}_C$*.*

Theorem 4.7 *Hypothesis* (H3) *is satisfied in each of the subregions* **RA** $-$ **RC**.

Theorem 4.8 *In subregion* **RA***,* $\mathcal{P} = \mathcal{D}_A$*,* $\mathcal{C}^\star_{\mathrm{bd}} = \mathcal{D}_A^{\mathrm{bd2}}$*, and* $N^\star = 8\ell^\star - 4$*.*

Theorem 4.9 *In subregion* **RB***,* $\mathcal{P} = \mathcal{D}_B$*,* $\mathcal{C}^\star_{\mathrm{bd}} = \mathcal{D}_B^{\mathrm{bd2}}$*, and* $N^\star = 8[q_{\ell^\star-1} + r_{\ell^\star-1-1}]$*.*

Theorem 4.10 *In subregion* **RC***,* $\mathcal{P} = \mathcal{D}_C$*,* $\mathcal{C}^\star_{\mathrm{bd}} = \mathcal{D}_C^{\mathrm{bd2}}$*, and* $N^\star = 8[q_{\ell^\star-1} + \sum_{c=1}^{\lfloor\sqrt{\ell^\star-1}\rfloor} r_{\ell^\star-c^2-1}]$*.*

Here, (r_k) and (q_k) are the coefficients of two generating functions defined in the appendix, which count polyominoes with fixed volume and minimal perimeter. The claims in Theorems 4.8–4.10 are valid for $\ell^\star \geq 4$ only. For $\ell^\star = 2, 3$, see Section 4.4.3.

4.1.4 Discussion

1. In (4.2) we take an annulus of width 3 without interaction instead of an annulus of width 1 as in Chapters 2 and 3. This allows us to prove that the model satisfies (H3), without having to deal with complications that arise when droplets are too close to the boundary of Λ. The theorems in Chapters 2 and 3 remain valid.

2. Theorems 4.7 and 4.8–4.10, together with the theorems presented in Chapter 2 and Chapter 3, complete our analysis for part of the subregion given by (4.12). Our results do not carry over to other values of the parameters, for a variety of reasons explained in Chapter 2, Section 2.2.2. In particular, for $\Delta_1 > U$ the critical droplets are square-shaped rather than rhombus-shaped. Moreover, (H2) is expected to be much harder to prove for $\Delta_2 - \Delta_1 < 2U$.

3. Theorems 4.8–4.10 show that, even within the subregion given by (4.12), the model-dependent quantities $\mathcal{C}^\star$ and $N^\star$, which play a central role in the metastability theorems in Chapter 2, are highly sensitive to the choice of parameters. This is typical for metastable behavior in multi-type particle systems, as explained in Chapter 2, Section 2.2.2.

4. The arguments used in the proof of Theorems 4.7 and 4.8–4.10 are geometric. Along any optimal path from $\square$ to $\boxplus$, as the energy gets closer to $\Gamma^\star$ the motion of the particles becomes more resticted. By analyzing this restriction in detail we are able to identify the shape of the critical droplets.

5. The fourth subregion is more subtle. The protocritical set $\mathcal{P}$ is somewhere between $\mathcal{D}_B$ and $\mathcal{D}_C$, and we expect $\mathcal{P} = \mathcal{D}_C$ for small Δ_1 and $\mathcal{D}_B \subsetneq \mathcal{P} \subsetneq \mathcal{D}_C$ for large Δ_1. The proof of Theorems 4.8–4.10 in Section 4.5 will make it clear where the difficulties come from.

Outline: In the remainder of this chapter we provide further notation and definitions (Section 4.2), state and prove a number of preparatory lemmas (Section 4.3), describe the motion of "tiles" along the boundary of a droplet (Section 4.4), and give the proof of Theorem 4.7 and 4.8–4.10 (Section 4.5). In the appendix we recall some standard facts about polyominoes with minimal perimeter.

4.2 Coordinates and definitions

Section 4.2.1 introduces two coordinate systems that are used to describe the particle configurations: standard and dual. Section 4.2.2 lists the main geometric definitions that are needed in the rest of the chapter.

4.2.1 Coordinates

1. A site $i \in \Lambda$ is identified by its *standard coordinates* $x(i) = (x_1(i), x_2(i))$, and is called odd when $x_1(i) + x_2(i)$ is odd and even when $x_1(i) + x_2(i)$ is even. The standard coordinates of a particle p in a configuration η are denoted by $x(p) = (x_1(p), x_2(p))$. The *parity* of a particle p in a configuration η is defined as $x_1(p) + x_2(p) + \eta(x(p))$ modulo 2, and p is said to be odd when the parity is 1 and even when the parity is 0.

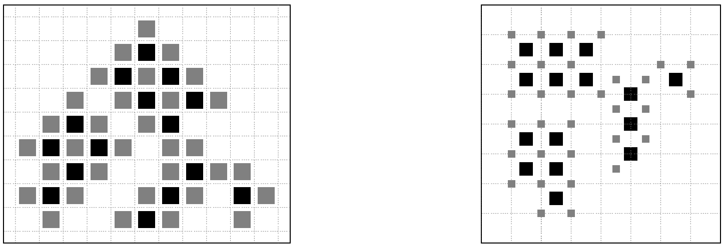
2. A site $i \in \Lambda$ is also identified by its *dual coordinates*

$$u_1(i) = \frac{x_1(i) - x_2(i)}{2}, \qquad u_2(i) = \frac{x_1(i) + x_2(i)}{2}. \tag{4.15}$$

Two sites i and j are said to be *adjacent*, written $i \sim j$, when $|x_1(i) - x_1(j)| + |x_2(i) - x_2(j)| = 1$ or, equivalently, $|u_1(i) - u_1(j)| = |u_2(i) - u_2(j)| = \frac{1}{2}$ (see Fig. 4.5).

3. For convenience, we take Λ to be the $(L + \frac{3}{2}) \times (L + \frac{3}{2})$ dual square with bottom-left corner at site with dual coordinates $(-\frac{L+1}{2}, -\frac{L+1}{2})$ for some $L \in \mathbb{N}$

with $L > 2\ell^\star$ (to allow for $H(\boxplus) < H(\square)$). Particles interact only in Λ^-, which is an $(L+\frac{1}{2}) \times (L+\frac{1}{2})$ dual square. This dual square, a *rhombus* in standard coordinates, is convenient because the local minima of H are rhombus-shaped as well (for more details see Chapter 3).



(a) (b)

Figure 4.5: A configuration represented in: (a) standard coordinates; (b) dual coordinates. Light-shaded squares are particles of type 1, dark-shaded squares are particles of type 2. In dual coordinates, particles of type 2 are represented by larger squares than particles of type 1 to exhibit the "tiled structure" of the configuration.

4.2.2 Definitions

1. A site $i \in \Lambda$ is said to be *lattice-connecting* in the configuration η if there exists a lattice path λ from i to $\partial^-\Lambda$ such that $\eta(j) = 0$ for all $j \in \lambda$ with $j \neq i$. We say that a particle p is lattice-connecting if $x(p)$ is a lattice-connecting site.

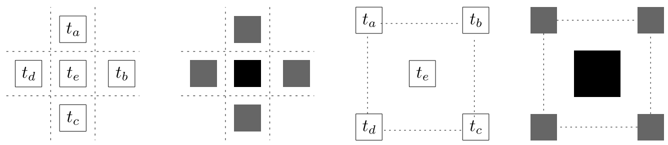
2. Two particles in η at sites i and j are called *connected* if $i \sim j$ and $\eta(i)\eta(j) = 2$. If two particles p_1 and p_2 are connected, then we say that there is an *active bond* b between them. The bond b is said to be *incident* to p_1 and p_2. A particle p is said to be *saturated* if it is connected to four other particles, i.e., there are four active bonds incident to p. The support of the configuration η, i.e., the union of the unit squares centered at the occupied sites of η, is denoted by $\mathrm{supp}(\eta)$. For a configuration η, $n_1(\eta)$ and $n_2(\eta)$ denote the number of particles of type 1 and 2 in η, and $B(\eta)$ denotes the number of active bonds. The energy of η equals $H(\eta) = \Delta_1 n_1(\eta) + \Delta_2 n_2(\eta) - UB(\eta)$.

3. Let $G(\eta)$ be the *graph* associated with η, i.e., $G(\eta) = (V(\eta), E(\eta))$, where $V(\eta)$ is the set of sites $i \in \Lambda$ such that $\eta(i) \neq 0$, and $E(\eta)$ is the set of pairs $\{i, j\}$, $i, j \in V(\eta)$, such that the particles at sites i and j are connected. A configuration η' is called a *subconfiguration* of η, written $\eta' \prec \eta$, if $\eta'(i) = \eta(i)$ for all $i \in \Lambda$ such that $\eta'(i) > 0$. A subconfiguration $c \prec \eta$ is called a *cluster* if the graph $G(c)$ is a maximal connected component of $G(\eta)$. The set of non-saturated particles in c is called the *boundary* of c, and is denoted by ∂c. Clearly, all particles in the same cluster have the same parity. Therefore the concept of parity extends from particles to clusters.

4. For a site $i \in \Lambda$, the *tile* centered at i, denoted by $\mathrm{t}(i)$, is the set of five sites consisting of i and the four sites adjacent to i. If i is an even site, then the tile is said to be even, otherwise the tile is said to be odd. The five sites of a tile are labeled a, b, c, d, e as in Fig. 4.6. The sites labeled a, b, c, d are called *junction sites*. If a particle p sits at site i, then $\mathrm{t}(i)$ is alternatively denoted by $\mathrm{t}(p)$ and is called the tile associated with p. In standard coordinates, a tile is a square of size $\sqrt{2}$. In dual coordinates, it is a unit square.

5. A tile whose central site is occupied by a particle of type 2 and whose junction sites are occupied by particles of type 1 is called a 2*–tile* (see Fig. 4.6). Two 2–tiles are said to be adjacent if their particles of type 2 have dual distance 1. A horizontal (vertical) 12*–bar* is a maximal sequence of adjacent 2–tiles all having the same horizontal (vertical) coordinate. If the sequence has length 1, then the 12–bar is called a 2*–tiled protuberance*. A cluster containing at least one particle of type 2 such that all particles of type 2 are saturated is said to be 2–tiled. A 2–tiled configuration is a configuration consisting of 2–tiled clusters only. A *hanging protuberance* (or hanging 2–tile) is a 2–tile where three particles of type 1 are adjacent to the particle of type 2 of the 2–tile only (see Fig. 4.17(b)).

Remark 4.11*A configuration consisting of a dual* 2*–tiled square of side length* $\ell^\star$ *belongs to* $\mathcal{X}_{\boxplus}$.



(a) (b) (c) (d)

Figure 4.6: Tiles: (a) standard representation of the labels of a tile; (b) standard representation of a 2–tile; (c) dual representation of the labels of a tile; (d) dual representation of a 2–tile.

6. The *tile support* of a configuration η is defined as

$$[\eta] = \bigcup_{p \in \varpi_2(\eta)} \mathrm{t}(p), \tag{4.16}$$

where $\varpi_2(\eta)$ is the set of particles of type 2 in η. Obviously, $[\eta]$ is the union of the tile supports of the clusters making up η. For a standard cluster c the *dual perimeter*, denoted by $P(c)$, is the length of the Euclidean boundary of its tile support $[c]$ (which includes an inner boundary when c contains holes). The dual perimeter $P(\eta)$ of a 2–tiled configuration η is the sum of the dual perimeters of the clusters making up η.

7. Denote by $\mathcal{V}_{\star,n_2}$ the set of configurations such that in $(\Lambda^-)^-$ the number of particles of type 2 is n_2. Denote by $\mathcal{V}^{4n_2}_{\star,n_2}$ the subset of $\mathcal{V}_{\star,n_2}$ where the number of active bonds is $4n_2$ and there are no non-interacting particles of type 1, i.e., the set of 2–tiled configurations with n_2 particles of type 2. A configuration η is called *standard* if $\eta \in \mathcal{V}^{4n_2}_{\star,n_2}$ and its tile support is a standard polyomino in dual coordinates (see Definition 3.6 below). A configuration η with $n_2(\eta)$ particles of type 2 is called *quasi-standard* if it can be obtained from a standard configuration with $n_2(\eta)$ particles of type 2 by removing some (possibly none) of the particles of type 1 with only one active bond, i.e., corner particles of type 1. Denote by $\bar{\mathcal{V}}_{\star,n}$ the set of configurations of *minimal energy* in $\mathcal{V}_{\star,n}$.

8. The state space $\mathcal{X}$ can be partitioned into manifolds:

$$\mathcal{X} = \bigcup_{n_2=0}^{|\Lambda|} \mathcal{V}_{\star,n_2}. \tag{4.17}$$

Two manifolds $\mathcal{V}_{\star,n}$ and $\mathcal{V}_{\star,n'}$ are called adjacent if $|n-n'|=1$. Note that transitions between two manifolds are possible only when they are adjacent and are obtained either by adding a particle of type 2 to $\partial^-\Lambda$ ($\mathcal{V}_{\star,n} \to \mathcal{V}_{\star,n+1}$) or removing a particle of type 2 from $\partial^-\Lambda$ ($\mathcal{V}_{\star,n} \to \mathcal{V}_{\star,n-1}$). Note further that $\square \in \mathcal{V}_{\star,0}$ and $\boxplus \in \mathcal{V}_{\star,(L-1)^2}$. Therefore, to realize the transition $\square \to \boxplus$, the dynamics must visit all manifolds $\mathcal{V}_{\star,n}$ with $n=1,\dots,(L-1)^2$. Abbreviate $\mathcal{V}_{\star,\le m} = \bigcup_{n=0}^{m} \mathcal{V}_{\star,n}$ and $\mathcal{V}_{\star,\ge m} = \bigcup_{n=m}^{|\Lambda|} \mathcal{V}_{\star,n}$.

9. For $\mathcal{Y} \subset \mathcal{X}$, $\hat\eta \in \mathcal{Y}$ and $x \in \Lambda\backslash \mathrm{supp}[\hat\eta]$, we write $\eta = (\hat\eta, x)$ to denote the configuration that is obtained from $\hat\eta$ by adding a particle of type 2 at site x. We write $\mathcal{Y}^{\mathrm{bd2}}$ to denote the set of configurations obtained from a configuration in $\mathcal{Y}$ by adding a particle of type 2 in $\partial^-\Lambda$, i.e., $\mathcal{Y}^{\mathrm{bd2}} = \bigcup_{\hat\eta\in\mathcal{Y}} \bigcup_{x\in\partial^-\Lambda} (\hat\eta, x)$. For $\omega\colon \square \to \boxplus$, let $\sigma_{\mathcal{Y}}(\omega)$ be the configuration in $\mathcal{Y}$ that is first visited by ω. Define

$$\begin{aligned} \Rsh\mathcal{Y} &= \bigcup_{\omega\colon\, \square\to\boxplus} \sigma_{\mathcal{Y}}(\omega), \\ \bar{\Rsh}\mathcal{Y} &= \bigcup_{\substack{\omega\colon\, \square\to\boxplus \\ \text{optimal}}} \sigma_{\mathcal{Y}}(\omega), \end{aligned} \tag{4.18}$$

called the *entrance*, respectively, the *optimal extrance* of $\mathcal{Y}$. With this notation we have $\mathcal{C}^\star_{\mathrm{bd}} = \bar{\ulcorner}\mathcal{G}(\square, \boxplus)$.

10. For $\mathcal{A}, \mathcal{B} \subset \mathcal{X}$, define

$$g(\mathcal{A},\mathcal{B}) = \{\eta \in \mathcal{B}\colon\ \exists \zeta \in \mathcal{A} \text{ and } \omega\colon\ \zeta \to \eta\colon\ n_2(\eta) \le n_2(\xi) \le n_2(\zeta),\ H(\xi) < \Gamma^\star\, \forall \xi \in \omega\},$$
$$\bar{g}(\mathcal{A},\mathcal{B}) = \{\eta \in \mathcal{B}\colon\ \exists \zeta \in \mathcal{A} \text{ and } \omega\colon\ \zeta \to \eta\colon\ n_2(\eta) \le n_2(\xi) \le n_2(\zeta),\ H(\xi) \le \Gamma^\star\, \forall \xi \in \omega\}. \tag{4.19}$$

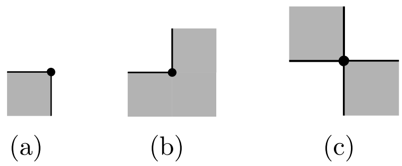


Figure 4.7: Corners of polyominoes: (a) one convex corner; (b) one concave corner; (c) two concave corners. Shaded mean occupied by a unit square.

11. A *unit hole* is an empty site such that all four of its neighbors are occupied by particles of the same type (either all of type 1 or all of type 2). An empty site with three neighboring sites occupied by a particle of type 1 is called a *good dual corner*. In the dual representation a good dual corner is a concave corner (see Fig. 4.7). The *surface* of $\eta \in \mathcal{X}$ is defined as

$$F(\eta) = \{x \in \Lambda\colon\ \exists\, y \sim x\colon\ \eta(y) = 1\}. \tag{4.20}$$

For $\eta \in \mathcal{X}$, let

$$\mathcal{T}(\eta) = 2P(\eta) + [\psi(\eta) - \phi(\eta)] = 2P(\eta) + 4[C(\eta) - Q(\eta)], \tag{4.21}$$

where $C(\eta)$ is the number of clusters in η, $P(\eta)$ the total length of the perimeter of these clusters, $Q(\eta)$ the number of holes, $\psi(\eta)$ the number of convex corners, and $\phi(\eta)$ is the number of concave corners. Note that $\mathcal{T}(\eta) = \sum_{c\in\eta} \mathcal{T}(c)$, where the sum runs over the clusters in η.

We also need the following definition:

Definition 4.12 [Alonso and Cerf [AC96].] *A polyomino (= a union of unit squares) is called monotone if its perimeter is equal to the perimeter of its circumscribing rectangle. A polyomino is called standard if its support is a quasi-square (i.e., a rectangle whose side lengths differ by at most one), with possibly a bar attached to one of its longest sides.*

4.3 Preparatory lemmas

In this section we collect a number of preparatory lemmas that are valid throughout the subregion given by (4.12). These lemmas will be needed in Section 4.5 to prove Theorems 4.7 and 4.8–4.10. In Section 4.3.1 we characterize $\vec{\bar{\mathcal{V}}}_{\star,\ell^\star(\ell^\star-1)+1}$ (Lemmas 4.14–4.15 below), in Section 4.3.2 we characterize $g(\{\square\},\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ and $\bar{g}(\{\square\},\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ (Lemma 4.15 below), and in Section 4.3.3 we characterize $\mathcal{G}(\square,\boxplus)$ (Lemmas 4.17–4.18 below).

An elementary observation is the following:

Lemma 4.13 *If $\eta \in \bar{\mathcal{V}}_{\star,n_2}$ with $\ell^\star(\ell^\star-1)+1 \le n_2 \le (\ell^\star)^2$, then η is 2–tiled and its dual perimeter is equal to $4\ell^\star$.*

Proof. Immediate from Lemmas 3.7–3.8 and 3.11 in Chapter 3, and also from Corollary 2.5 in [AC96]. ★

4.3.1 Characterization of $\vec{\bar{\mathcal{V}}}_{\star,\ell^\star(\ell^\star-1)+1}$

Lemma 4.14 *Let ρ be a 2–tiled configuration with $\ell^\star(\ell^\star-1)$ particles of type 2 and with dual tile support equal to a rectangle of side lengths $\ell^\star,(\ell^\star-1)$ (i.e., ρ is a standard configuration).*
(1) If $\eta \neq \rho$ is a 2–tiled configuration with $\ell^\star(\ell^\star-1)$ particles of type 2, then $H(\eta) > \Gamma^\star - \Delta_2$.
(2) If $\eta \neq \rho$ is a configuration with $\ell^\star(\ell^\star-1)$ particles of type 2 such that $[\eta] \neq [\rho]$, then $H(\eta) > \Gamma^\star - \Delta_2$.
(3) If $\eta \neq \rho$ is a configuration with $\ell^\star(\ell^\star-1)$ particles of type 2 obtained from ρ by removing at least one of the "non-corner" particles of type 1 in ρ (note that η and ρ have the same dual tile support), then $H(\eta) > \Gamma^\star - \Delta_2$.

Proof. (1) Since η is a 2–tiled configuration, it follows from Lemma 3.8 in Chapter 3 that $H(\eta)-H(\rho) = \frac{1}{4}[\mathcal{T}(\eta)-\mathcal{T}(\rho)]\Delta_1$, because the energy difference between the two configurations only depends on the difference in the number of particles of type 1. From Lemma 3.7 in Chapter 3 it follows that $\mathcal{T}(\eta) > \mathcal{T}(\rho)$. From the definition of $\mathcal{T}$ in (4.21) and Eq. (3.20) in Chapter 3 we have that, for any 2–tiled η, $\mathcal{T}(\eta) = 4k$ for some $k \in \mathbb{N}$. Hence $\mathcal{T}(\eta)-\mathcal{T}(\rho) \ge 4$, and so $H(\eta)-H(\rho) \ge \Delta_1$. The claim now follows by observing that $H(\rho) = \Gamma^\star + \varepsilon - \Delta_1 - \Delta_2$ and $\varepsilon > 0$.

(2) First consider the case where η consists of a single cluster. Then there exists a configuration η', obtained from η by saturating all particles of type 2, such that $H(\eta') \le H(\eta)$ with equality if and only if $\eta' = \eta$. Clearly, $[\eta] = [\eta']$. By part (1), we

have $H(\eta) \geq H(\eta') > \Gamma^\star - \Delta_2$. If η consists of clusters $c_1, \ldots, c_m$ with $m \in \mathbb{N}\backslash\{1\}$, then observe that $H(\eta) = \sum_{i=1}^m c_i$. Let $\eta^{n_2(c_i)}$ denote any standard configuration with $n_2(c_i)$ particles of type 2. By Lemmas 3.9 and 3.12 in Chapter 3, we have $H(\eta) = \sum_{i=1}^k H(c_i) \geq \sum_{i=1}^k H(\eta^{n_2(c_i)})$. Since ρ is a standard configuration, it follows from Lemma 3.7 in Chapter 3 that $\sum_{i=1}^k \mathcal{T}(\eta^{n_2(c_i)}) > \mathcal{T}(\rho)$, and so, as in the proof of part (1), $\sum_{i=1}^k \mathcal{T}(\eta^{n_2(c_i)}) - \mathcal{T}(\rho) > 4$. Using (3.36) in Chapter 3 for the energy of a standard configuration, we obtain that $\sum_{i=1}^k H(\eta^{n_2(c_i)}) - H(\rho) = \frac{1}{4}[\sum_{i=1}^k \mathcal{T}(\eta^{n_2(c_i)}) - \mathcal{T}(\rho)]\Delta_1$, from which we get the claim.

(3) Let $m \in \mathbb{N}$ denote the number of non-corner particles of type 1 removed from ρ to obtain η. Then $H(\eta) \geq H(\rho) + m(2U - \Delta_1) \geq H(\rho) + 2U - \Delta_1$ (because each of the non-corner particles of type 1 in ρ has at least 2 active bonds). Substituting the value of $H(\rho)$ into the latter expression, we obtain $H(\eta) \geq \Gamma^\star - \Delta_1 - \Delta_2 + \varepsilon + 2U - \Delta_1$. The claim follows by observing that $\Delta_1 < U$. ★

Lemma 4.15 (1) *All paths in* $(\square \to \boxplus)_{\mathrm{opt}}$ *enter the set* $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ *via a configuration* $(\hat\eta, x)$ *with* $\hat\eta \in \mathcal{V}_{\star,\ell^\star(\ell^\star-1)}$ *a quasi-standard configuration and* $x \in \partial^-\Lambda$.
(2) *All paths in* $(\square \to \boxplus)_{\mathrm{opt}}$ *enter the set* $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ *via a configuration* $(\hat\eta, x)$ *with* $\hat\eta \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ *such that* $\Phi(\square, \hat\eta) \leq \Gamma^\star$, *i.e.,* $\hat\eta \in \bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, *and* $x \in \partial^-\Lambda$. *Consequently,* $\bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ *is a gate for the transition* $\square \to \boxplus$.

Proof. (1) This is immediate from Lemma 4.14.

(2) By Theorem 3.5 in Chapter 3 (which identifies $\Gamma^\star$) and Lemmas 3.9–3.10 in Chapter 3 (which determine the energy of configurations in $\bar{\mathcal{V}}_{\star,n}$ for all n), if $\eta \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$, then $H(\eta) = \Gamma^\star - \Delta_2$. We argue by contradiction. Suppose that $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ enters $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ via a configuration $\zeta = (\hat\zeta, x)$ with $\zeta \in \mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}\backslash\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ and $x \in \partial^-\Lambda$. Then $H(\zeta) = H(\hat\zeta) + \Delta_2 > \Gamma^\star$, because $H(\zeta) > \Gamma^\star - \Delta_2$. Hence ω is not optimal. ★

4.3.2 Characterization of $g(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ and $\bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$

Definition 4.16 (a) *For* $n \in \mathbb{N}$, *let* $\hat{\mathcal{S}}_n$ *be the set of standard configurations with* n *particles of type* 2.
(b) *Let* $\omega \colon \square \to \boxplus = (\square, \ldots, \xi, \eta, \zeta, \ldots, \boxplus)$. *Write* $P_\omega(\eta)$ *to denote the part of* ω *from* $\square$ *to* ξ *and* $S_\omega(\eta)$ *to denote the part of* ω *from* ζ *to* $\boxplus$. *Any configuration in* $P_\omega(\eta)$ *is called a predecessor of* η *in* ω, *while any configuration in* $S_\omega(\eta)$ *is*

called a successor of η in ω. The configurations ξ and ζ are called the immediate predecessor, respectively, the immediate successor of η in ω.

Lemma 4.17 (1) *For every $\zeta \in \bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ there is a standard configuration $\bar{\eta} \in \hat{\mathcal{S}}_{\ell^\star(\ell^\star-1)+1}$ such that $\zeta \in \bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$.*
(2) *For every $\zeta \in g(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ there is a standard configuration $\bar{\eta} \in \hat{\mathcal{S}}_{\ell^\star(\ell^\star-1)+1}$ such that $\zeta \in g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. Consequently,*

$$g(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \bigcup_{\bar{\eta} \in \hat{\mathcal{S}}_{\ell^\star(\ell^\star-1)+1}} g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}). \tag{4.22}$$

Proof. (1) Pick $\zeta \in \bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. Let $\omega\colon \square \to \zeta$ be such that $\max_{\xi\in\omega} H(\xi) \leq \Gamma^\star$. Let η be the configuration visited by ω when it enters the set $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ for the last time before visiting ζ. Write ω as $\omega_1 + \omega_2$, where ω_1 is the part of ω from $\square$ to η and ω_2 is the part of ω from η to ζ. By Lemma 4.14, we have $\eta = (\hat{\eta}, x)$, where $\hat{\eta}$ is a quasi-standard configuration in $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)}$ and $x \in \partial^-\Lambda$, otherwise $H(\eta) > \Gamma^\star$. We will show that there is a standard configuration $\bar{\eta} \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ and a path $\omega_3\colon \eta \to \bar{\eta}$ such that $H(\xi) \leq H(\eta)$ and $n_2(\xi) = \ell^\star(\ell^\star-1)+1$ for all $\xi \in \omega_3$.

Let $\tilde{\eta}$ be the standard configuration in $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)}$ with the same tile support as $\hat{\eta}$. This configuration exists because every quasi-standard configuration whose support lies in Λ^- has no particle of type 2 in $\partial^-\Lambda^-$. (The latter is due to the fact that, in a quasi-standard configuration with $\ell^\star(\ell^\star-1)$ particles of type 2, each site that is occupied by a particle of type 2 has at least three neighboring sites occupied by a particle of type 1, and all sites in $\partial^-\Lambda^-$ have at most two adjacent sites in Λ^-.) Let $\bar{\eta}$ the standard configuration in $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ obtained from $\tilde{\eta}$ by adding a protuberance, with the particle of type 2 in this protuberance located at a site $y^\star$ on one of the longest sides of the rectangular cluster of $\tilde{\eta}$. This is always possible because at least one of the longest sides of $[\tilde{\eta}]$ is far away from $\partial^-\Lambda$.

Consider the path $S_{\omega_2}(\eta)$. Since η is the configuration visited by ω when the set $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ is entered for the last time before visiting ζ, all configurations in $S_{\omega_2}(\eta)$ have at least $\ell^\star(\ell^\star-1)+1$ particles of type 2. In particular, the particle of type 2 in x cannot leave Λ. We refer to this particle as the "floating particle". Observe that $H(\eta) \geq \Gamma^\star + \varepsilon - \Delta_1$, with equality if and only if $\hat{\eta}$ is standard. This implies that only moves of the floating particle are allowed until it enters Λ^- (particles in $\partial^-\Lambda$ cannot have active bonds). Furthermore, since $L > 2\ell^\star$ (and hence the sides of $\hat{\eta}$ are smaller than the sides of Λ), it follows that all sites $y \in \Lambda^-$ such that $y \notin \mathrm{supp}(\hat{\eta})$ are lattice-connecting. In particular, there exists a lattice path $\lambda = x_0, x_1, \ldots, x_m$ in Λ for some $m \in \mathbb{N}$ with $x_0 = x$ and $x_m = y^\star$.

Let ω_3 be the path from η to $\bar{\eta}$ obtained by first letting the floating particle move along the lattice path λ until it reaches site $y^\star$ and then saturating all the particles of type 2 in $(\hat{\eta}, y^\star)$. Note that $H(\hat{\eta}, y^\star) \leq H(\eta) - U$ and that all configurations in γ_3 have at least as many active bonds as η. Therefore $H(\xi) \leq H(\eta)$ for all $\xi \in \omega_3$.

Let $\hat{\omega}_3$ denote the path from $\bar{\eta}$ to η obtained by inverting ω_3. Then, by construction, $\tilde{\omega} = \hat{\omega}_3 + \omega_2$ is a path from $\bar{\eta}$ to ζ such that $H(\xi) \leq \Gamma^\star$ and $n_2(\xi) \geq \ell^\star(\ell^\star - 1) + 1$ for all $\xi \in \tilde{\omega}$.

(2) Same as part (1). ★

4.3.3 Characterization of $\mathcal{G}(\square, \boxplus)$

Lemma 4.18 (1) *All saddles in $\mathcal{V}_{\star,\leq \ell^\star(\ell^\star-1)}$ are unessential.*
(2) *Let $\zeta \in \mathcal{V}_{\star,\leq \ell^\star(\ell^\star-1)+1}$ be such that $H(\zeta) = \Gamma^\star$. Let $\mathcal{O}(\zeta) = \{\omega \in (\square \to \boxplus)_{\mathrm{opt}} \colon \omega \ni \zeta\}$ be the set of optimal paths visiting ζ. If all paths in $\mathcal{O}(\zeta)$ visit $g(\{\square\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ after visiting ζ, then ζ is unessential.*

Proof. (1) Let $\zeta \in \mathcal{V}_{\star,\leq \ell^\star(\ell^\star-1)}$ be a configuration such that $H(\zeta) = \Gamma^\star$. By Lemma 4.15(2), we have (recall Definition 4.2(e)) $S(\omega)\backslash\{\zeta\} \neq \emptyset$ for all $\omega \in \mathcal{O}(\zeta)$, i.e., all paths in $\mathcal{O}(\zeta)$ visit at least one other saddle configuration. Pick $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$. By Lemma 4.15(1), ω (last) enters the set $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ via a configuration (ρ_i, x) with ρ_i a quasi-standard configuration obtained from the standard configuration $\rho_0 \in \mathcal{V}_{\star,\ell^\star(\ell^\star-1)}$ by removing i corner particles of type 1, and $x \in \partial^-\Lambda$. It is clear that the configuration visited by ω just before (ρ_i, x) is ρ_i. Write $\omega = \omega_1 + \omega_2$, where ω_1 is a path from $\square$ to ρ_i and ω_2 is a path from ρ_i to $\boxplus$. Obviously, $\zeta \in \omega_1$. Moreover, $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ implies that $H(\rho_i, x) \leq \Gamma^\star$ and, consequently, $H(\rho_i) \leq \Gamma^\star - \Delta_2$. Furthermore, $H(\rho_j) < H(\rho_i)$ for $j < i$. Let $\omega_3 \colon \square \to \rho_0$ be a path from $\square$ to ρ_0 such that $H(\xi) < \Gamma^\star$ for all $\xi \in \omega_3$ (e.g. follow the construction of the "reference path" in Chapter 3), and let $\omega_4 \colon \rho_0 \to \rho_i$ be the path obtained by, iteratively, detaching and moving out of Λ one corner particle of type 1 until configuration ρ_i is reached. It is easy to see that $\max_{\xi \in \omega_4} H(\xi) < \Gamma^\star$. Consider the path $\hat{\omega} = \omega_3 + \omega_4 + \omega_2$. By construction, $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ and $S(\hat{\omega}) \subset S(\omega)\backslash\{\zeta\}$. Finally, observe that the same argument holds for any $\omega \in \mathcal{O}(\zeta)$.

(2) Since $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) \subset \mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$, all optimal paths from $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ to $\boxplus$ must visit the set $\vec{\Gamma}\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$. Therefore $S(\omega)\backslash\{\zeta\} \neq \emptyset$ for all $\omega \in \mathcal{O}(\zeta)$, since all configurations in $\vec{\Gamma}\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ have energy $\Gamma^\star$. Pick $\omega \in \mathcal{O}(\zeta)$, and let η be the first configuration in $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ visited by ω after visiting ζ. Let ω_1 be the part of ω from $\square$ to η and ω_2 the part of ω from η to $\boxplus$. Since $\eta \in g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, there is a path ω_3 from $\square$ to η such that

$H(\sigma) < \Gamma^\star$ for all $\sigma \in \omega_3$. Let $\hat{\omega} = \omega_3 + \omega_2$. By construction, $\hat{\omega} \in (\square \to \boxplus)_{\mathrm{opt}}$ and $S(\hat{\omega}) \subseteq S(\omega)\backslash\{\zeta\}$. Finally, observe that the same argument holds for all $\omega \in \mathcal{O}(\zeta)$. ★

Lemma 4.19 *If* $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, *then* $\mathcal{C}^\star_{\mathrm{bd}} \subset g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ *and* $\mathcal{P} \subset g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$.

Proof. By Lemma 4.15(2), if $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, then $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ is a gate for the transition $\square \to \boxplus$. Since $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ is a gate, there exists a $\mathcal{W} \subset g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ that is a minimal gate for the transition $\square \to \boxplus$. Let $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$. Since $\mathcal{W} \subset \mathcal{G}(\square, \boxplus)$ and $\omega \cap \mathcal{W} \neq \emptyset$, it follows that $\omega \cap \mathcal{G}(\square, \boxplus) \cap g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}} \neq \emptyset$. Combining Lemmas 4.15 and 4.18, it follows that if $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, then all saddles in $\mathcal{V}_{\star,\leq\ell^\star(\ell^\star-1)+1}$ are unessential and, by Lemma 4.3, do not belong to $\mathcal{G}(\square, \boxplus)$. Therefore the first configuration in $\mathcal{G}(\square, \boxplus)$ visited by ω is an element of $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$. Since the choice of $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ is arbitrary, we conclude that $\mathcal{C}^\star_{\mathrm{bd}} \subset g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$.

It remains to show that $\mathcal{P} \subset g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. The proof is by contradiction. Pick $\hat{\eta} \in \mathcal{P}\backslash g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. Since $\mathcal{C}^\star_{\mathrm{bd}} \subset g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$, there is a configuration $\eta \in g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ obtained in a single step from $\hat{\eta}$. Clearly, $\hat{\eta} \in \mathcal{V}_{\star,\geq\ell^\star(\ell^\star-1)+1}$, since the number of particle of type 2 in Λ changes at most by one at each step. Since, by Lemma 4.15 and the hypothesis $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, all paths in $(\square \to \boxplus)_{\mathrm{opt}}$ enter $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ by adding a particle of type 2 in $\partial^-\Lambda$ to a configuration in $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, it follows that $\hat{\eta} \in \mathcal{V}_{\star,\geq\ell^\star(\ell^\star-1)+2}$ by assumption. ★

4.4 Motion of 2–tiles

In Section 4.4.1 we study the motion of 2–tiles. In Section 4.4.2 we derive some restrictions on the transitions between configurations with different tile support. In Section 4.4.3 we identify the critical droplets for small values of $\ell^\star$, namely, $\ell^\star = 2, 3$.

4.4.1 Motion of dimers of 2–tiles

Definition 4.20 (a) *Two configurations η and η' (with the same tile support) are called equivalent if there is a path $\omega\colon \eta \to \eta'$ (possibly of length zero) such that all configuration in ω have the same tile support and $\Phi(\eta, \eta') < \Gamma^\star$. In words,*

two configurations are equivalent if it is possible to go from one to the other via a sequence of moves of particles of type 1 *without reaching energy level* $\Gamma^\star$.
(b) *A heavy-step is a sequence of moves realizing the transition between two configurations* η *and* η' *with different tile support. Note that a heavy-step is completed by moving, removing or adding a particle of type* 2 *in* Λ.

Let $\eta \in \mathcal{V}_{\star,n_2}$ and $\bar\eta \in \bar{\mathcal{V}}_{\star,n_2}$. By Lemma 4.1 and the proof of Lemma 3.9 in Chapter 3, both $B(\bar\eta)$ and $n_1(\bar\eta)$ are constant in $\bar{\mathcal{V}}_{\star,n_2}$.

Definition 4.21 (a) *A configuration* $\eta \in \mathcal{V}_{\star,n_2}$ *is said to have* m *broken bonds if* $B(\eta) = B(\bar\eta) - m$ *for all* $\bar\eta \in \bar{\mathcal{V}}_{\star,n_2}$. *The number of broken bonds in configuration* η *is denoted by* $B^-(\eta)$.
(b) *A configuration* $\eta \in \mathcal{V}_{\star,n_2}$ *is said to have* n *extra particles of type* 1 *if* $n_1(\eta) = n_1(\bar\eta) + n$ *for all* $\bar\eta \in \bar{\mathcal{V}}_{\star,n_2}$. *The number of extra particles of type* 1 *in configuration* η *is denoted by* $n_1^+(\eta)$.
(c) $B(p,\eta)$ *denotes the number of active bonds adjacent to particle* p *in configuration* η.
(d) *A dimer consists of two adjacent particles of different type such that the particle of type* 1 *is lattice-connecting and has only one active bond (i.e., is a corner particle of type* 1*). The particle of type* 2 *belonging to a dimer is called a corner particle of type* 2.
(e) *A particle of type* 2 *in a* 2*–tiled configuration* η *is called external if it can be moved without moving any other particle of type* 2 *in* η *(see Fig.* 4.14*).*

In this section we will exhibit two methods to move a dimer in a configuration η to a good dual corner of the cluster it belongs to (see Fig. 4.8). The configuration η' that is obtained in this way satisfies $H(\eta') \le H(\eta)$. In particular, we will exhibit two different choices for a path ω from η as in Fig. 4.8(a) to η' as in Fig. 4.8(b), and we will determine $\max_{\xi\in\omega} H(\xi)$. In what follows we write $\Delta H(\omega) = H(\tilde\eta) - H(\eta)$, where $\tilde\eta$ is the configuration that is reached after the last step in ω.

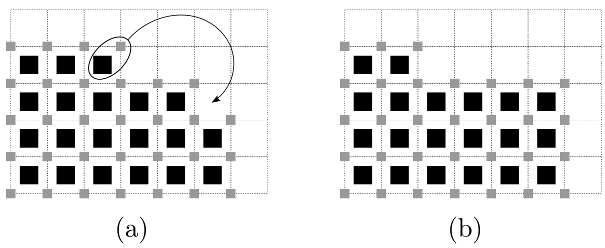


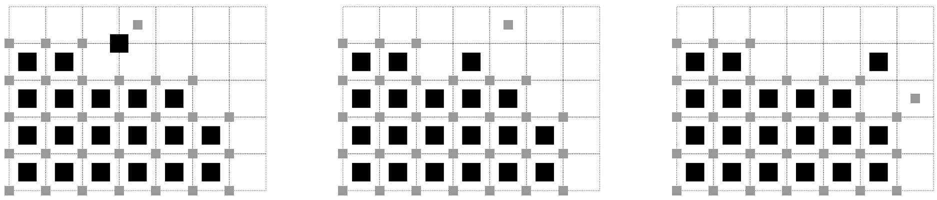
Figure 4.8: Motion of a 2–tile.

Lemma 4.22 *A* 2*–tile can be moved within energy barrier* $3U$ *and* $U + 4\Delta_1$.

Proof. We will give examples that are paradigmatic for the general case. Let p, q denote, respectively, the particle of type 2 and of type 1 of the dimer that we want to move.

1. The first method is achieved within energy barrier $3U$ energy (i.e., $\max_{\xi\in\omega} H(\xi) = 3U$) and goes as follows (see Fig. 4.9). First, particle q is moved one step North-East ($\Delta H(\omega) = U$). Next, also particle p is moved one step North-East ($\Delta H(\omega) = 3U$; see Fig. 4.9(a)). After that, particle p is moved one step South-East ($\Delta H(\omega) = 2U$), and particle q is moved in two steps to the site at dual distance $2\sqrt{2}$ from particle p in the North-East direction ($\Delta H(\omega) = 2U$; see Fig. 4.9(b)). It is possible to continue following a pattern of this type until particle p is adjacent only to the (original) corner particle of type 1 at the end of the bar "just below" p ($\Delta H(\omega) = 3U$; see Fig. 4.9(c)). Call η_1 the configuration reached after this last step. Particle q can now be moved to the site at dual distance $2\sqrt{2}$ from particle p in the South-East direction ($\Delta H(\omega) = 3U$; see Fig. 4.9(c)). Call this configuration η_2. Move particle p first one step South-East ($\Delta H(\omega) = 3U$) and then one step South-West ($\Delta H(\omega) = U$). Finally, move particle q to the free site adjacent to p ($\Delta H(\omega) = 0$).

Remark 4.23 *Note that from η_2 to η' particle p moves in the South direction via the same mechanism that was used to move in the East direction from η to η_1. This symmetry in the motion of the dimer around a corner of the cluster will be used also in the sequel.*



(a) (b) (c)

Figure 4.9: A dimer is moved to a corner within energy barrier $3U$.

2. The second method is achieved within energy barrier $U + 4\Delta_1$ (i.e., $\max_{\xi\in\omega} H(\xi) = U + 4\Delta_1$) and goes as follows (see Fig. 4.10). First, move particle q one step in the North-East direction ($\Delta H(\omega) = U$), and let two extra particles of type 1 enter Λ and reach the two sites at dual distance 1 from q in the West and the South direction ($\Delta H(\omega) = U + 2\Delta_1$). Next, move particle p one step in the North-East direction ($\Delta H(\omega) = U + 2\Delta_1$, see Fig. 4.10(a)). After that, move the particle of type 1 at dual distance 1 in the West direction from p to the site adjacent to p in the South-West direction ($\Delta H(\omega) = U + 2\Delta_1$), let one extra particle of type 1 enter Λ ($\Delta H(\omega) = 2 + 3\Delta_1$), and move this particle to the site at dual distance 1 in the West direction from p ($\Delta H(\omega) = 3\Delta_1$, see Fig. 4.10(b)).

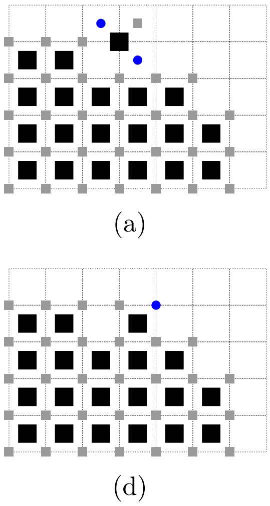


Figure 4.10: A dimer is moved to a corner within energy barrier $U + 4\Delta_1$. The small circles represent the extra particles of type 1 with respect to those in the starting configuration.

Move the particle adjacent to p in the South-East direction one step in the North-East direction ($\Delta H(\omega) = U + 3\Delta_1$). Move p one step in the South-East direction ($\Delta H(\omega) = U + 2\Delta_1$, see Fig. 4.10(c)). Afterwards, use one of the free particles of type 1 to saturate p ($\Delta H(\omega) = +3\Delta_1$), and remove the other free particles of type 1 from Λ ($\Delta H(\omega) = 2\Delta_1$, see Fig. 4.10(d)). The same procedure can be repeated until the configuration in Fig. 4.10(e) is reached ($\Delta H(\omega) = 3\Delta_1$). Next, let a particle enter Λ and reach the site at dual distance 1 in the East direction from p, and move one step in the South-East direction the particle adjacent to p in the South-East direction ($\Delta H(\omega) = U + 4\Delta_1$, see Fig. 4.10(f)). Next, move p in the Sout-East direction ($\Delta H(\omega) = U + 4\Delta_1$), saturate it with one of the free particles of type 1, and remove the other particles of type 1 from Λ ($\Delta H(\omega) = 2\Delta_1$). Now particle p can be moved in the South direction in the same way it was moved in the East direction within energy barrier $U + 3\Delta_1$. ★

By Lemma 4.15, we know that any path in $(\square \to \boxplus)_{\text{opt}}$ enters the set $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ when a particle of type 2 is added in $\partial^-\Lambda$ to a configuration in $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. By Lemma 4.17, we know that $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ can be determined by looking at all the configurations that can be reached starting from the standard configurations in $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ without changing the number of particles of type 2 in Λ and taking into account all the moves that are possible within energy barrier Δ_2. Note that different configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ necessarily have different tile support, and so to move between these classes of configurations it is necessary to perform a sequence of heavy-steps.

Remark 4.24 *Note that, from the point of view of the maximal energy barrier that needs to be overcome to go from η to η', for $\Delta_1 > \frac{1}{2}U$ the first method is more efficient while fOr $\Delta_1 < \frac{1}{2}U$ the second method is more efficient.*

Remark 4.25 *Starting from a 2–tiled configuration with a monotone dual support inscribed in a rectangle of side lengths l_1, l_2 ("far enough" from the boundary of Λ), it is possible to reach, via one of the two mechanisms described above, all the 2–tiled configurations with a monotone dual support and the same circumscribing rectangle.*

4.4.2 Restriction on heavy-steps

Lemma 4.26 *Let $\Delta_2 < 3U + \Delta_1$ and $\eta \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$. If the first heavy-step starting from η (that does not change the number of particles of type 2) does not result in the motion of a corner particles of type 2 along the edge where in η it shares a bond with a corner particle of type 1, then it is not possible to reach a new configuration $\eta' \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ within energy barrier Δ_2.*

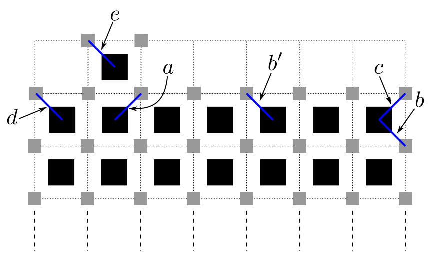


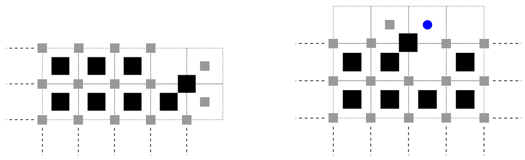
Figure 4.11: Types of edges for the first possible heavy-step starting from a standard configuration.

Proof. It is clear that the first heavy-step can only involve one of the external particles of type 2. For the proof we refer to Fig. 4.11, where a prototype configuration $\bar{\eta} \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ is represented.

We will show that if a heavy-step is performed along one of the edges a, b or b', then it is not possible to reach a new configuration $\eta' \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ without exceeding energy barrier Δ_2. These edges are representatives of the possible types of edges along which the first heavy-step is possible without involving the motion of a corner particle of type 2 along the edge where it shares a bond with a corner particle of type 1.

1. Assume that the first heavy-step is along edge a. Let (u, v) denote the dual coordinates of the particle p_1 of type 2 we want to move. Let $\eta_1 \notin \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ be the configuration that is reached when p_1 is moved, along edge a, to the site with dual coordinates $(u + \frac{1}{2}, v + \frac{1}{2})$, and let η_0 be the configuration visited just before the heavy-step is performed. When η_1 is reached, either the site with dual coordinates $(u+1, v+1)$ is empty or it is occupied by a particle of type 1. Without loss of generality, we may assume that η_1 does not contain free particles of type 1, since these particles could be iteratively removed from Λ while decreasing the energy of the configuration. Similarly, we may assume that all particles of type 1 that do not interfere with the heavy-step that is performed are still in Λ, since in $\bar{\eta}$ they had at least one active bond and thier removal would increase the energy of the configuration (since $\Delta_1 < U$). In the former case, $B(\eta_1) = B(\bar{\eta}) - 5$, and so $H(\eta_1) - H(\bar{\eta}) = 5U - \Delta_1 > \Delta_2$. In the latter case, $B(\eta_1) = B(\bar{\eta}) - 4$, and so $H(\eta_1) - H(\bar{\eta}) = 4U > \Delta_2$.

2. Assume that the first heavy-step is along edge b (see Fig. 4.12(a)). Again, let $w = (u, v)$ denote the dual coordinates of the particle p_1 of type 2 we want to move. Denote by q_1 and q_2 the particles of type 1 sitting in $\bar{\eta}$, respectively, at the sites with dual coordinates $(u+\frac{1}{2}, v-\frac{1}{2})$ and $(u+\frac{1}{2}, v-\frac{1}{2})$. Let $\eta_1 \notin \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ be the configuration obtained by moving particle p_1 to the site x with dual coordinates $(u + \frac{1}{2}, v - \frac{1}{2})$, and let η_0 be the configuration visited just before the heavy-step is performed. When particles p_1 reaches site x, it has at most two active bonds, depending on whether the dual sites $y_1 = (u + 1, v - 1)$ and $y - 2 = (u + 1, v)$ are empty or occupied by a particle of type 1. If both y_1 and y_2 are empty, then $H(\eta_1) - H(\bar{\eta}) = 5U - 2\Delta_1 > \Delta_2$ (again we assume that Λ does not contain free particles of type 1 and all other particles of type 2 are saturated). If only one dual site between y_1 and y_2 is occupied, then, arguing as before, we get $H(\eta_1) - H(\bar{\eta}) = 4U > \Delta_2$ if particle q_2 is still inside Λ and $H(\eta_1) - H(\bar{\eta}) = 4U - \Delta_1 > \Delta_2$ if particle q_1 has been removed from the Λ. If both y_1 and y_2 are occupied, then $H(\eta_1) - H(\bar{\eta}) = 3U$ (again we assume that there are no free particles of type 1 in Λ). Note that, since $\Delta_2 < 3U + \Delta_1$, no particle of type 1 is allowed to enter Λ nor is it allowed to break any active bond. Therefore the only moves that are possible starting from η_1 are those that do not increase the energy. Only two moves are possible. Either the particle of type 2 is moved back from site x to site w, or the particle q_3 of type 1 sitting at the dual site $y_3 = (u - \frac{1}{2}, v + \frac{1}{2})$ is moved to site x. In the former case, it is clear that the configuration that is reached is η_0 and the move produces a non-self-avoiding path. In the latter case, we reach a configuration $\eta_2 \notin \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ with the same energy as η_1. But now the only move that does not increase the energy is the motion of q_3 back to y_3, which again produces a non-self-avoiding path.



(a) (b)

Figure 4.12: Two choices for the first heavy-step that are too costly.

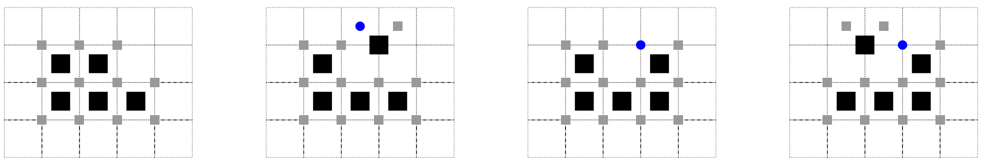
3. The case where the first heavy–step is performed along edge b' is similar to the previous case (see Fig. 4.12(b)). ★

We see from Lemma 4.18 that $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})^{\mathrm{bd2}}$ is a good candidate for $\mathcal{C}^\star_{\mathrm{bd}}$.

4.4.3 Small values of $\ell^\star$

In Section 4.5 we will identify the geometry of the protocritical and critical configurations for $\ell^\star \geq 4$, i.e., for the subregion $\Delta_2 > 4U - \frac{4}{3}\Delta_1$. The analysis will show that the set $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ consists of all the configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$. The region $\Delta_2 \leq 4U - \frac{4}{3}\Delta_1$ is denoted by **RT**.

For $\ell^\star = 2$ this set consists of those 2–tiled configurations whose dual tile support is either a 2×2 square from which a corner has been removed or a 3×1 rectangle. For $\ell^\star = 3$ it consists of those 2–tiled configurations whose dual tile support is either a 3×2 rectangle plus a "protuberance" on one of the four sides or a 3×3 square from which two corners have been removed. This can be easily verified by noting that it is possible to move a tile protuberance within energy barrier $4U - 2\Delta_1 < \Delta_2$ and that it is possible to "slide" an external 12–bar of length 2 within energy barrier $2U + \Delta_1 < \Delta_2$, as described next (see Fig. 4.13).



(a) (b) (c) (d)

Figure 4.13: Sliding a 12–bar of length 2.

We construct a path ω from configuration η of Fig. 4.13(a) to configuration η' obtained by shifting the 12–bar of length 2 in the East direction by one dual unit. Let p_1 denote the Eastern-most particle of type 2 of the 12–bar and p_2 the other particle of type 2. Let q_1 be the particle of type 1 adjacent to p_1 in the North-East direction, q_2 the particle of type 1 adjacent to p_1 in the North-West direction, and q_3 the particle of type 1 adjacent to p_2 in the North-West direction. Move q_1 one step North-East ($\Delta H(\omega) = U$), let an extra particle q_4 of type 1 enter Λ ($\Delta H(\omega) = U + \Delta_1$), and let this particle reach the site at dual distance 1 in the West direction from q_1, and move p_1 one step North-East ($\Delta H(\omega) = 2U + \Delta_1$; see Fig.4.13(b)). Then, without increasing the energy of the configuration, move p_2, q_1 and q_4 subsequently one step South-East ($\Delta H(\omega) = \Delta_1$; see Fig. 4.13(c)). Afterwards, move first q_2 and q_3 one step North-East ($\Delta H(\omega) = 2U + \Delta_1$) and p_2 one step North-East ($\Delta H(\omega) = 2U + \Delta_1$; see Fig. 4.13(d)). Finally, move p_2 one step South-East, use q_2 to saturate p_2, and remove q_3 from Λ ($\Delta H(\omega) = 0$).

It turns out that in each of these cases $\mathcal{P} = \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ and $\mathcal{C}^\star_{\mathrm{bd}} = \bar{\mathcal{V}}^{\mathrm{bd2}}_{\star,\ell^\star(\ell^\star-1)+1}$. The proofs are essentially analogous to those that will be given in Section 4.5.1 below.

4.5 Geometry of critical configurations

In this section we prove Theorems 4.7 and 4.8–4.10.

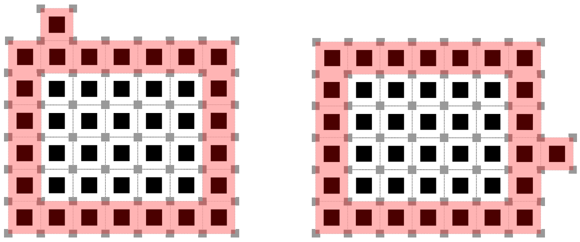
In Sections 4.5.1–4.5.3 we will identify $\mathcal{P}$ and $\mathcal{C}^\star_{\mathrm{bd}}$ for the subregions **RA**, **RB** and **RC**, respectively. Once the structure of the configurations in $\mathcal{P}$ and $\mathcal{C}^\star_{\mathrm{bd}}$ are identified, (H3-a) and (H3-b) will follow immediately. To prove (H3-c), we will show the existence of a $\zeta \in \mathcal{C}^\star_{\mathrm{att}}(\hat{\eta})$ such that $\Phi(\zeta, \boxplus) < \Gamma^\star$ (i.e., the existence of a “good site” in $\hat{\eta}$). Due to the fact that Λ has a border of width 3 where there is no interaction between particles, it will be immediate that such a good site can always be reached by a particle of type 2 in $\partial^-\Lambda$ without touching the cluster. Finally, to see that all $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ pass through $\mathcal{C}^\star_{\mathrm{att}}$, we observe that, as long as the free particle of type 2 does not attach itself to the cluster, the energy cannot drop below $\Gamma^\star$ and hence no other particle is allowed to enter Λ. In particular, this implies that the set $\mathcal{V}_{\star,\geq\ell^\star(\ell^\star-1)+2} \ni \boxplus$ cannot be reached.

In each of the following sections we look at a specific standard configuration, labelled by the position of the lower-left particle, acting as the representative of the set of all standards configurations that are obtained by translation and rotation. Each section is split into three parts: (1) identification of $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ and $\bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ via the motion of 2–tiles between dual corners; (2) existence of a good site via the construction of a path to $\boxplus$ below energy level $\Gamma^\star$; (3) identification of $\mathcal{P}$ and $\mathcal{C}^\star_{\rm bd}$.

4.5.1 Region RA

In this section we prove Theorem 4.8.

Let $\mathcal{D}_A$ be the set of 2–tiled configurations with $\ell^\star(\ell^\star-1)+1$ particles of type 2 whose dual tile support is a rectangle of side lengths $\ell^\star, \ell^\star-1$ plus a protuberance on one of the four side of the rectangle (see Fig. 4.14).



(a) (b)

Figure 4.14: Two examples of configurations in $\mathcal{D}_A$ for $\ell^\star = 7$. The external particles of type 2 are those lying in the shaded area.

Definition 4.27 *A path ω from $\eta \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ to $\eta' \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ such that $n_2(\xi) = n_2(\eta)$ for all $\xi \in \omega$ is called a modifying path from η to η'.*

With this definition, a configuration $\eta' \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ belongs to $\bar{g}(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ (respectively, $g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$) with $\bar\eta$ a standard configuration in $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ if and only if there is a modifying path from $\bar\eta$ to η' that does not exceed (respectively, stays below) energy level $\Gamma^\star$.

Remark 4.28 *Note that if there is a path $\omega\colon\ \eta \to \eta'$ that does not exceed (stay below) $\Gamma^\star$, then there is also a path $\omega'\colon\ \eta \to \eta'$ that does the same without ever completing a heavy-step and reaching a configuration that is equivalent to a configuration that has already been visited.*

Identification of $g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ and $\bar{g}(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$

Lemma 4.29 $g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \bar{g}(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \mathcal{D}_A$.

Proof. Let ρ be a configuration consisting of 2–tiled dual rectangle with horizontal side length $\ell^\star$ and vertical side length $\ell^\star-1$ whose top-rightmost 2–tile is centered at site (a_ρ, b_ρ). Let $\bar{\eta}$ be the 2–tiled standard configuration obtained from ρ by adding a 2–tiled protuberance centered at (dual) site $x = (a_\rho + 1, b_\rho + 1)$ (see Fig. 4.11). Observe that $H(\bar{\eta}) = \Gamma^\star - \Delta_2$. Let y be one of the two sites of the tile centered at x that is occupied by a particle of type 1 with only one active bond. It is easy to check that $\mathcal{D}_A \subseteq g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. Indeed, it is enough to consider the configuration (ρ, y) obtained from $\bar{\eta}$ by first detaching and removing the two corner particles of type 1 adjacent to x and then moving the particle of type 2 from x to y, which gives $\Phi((\rho, y), \eta) < \Gamma^\star$ for all $\eta \in \mathcal{D}_A$. Note that this is true irrespective of the distance of η to the boundary of Λ.

To conclude the proof we will show that all modifying paths starting from $\bar{\eta}$ either lead to a configuration in $\mathcal{D}_A$ or exceed energy level $\Gamma^\star$. Note that we are interested only in those modifying paths consisting of at least one heavy-step, otherwise the only configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ that can be reached from $\bar{\eta}$ is $\bar{\eta}$ itself. In other words, since all configurations in $\mathcal{D}_A$ consist of a 2–tiled dual rectangle plus a 2–tiled protuberance, we have to show that, without exceeding energy level $\Gamma^\star$, i.e., within energy barrier Δ_2, the only configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ that can be reached via a path consisting of configurations with $\ell^\star(\ell^\star - 1) + 1$ particles of type 2 are obtained by "moving" the 2–tiled protuberance.

Let $\eta \in \bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, and let ω be a modifying path from $\bar{\eta}$ to η such that $H(\xi) \leq \Gamma^\star = H(\bar{\eta}) + \Delta_2$ for all $\xi \in \omega$. Note that, since $\Delta_2 < 3U$, we have $B^-(\xi) \leq 2$ for all $\xi \in \omega$. Furthermore, in $\mathcal{D}_A \backslash (\mathcal{D}_A \cap \mathbf{RT})$ we have $\Delta_1 > \frac{1}{2}U$ and $\Delta_2 > U + 3\Delta_1$. This implies that, for $\xi \in \omega$,

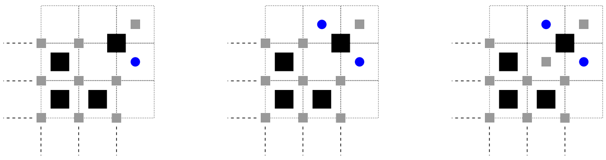
(i) if $B^-(\xi) = 1$, then $n_1^+(\xi) \leq 2$;
(ii) if $B^-(\xi) = 2$, then $n_1^+(\xi) \leq 1$.

Fig. 4.11 shows the different classes of edges along which the first heavy–step of a modifying path is possible. We will group modifying paths according to the edge along which the first heavy-step is made. Note that $\Delta_2 < 3U + \Delta_1$ in region **RA** and so Lemma 4.26 applies. Therefore, as a first possible heavy-step, we need to consider only those consisting of the motion of a corner particle of type 2 along the edge where it shares a bond with a corner particle of type 1. In order to identify particles and edges, we refer to Fig. 4.11.

Step 1:

Claim 4.30 *All modifying paths starting with a heavy-step involving a particle of type* 2 *other than that in the protuberance exceed energy level* $\Gamma^\star$*.*

Proof. **1.** Asumme that he first heavy-step is along edge c. Let x be the site where the particle p_1 that we want to move sits in configuration $\bar{\eta}$. Let η_{1-} be the configuration visited just before the first heavy-step is performed, and let η_1 be



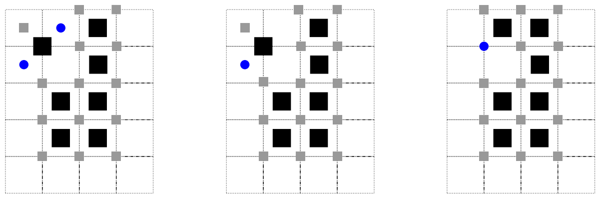
(a) (b) (c)

Figure 4.15: Region **RA**, first heavy–step along edge c.

the configuration that is reached when p_1 is moved one step North-East to site y. There are four possible cases.

- $B(p_1, \eta_1) = 0$. Let us assume that all free particles of type 1 are removed from Λ. Then $H(\eta_1) - H(\bar{\eta}) = 4U - \Delta_1 > \Delta_2$ and hence the path exceeds energy level $\Gamma^\star$.
- $B(p_1, \eta_1) = 1$: $H(\eta_1) - H(\bar{\eta}) = 3U > \Delta_2$.
- $B(p_1, \eta_1) = 2$. Let us assume that the two sites occupied by a particle of type 1 are y_1 (South-East of y) and y_2 (North-East of y). Since $\Delta_1 < U$, the least expensive way in terms of energy cost to have $B(p_1, \eta_1) = 2$ is achieved by bringing one extra particle of type 1 in Λ (see Fig. 4.15(a)): $H(\eta_1) - H(\bar{\eta}) = 2U + \Delta_1$. Therefore, starting from η_1, only moves that do not increase the energy are possible. Since η_1 is not equivalent to any configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$, at least one extra heavy-step is necessary from η_1. By Remark 4.28, the first heavy-step from η_1 cannot be completed by moving p_1 back to x. Before the next heavy-step is performed, the only moves from η_1 that do not increase the energy further are motions of particles of type 1 with one active bond to or from a site adjacent to p_1. In particular, it is not possible to bring inside Λ any other particle or type 1. Any possible sequence of such moves cannot change the energy of the configuration. When the next heavy-step is completed, at least one extra bond is added and energy level $\Gamma^\star$ is exceeded.
- $B(p_1, \eta_1) = 3$ (see Fig. 4.15(b)). Similarly to the previous case, the least expensive way to have $B(p_1, \eta_1) = 3$ is achieved by bringing two extra particles of type 1 inside Λ. From η_1 at least one other heavy-step is necessary, and moves that increase the energy are not allowed. As in the previous case, only motions of particles of type 1 that do not decrease the number of bonds are allowed (see, for instance, Fig. 4.15(c)), and the completion of the next heavy-step exceeds energy level $\Gamma^\star$.

2. Assume that the first heavy–step is along edge d. Let x be the site where



(a) (b) (c)

Figure 4.16: Region **RA**, first heavy–step along edge d.

the particle p_1 that we want to move sits in configuration $\bar{\eta}$. Let η_{1-} be the configuration visited just before the first heavy-step is performed, and let η_1 the configuration that is reached from η after moving p_1 one step North-West along the edge d to site y. Also, let p_2 denote the particle of type 2 in the tile protuberance, and p_3 the particle of type 2 at dual distance one from p_1 in the South direction in configuration $\bar{\eta}$. As in the previous case, after the heavy-step is performed we must have $B(p_1, \eta_1) \geq 2$.

- $B(p_1, \eta_1) = 3$. The best choice is when $B^-(\eta_1) = 1$ and $n_1^+(\eta_1) = 2$ (see Fig. 4.16(a)). From η_1 only moves that do not increase the energy are possible. There is only possible one non-backtracking move: the particle of type 1 South-West of x is moved one step North-East. After this move, it is only possible to move the particle of type 1 South-West of p_1 one step South-West. The configuration that is reached does not belong to $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ and no other move is allowed (this is the analogue of $B(p_1, \eta_1) = 3$ in the previous case).

- $B(p_1, \eta_1) = 2$. As in the previous case, the choice that minimizes the energy of η_1 is such that $B^-(\eta_1) = 2$ and $n_1^+(\eta_1) = 1$, and the particles of type 1 adjacent to p_1 sit at sites y_1 and y_2, respectively, South-West and North-West of y (see Fig. 4.16(b)). It is easy to see that this is the choice that allows for "more freedom" of the path, in the sense that it is the only choice from which it is possible to complete a further heavy-step. Therefore, only moves that do not increase the energy are allowed starting from η_1, and again note that no other particle of type 1 is allowed to enter Λ. From η_1 at least one other heavy-step is necessary. This means that from η_1 it is only possible to move p_1 one step North-East to site z (this case will be examined afterwards) or to start a sequence of moves of particles of type 1 to or from a site adjacent to p_1. Any possible sequence of such moves cannot decrease the energy of the configuration and only a heavy-step can be completed by moving p_1 one step North-East to site z to reach configuration η_2. Clearly, the configurations the path can reach (strictly) below $\Gamma^\star$ from η_2 are the same as those that can be reached from η_3 by saturating p_1 with the two free particle of type 1 (see Fig. 4.16(c)). Arguing as in the previous case, we see that the only heavy-step possible without exceeding energy level $\Gamma^\star$ from η_3 is the one that is completed by moving p_1 back to site y (configuration η_4). The transition from η_3 to η_4 can be treated in the same way as that from $\bar{\eta}$ to η_1, and so we conclude that from η_4 it is only possible to reach a configuration equivalent to $\bar{\eta}$.

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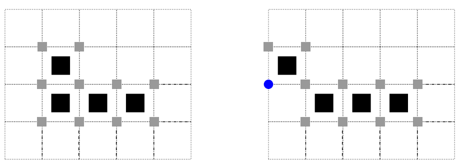
Step 2:

Claim 4.31 *Let the first step of a modifying path starting from a configuration in $\mathcal{D}_A$ involve the particle p of type 2 in the protuberance. If p is not re-attached to the main cluster before the next heavy-step is completed, then the path exceeds energy level $\Gamma^\star$ before reaching a configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$.*

Proof. The proof of this claim will be deferred to the proof of Lemma 4.35, Step 1, in Section 4.5.2. There it will be shown that the same claim holds also in region **RB**, where the values that Δ_2 can take are larger than those that Δ_2 can take in **RA**. ★

Depending on its starting position, the protuberance can be re-attached in two possible ways: either the particle of type 2 shares two particles of type 1 with the other particles of type 2 in the cluster (see Fig. 4.17(a)), or it shares only one particle of type 1 (see Fig. 4.17(b)). In both cases we consider the evolution of the path to a 2–tiled configuration that is equivalent to the one reached the moment the particle of type 2 joins the main cluster. In the first case, the configuration is again in the class $\mathcal{D}_A$, and hence the same kind of argument can be repeated. In the second case, the following statement allow us to conclude the proof of Lemma 4.29.



(a) (b)

Figure 4.17: Modifying paths may create hanging protuberances.

In the first case, the configuration is again in the class $\mathcal{D}_A$ and, hence, the same kind of analysis can be repeated. In the second case, the following statement allow us to conclude the proof of the lemma.

Step 3:

Claim 4.32 *From a configuration consisting of a 2–tiled rectangle plus a hanging protuberance it is not possible to reach a configuration in* $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}\backslash\mathcal{D}_A$ *without exceeding energy level* $\Gamma^\star$.

Proof. Let η_0 be the configuration of Fig. 4.17(b), η_1 the configuration reached when the first heavy-step from η_0 is completed, and η_{1-} the configuration visited by the path just before η_1. Let p_1 be the particle of type 2 in the hanging protuberance and p_2 the particle of type 2 at dual distance $\sqrt{2}$ in the South-East direction from p_1. Let q_1 denote the particle of type 1 shared by p_1 and p_2. We will show that if the first heavy-step from η_0 is not completed by moving p_1 one step North-East of one step South-West (the two cases are analogous), then the path exceeds energy level $\Gamma^\star$. From Lemma 4.26 and Step 1 it follows that, in order to prove the claim, we need to consider only the heavy-steps completed by moving p_1 North-West or South-East and p_2 North-West.

- Assume that p_1 is moved one step South-East. Observe that $B(p_1,\eta_1) \leq 2$ and $B(p_2,\eta_1) \leq 3$. Clearly, since $\Delta_1 < U$, the choice that is most favorable from the point of view of energy is when p_1 has 2 active bonds and p_2 has 3 active bonds. It is clear that, since η_1 is reached from η_{1-} via the motion of a particle of type 2, the two configurations have the same particles of type 1 placed at the same sites. Since $B(p_1,\eta_1) = 2$, there is no advantage in having more than two particles of type 1 adjacent to p_1 in η_{1-}, since one bond will be lost anyway with the motion of p_2. It follows that $H(\eta_1) - H(\bar{\eta}) = 3U + \Delta_1 > \Delta_2$ (see Fig. 4.18(a)). Arguing in the same way, we see that in the case where the first heavy-step from η_0 is completed by moving p_2 one step North-West, we have $H(\eta_1) - H(\bar{\eta}) = 3U + 2\Delta_1 > \Delta_2$ (see Fig. 4.18(b)). (Note that $3U + \Delta_1 > \Delta_2$ also in region **RB**, and so these moves will be forbidden there as well.)
- Assume that the first heavy-step is in the North-West direction. Then the only possibility without exceeding energy level $\Gamma^\star$ is when $B(p_1,\eta_1) = 2$. This is achieved, for instance, by moving the two particles of type 1 on the West side of p_1 one step North-West before completing the heavy-step. Since η_1 has two broken bonds, it is not possible to break any extra bond, and hence no extra heavy-step is possible as long as the particle of type 1 does not reach a site adjacent to p_1. Let η_2 be such a configuration (see Fig. 4.18(d)). Since η_2 has one broken bond and one extra particles of type 1, the next heavy-step (completed by moving either p_1 or p_2) cannot break more than one bond, but clearly this is impossible.
- Assume that the first heavy-step is completed by moving p_1 North-East (see

Fig. 4.18(c)). Then η_1 is a configuration that can be reached with one heavy-step from a configuration in $\mathcal{D}_A$, and hence the claim in Step 2 holds. This can be done by moving the two particles of type 1 North of p_1 one step North-East (breaking two active bonds), moving p_1 one step North-East ($\Delta H = 0$) and removing the free particle of type 1 froma Λ ($\Delta H = -\Delta_1$).

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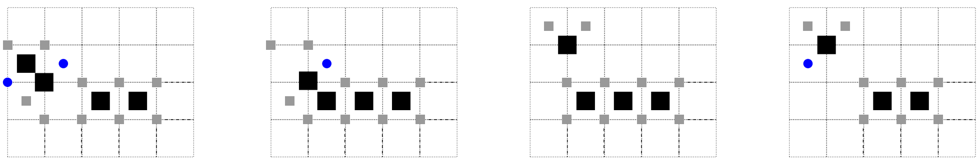


(a) (b) (c) (d)

Figure 4.18: Region **RA**, first heavy–step along edge e.

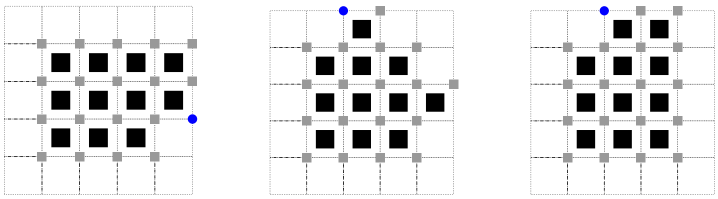
Existence of a good site

Lemma 4.33 *For all $\hat{\eta} \in \mathcal{D}_A$, there exists an $x \in F(\hat{\eta})$ such that $\Phi((\hat{\eta}, x), \boxplus) < \Gamma^\star$.*

Proof. Configurations in $\mathcal{D}_A$ consist of a dual 2–tiled square and a protuberance on one of the four sides. If the protuberance is on the longest side, then the rectangle circumscribing the cluster is a square of side length $\ell^\star$. Conversely, if the protuberance is on one of the shortest sides, then the rectangle circumscribing the cluster has side lengths $\ell^\star - 1, \ell^\star + 1$. Without loss of generality, we assume that the longest side of the rectangle is horizontal and that the protuberance is on the North side of the rectangle when it is attached to the longest side and on the East side when it is attached to the shortest side.

- Assume that the protuberance is on the longest side. Let x be the central site of a tile adjacent to the protuberance to the North side of the rectangle. After a particle of type 2 has entered Λ and has been moved to x, a configuration with energy $\Gamma^\star - 3U$ is reached. The particle at site x can be saturated within the energy barrier Δ_1, to reach a configuration with energy $\Gamma^\star - \Delta_2 - \varepsilon < H(\eta)$ for all $\eta \in \mathcal{D}_A$, consisting of a rectangle of side lengths $\ell^\star, \ell^\star - 1$ plus a 12–bar of length 2 on its (longest) north-side. Then, within energy barrier Δ_2, the 12–bar can be completed to obtain a 2–tiled dual square of side length $\ell^\star$. The claim in the lemma follows from Remark 4.11. Such a configuration is supercritical (and has energy smaller than the standard configuration with $\ell^\star(\ell^\star - 1)$ particles of type 2). Therefore it can grow until $\boxplus$ is reached while staying below energy level $\Gamma^\star$.

- Assume that the protuberance is on the shortest side. Let x be the central site of a tile adjacent to the protuberance to the East side of the rectangle. After a particle of type 2 has entered Λ and has been moved to x, a configuration with energy $\Gamma^\star - 3U$ is reached. The particle at site x can be saturated within energy barrier Δ_1, to reach a configuration with energy $\Gamma^\star - \Delta_2 - \varepsilon < H(\eta)$ for all $\eta \in \mathcal{D}_A$, consisting of a rectangle of side lengths $\ell^\star, \ell^\star - 1$ plus a 12–bar of length 2 on its shortest (see Fig. 4.19(a)).



(a) (b) (c)

Figure 4.19: Region **RA**, first heavy–step along edge e.

Let y be the central site of a tile adjacent to the North side of the rectangle of side lengths $\ell^\star, \ell^\star - 1$. One of the dimers of the 12–bar of length 2 can be moved within energy barrier $3U$ (note that $3U - \Delta_2 - \varepsilon < 0$) to the north Side of the rectangle (as described in Section 4.4.1), with the particle of type 2 at site y, to reach a configuration with energy $\Gamma^\star - \Delta_2 - \varepsilon + U$. The particle of type 2 can be saturated using one of the corner particle of type 1 adjacent to the protuberance that is left on the East side. This is done within energy barrier U, and the resulting configuration again has energy $\Gamma^\star - \Delta_2 - \varepsilon + U$ (see Fig. 4.19(b)). Finally, move the pending dimer that is left on the East side to a corner adjacent to the tile centered at site y (see Fig. 4.19(c)). As described in Section 4.4.1, this can be done within energy barrier $2U$ (since the particle of type 2 of the dimer has only one neighboring corner particle of type 1). The configuration obtained in this way consists of a rectangle of side lengths $\ell^\star, \ell^\star - 1$ plus a 12–bar of length 2 on its longest North-side. It is now possible to continue as in the previous case. Note that, to move the 12–bar of length 2 from the East side to the North side, we implicitly assumed that these sides of the rectangle are far from the boundary of Λ.

Now suppose that the protuberance was originally on a side of the rectangle close to $\partial^- \Lambda$. Then we can proceed in the following way. After the 12–bar of length 2 has been completed, it is possible to complete the 12–bar below energy level $\Gamma^\star$ and obtain a 2–tiled rectangle of side lengths $\ell^\star+1, \ell^\star-1$. From this configuration it is possible to iteratively remove $\ell^\star-3$ corner 2–tiles from the shortest side of the rectangle that is far from $\partial^-\Lambda$, in order to obtain a 2–tiled configuration where the 12–bar of length 2 is far from $\partial^-\Lambda$ as well. Clearly, this can be achieved below energy level $\Gamma^\star$. It is now possible to proceed as in the previous case, observing that either the North side or the South side of the rectangle is far from $\partial^-\Lambda$.

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Identification of $\mathcal{P}$ and $\mathcal{C}^\star_{\mathrm{bd}}$

Lemma 4.34 $\mathcal{P} = \mathcal{D}_A$ *and* $\mathcal{C}^\star_{\mathrm{bd}} = \mathcal{D}_A^{\mathrm{bd2}}$.

Proof. All configurations in $\mathcal{D}_A^{\mathrm{bd2}}$ have energy $\Gamma^\star$. We will show that all configurations in $\mathcal{D}_A^{\mathrm{bd2}}$ are essential saddles, and therefore belong to $\mathcal{G}(\square, \boxplus)$ by Lemma 4.3. Pick $\eta = (\hat{\eta}, x)$ in $\mathcal{D}_A^{\mathrm{bd2}}$.

Let $\mathcal{U}(\eta)$ be the set of optimal paths entering $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ via configuration η. Pick $\omega \in \mathcal{U}(\eta)$ such that $H(\xi) < \Gamma^\star$ for all $\xi \in P_\omega(\eta)$ and $S_\omega(\eta) = \{(\hat{\eta}, y_1), \dots, (\hat{\eta}, y_m), \dots, \boxplus\}$, with $y_i \notin \partial^-\Lambda$ for all $i \in 1, \dots, m$ and y_m in $F(\hat{\eta})$ such that $H(\xi) < \Gamma^\star$ for all $\xi \in S_\omega((\hat{\eta}, y_m))$. Note that such a path ω exists because:

(i) $\hat{\eta} \in g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ by Lemma 4.29;
(ii) there exists an $y_m \in F(\hat{\eta})$ such that $\Phi((\hat{\eta}, y_m)) < \Gamma^\star$ by Lemma 4.33;
(iii) in configuration η there exists a lattice path of empty sites $y_1, \dots, y_m$ with $y_1 \sim x$ and $y_i \notin \partial^-\Lambda$ for all $i \in 1, \dots, m$, since for all $x \in \partial^-\Lambda$ there exists an $y \sim x$ such that $y \notin \partial^-\Lambda$ (by the shape of Λ), and $[\hat{\eta}]$ is "sufficiently far" from $\partial^-\Lambda$ (i.e., there is a border of width 3 in Λ where particles do no interact).

Next, note that all saddles in $S_\omega(\eta)$ are configurations of the type $\eta' = (\hat{\eta}, u)$, $u \notin \partial^-\Lambda$. Recall Definition 4.2(e). We have to show that $S(\omega') \not\subseteq S(\omega)\backslash\{\eta\}$ for all $\omega' \in (\eta, \eta')_{\mathrm{opt}}$. Consider the partition $(\square \to \boxplus)_{\mathrm{opt}} = (\mathcal{U}(\eta), \mathcal{U}^c(\eta))$ with $\mathcal{U}^c(\eta) = (\square \to \boxplus)_{\mathrm{opt}} \backslash \mathcal{U}(\eta)$. If $\omega' \in \mathcal{U}(\eta)$, then $S(\omega') \not\subseteq S(\omega)\backslash\{\eta\}$ because $\eta \in \omega'$. If, on the other hand, $\omega' \in \mathcal{U}^c(\eta)$, then, by Lemma 4.15(1), ω' enters the set $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ via some configuration $\zeta = (\hat{\zeta}, z)$ with $H(\zeta) = \Gamma^\star$ and $z \in \partial^-\Lambda$ that does not belong to $S(\omega)$ (by the construction of ω). Since the choice of $\eta \in \mathcal{D}_A^{\mathrm{bd2}}$ was arbitrary, we conclude that all configurations in $\mathcal{D}_A^{\mathrm{bd2}}$ are essential saddles, and hence that $\mathcal{D}_A^{\mathrm{bd2}} \subset \mathcal{G}(\square, \boxplus)$.

To prove that $\mathcal{D}_A^{\mathrm{bd2}} = \mathcal{C}_{\mathrm{bd}}^\star$, i.e., $\mathcal{D}_A^{\mathrm{bd2}}$ is the entrance of the essential gate, we will show that, for any path $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$, any configuration $\zeta \in \mathcal{S}(\square, \boxplus)$ that is visited by ω before some configuration in $\mathcal{D}_A^{\mathrm{bd2}}$ is an unessential saddle and therefore does not belong to $\mathcal{G}(\square, \boxplus)$.

- We show that all saddles in $\mathcal{V}_{\star,\leq \ell^\star(\ell^\star-1)+1}$ are unessential. To that end, we pick $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ and we let $\zeta \in \omega$ be such that $H(\zeta) = \Gamma^\star$ and $n_2(\zeta) \leq \ell^\star(\ell^\star - 1) + 1$. By Lemma 4.15(1), all optimal paths enter $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ via a configuration in $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+2})^{\mathrm{bd2}}$. Hence, after visiting ζ, ω must visit $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+2})$ before entering $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$. By Lemma 4.29, combined with Lemma 4.17, we have $\bar{g}(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+2}) = g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+2})$. The claim now follows via Lemma 4.18(1).
- For all $\omega \in (\square \to \boxplus)_{\mathrm{opt}}$ such that $\xi \in S(\omega)$ and $\xi \in \mathcal{V}_{\star,\geq \ell^\star(\ell^\star-1)+2} \backslash \mathcal{D}_A^{\mathrm{bd2}}$, there exists an $\eta \in \mathcal{D}_A^{\mathrm{bd2}}$ such that $\eta \in P_\omega(\xi)$. Indeed, by Lemmas 4.15(1) and 4.29, all optimal paths enter $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ via a configuration in $\mathcal{D}_A^{\mathrm{bd2}}$.
- To conclude, we need to show that $\mathcal{P} = \mathcal{D}_A$. The inclusion $\mathcal{P} \supseteq \mathcal{D}_A$ is immediate, since all $\eta = (\hat{\eta}, x) \in \mathcal{D}_A^{\mathrm{bd2}} = \mathcal{C}_{\mathrm{bd}}^\star$ are obtained, in a single step, by adding a particle of type 2 at the boundary of Λ to a configuration $\hat{\eta} \in g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \mathcal{D}_A$. To see that $\mathcal{P} \subseteq \mathcal{D}_A$, suppose that there is a configuration $\hat{\eta} \in \mathcal{P} \backslash \mathcal{D}_A$. Let $\hat{\eta}'$ be the configuration in $\mathcal{C}_{\mathrm{bd}}^\star = \mathcal{D}_A^{\mathrm{bd2}}$ obtained in a single step from $\hat{\eta}$. Observe that $\mathcal{D}_A^{\mathrm{bd2}} \subset \Rsh\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$. Since, by Lemma 4.15(1), all optimal paths enter $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+2}$ by adding a particle of type 2 at $\partial^-\Lambda$ to a configuration in $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \mathcal{D}_A$, it follows that $\hat{\eta} \in \mathcal{V}_{\star,\geq \ell^\star(\ell^\star-1)+2}$. Indeed, by assumption, this configuration cannot be in $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \mathcal{D}_A$. In particular, it follows that $\hat{\eta} \in \mathcal{V}_{\star,\geq \ell^\star(\ell^\star-1)+2} \backslash \mathcal{D}_A^{\mathrm{bd2}}$. But this means that there is a path $\hat{\omega} \in (\square \to \boxplus)_{\mathrm{opt}}$ that reaches $\hat{\eta} \in \mathcal{V}_{\star,\geq \ell^\star(\ell^\star-1)+2} \backslash \mathcal{D}_A^{\mathrm{bd2}}$ and does not contain any configuration in $\mathcal{G}(\square, \boxplus)$. In particular, $\hat{\omega}$ does not contain any configuration in $\mathcal{D}_A^{\mathrm{bd2}}$. But this is a contradiction, since by Lemmas 4.15(1) and 4.29, all optimal paths enter $\mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ via a configuration in $\mathcal{D}_A^{\mathrm{bd2}}$.

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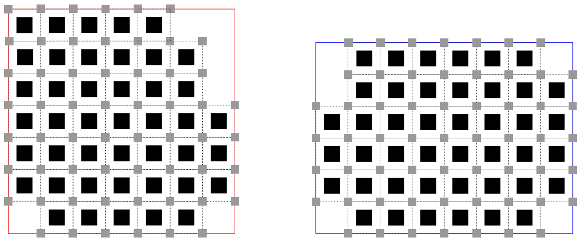
4.5.2 Region RB

In this section we prove Theorem 4.9.

Let $\mathcal{D}_B$ be the set of 2–tiled configurations with $\ell^\star(\ell^\star - 1) + 1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing rectangle has side lengths either $\ell^\star, \ell^\star$ or $\ell^\star+1, \ell^\star-1$ (see Fig. 4.20). Note that $\mathcal{D}_B \supseteq \mathcal{D}_A$.



(a) (b)

Figure 4.20: Two examples of configurations in $\mathcal{D}_B$ for $\ell^\star = 7$.

Identification of $g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ and $\bar g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$

There are configurations in $\mathcal{D}_B$ that cannot be reached within energy level $\Gamma^\star$. These configurations have support near the boundary of Λ and for $\Lambda \to \mathbb{Z}^2$ form a negligible fraction of $\mathcal{D}_B$.

Lemma 4.35 $g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \bar g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) \subseteq \mathcal{D}_B$.

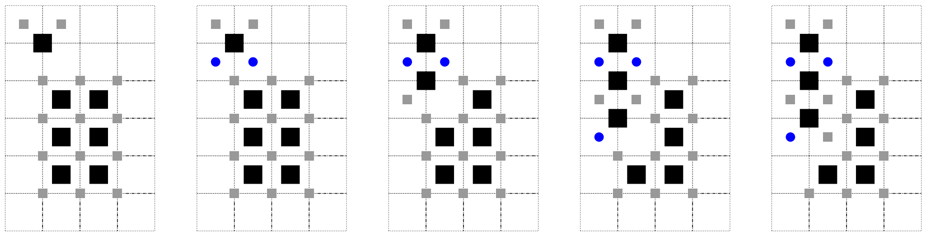
Proof. Note that in $\mathcal{D}_B$, for $\xi \in \mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ the following conditions are satisfied

(i) $B^-(\sigma) = 1$: $n_1^+(\sigma) \le 3$;
(ii) $B^-(\sigma) = 2$: $n_1^+(\sigma) \le 1$.
(iii) $B^-(\sigma) = 3$: $n_1^+(\sigma) \le 0$.

Observe that $\Delta_2 \le 3U + \Delta_1$ throughout region **RB**, and therefore Lemma 4.26 applies. This means that any heavy-step, completed without exceeding energy levl $\Gamma^\star$ and starting from a configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$, necessarily involves a corner particle of type 2 that is moved along the edge where it shares a bond with a corner particle of type 1.

From Remark 4.25 it follows that all 2–tiled configurations with a monotone dual support, a circumscribed rectangle of side lengths $(\ell^\star, \ell^\star)$ or $(\ell^\star-1, \ell^\star+1)$, and with a fixed lower left corner far enough from $\partial^-\Lambda$, belong to $g(\bar\eta, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. It remains to show that all other configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ cannot be reached without exceeding energy level $\Gamma^\star$. As in the case of the analogous lemma for region **RA**, the proofs comes in various steps.

Step 1: Let the first step of a modifying path starting from a configuration in $\mathcal{D}_A$ involve the particle p of type 2 in the protuberance. If p is not re-attached to the main cluster before the next heavy-step is completed, then the path exceeds energy level $\Gamma^\star$ before reaching a configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$. Therefore we may consider a path whose first heavy-step involves the protuberance and whose second heavy-step does not.



(a) η_1 (b) η_2 (c) η_3 (d) η_4 (e) η_5

Figure 4.21: The presence of a detached 2–tile precludes the motion of other 2–tiles.

Let $\bar{\eta}$ be a standard configuration whose protuberance on the North side belongs to the Western-most bar, and let η_1 (see Fig. 4.21(a)) be the configuration reached by completing a heavy-step that moves the particle p_1 in the protuberance one step North-West. Since the second heavy-step of the path does not involve a motion of p_1, we may assume that from configuration η_2 (see Fig. 4.21(b)) the path saturates particle p_1 with two extra particles of type 1. It will become clear later on that this choice for η_0 and η_1 is the most interesting, since after the next heavy-step is completed the particle of type 2 that is moved can share two particles of type 1 with p_1.

Let p_2 be the North-West particle of type 2 in the 2–tiled rectangle of η_2, p_3 the particle of type 2 below p_2, and p_4 the particle of type 2 East of p_2. It is easy to check that any heavy-step completed by moving any other corner particle of type 2 other than p_2 leads to an energy above $\Gamma^\star$. Since η_2 has two extra particle of type 1, the next heavy-step must be completed by breaking at most one bond. (Note that in η_2 all external particles of type 1 are saturated and hence at least one bond must be broken.) This means that the next particle of type 2 must be moved from one good dual corner to another, and the corner must be created by breaking exactly one bond. It follows that the only heavy-step from η_2 that can be completed is the one obtained by moving p_2 one step North-West with a particle of type 1 sitting South-West of it (configuration η_3; see Fig. 4.21(c)). From η_3 it is not allowed to break other bonds. As a consequence, the only heavy-steps that are possible are completed by moving p_4 South-East or p_3 North-East. These two cases are analogous. We describe the second one.

When p_2 is moved North-East, the total number of bonds cannot be decreased. This can be achieved by moving one step North-West the particle of type 1 adjacent to p_3 in η_3, and with the help of one extra particle of type 1 reaching the South-West of the "destination" of p_3 (configuration η_4; see Fig. 4.21(d)). From η_4 it is not allowed to increase the energy. Since in η_4 all particles of type 2 have at least three active bonds, the motion of the next particle of type 2 must be from a good dual to another. But from η_4 only the motion of corner particles of type 1 is allowed (configuration η_5; see Fig. 4.21(e)), and it is not possible to create a good dual corner without bringing a further extra particles of type 1 inside Λ. Hence the path cannot be extended with another heavy-step without exceeding energy level $\Gamma^\star$.

Step 2: In this step we will consider the evolution of those paths that visit a 2–tiled configuration having a hanging protuberance. For definiteness, we take η to be a configuration consisting of a 2–tiled rectangle plus a hanging protuberance at the North-West corner (see Fig. 4.17(b)). Let p_1 be the particle of type 2 in the hanging protuberance, and let p_2 be the particle of type 2 South-East of p_1.

If the first heavy-step from η is not completed by moving p_1 in the North-West, South-West or North-East direction, then the path exceeds energy level $\Gamma^\star$ before reaching a configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$. From Step 3 in the proof of Lemma 4.34, we already know that it is not possible to move p_1 South-East nor p_2 North-West. We will investigate what happens when some other corner particle of type 2 is moved to complete the first heavy-step from η.

Suppose that the first heavy-step is completed by moving particle p_3 of type 2 in the North-East corner tile of the rectangle (configuration η_1). It is easy to see that this move is only possible below energy level $\Gamma^\star$ when, in η_1, p_3 has three adjacent particles of type 1. This can be achieved by bringing inside Λ two extra particles of type 1 (see Fig. 4.22). From η_1 it is not possible to further increase the energy without exceeding energly level $\Gamma^\star$, and it is immediate that no other heavy-step is allowed.

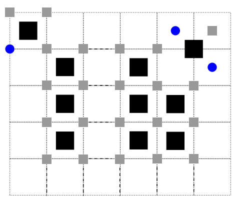
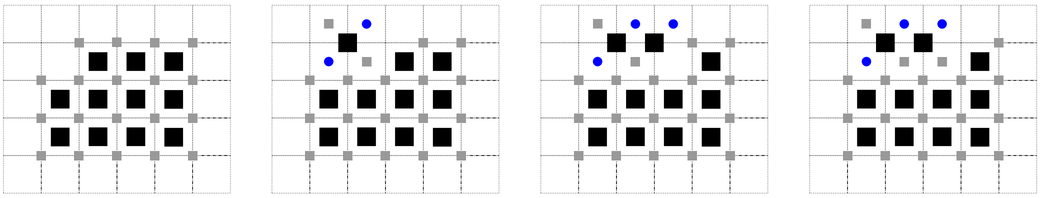


Figure 4.22: The presence of a hanging protuberance precludes the motion of other 2–tiles.

Step 1 and 2 imply the following. A modifying path that does not exceed energy level $\Gamma^\star$ and starts with any heavy-step involving the particle of the protuberance must "go back" to a configuration equivalent to a configuration in $\mathcal{D}_A$ before some other particle of type 2 can be moved.

Step 3: Let the first heavy-step from a configuration $\eta_0 \in \mathcal{D}_B$ be completed by moving a corner particle p of type 1 belonging to a 12–bar of dual length $m \geq 3$. If p is not re-attached to the main cluster before the next heavy-step is completed, then the path exceeds energy level $\Gamma^\star$ before reaching a configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$.



(a) η_0 (b) η_1 (c) η_2 (d) η_3

Figure 4.23: First heavy-step from a bar of length ≥ 3.

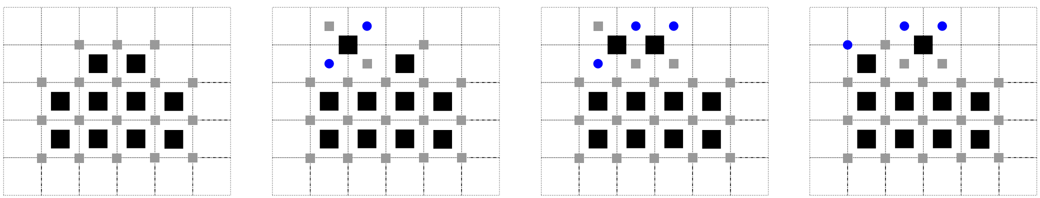
Let η_0 be as in Fig. 4.23(a), and let p_1, p_2 and p_3 be the first three particles of type 2, starting from the West, of the Northern-most 12–bar. Let the first heavy-step from η_0 be completed by moving p_1 North-West. Since we are assuming that the second heavy-step is not completed by moving p_1, we may consider the path from η_1 that is obtained by saturating p_1 with two extra particles of type 1 and by moving the particle North-West of p_2 one step South-West (see Fig. 4.23(b)). Note that η_1 can be reached within energy barrier $U + 3\Delta_1$.

Since from η_1 it is not allowed to break another extra bond, the only possible heavy-step is the one obtained by moving p_2 North-West after an extra particle of type 1 has entered Λ and has reached a site adjacent to the destination of p_2 (configuration η_2; see Fig. 4.23(c)). From η_2 it is not possible to further increase the energy without exceeding level $\Gamma^\star$, and a further heavy-step is therefore not possible.

Remark: Note that the key observations here are the following. After p_1 has moved, two extra particles of type 1 are required to saturate it. The presence of two extra particles of type 1 forces the path to evolve without breaking extra bonds. Since all the external particles of type 2 other than p_1 have at least three active bonds, the motion must necessarily be towards a good dual corner (a site with three neighbors occupied by a particles of type 1). Note that when a particle is moved, it changes its parity and only particles with the same parity can interact. When the second particle p_2 of type 2 is moved, it takes the parity of the particles in the tile p_1 belongs to. But after p_2 is moved, it can share at most two particles of type 1 with p_1, and hence another particle of type 1 is needed. This leads to a configuration with 3 extra particles of type 1 and one broken bond, and hence it is not allowed to make moves that increase the energy. In particular, it is not allowed to bring inside Λ other particles of type 1, and only particles of type 1 with one active bond can be moved. Note that, again, all particles of type 2 have at least three active bonds. Hence, a further heavy-step would only be possible if a good dual corner can be created close to a particle of type 2 without decreasing the number of bonds. These observations are key in order to explore what configurations can be reached by a modifying paths without exceeding $\Gamma^\star$.

Step 4: Let the first heavy-step from a configuration $\eta_0 \in \mathcal{D}_B$ be completed by moving a corner particle p_1 of type 2 belonging to a 12–bar of dual length $m = 2$. If the path does not exceed energy level $\Gamma^\star$, then one of the following must happen:

- Particle p is re-attached to the cluster before any other particle of type 2 is moved.
- If p_1 denotes the other particle of type 2 in the bar, then the path reaches a configuration η_d where p_1 and p_2 are saturated (with the help of three extra particles of type 2), belong to the same cluster and are at dual distance $\sqrt{2}$ from its location in η_0 (see Fig. 4.24(c)). From η_d, the first heavy-step (without backtracking) must be completed by re-attaching p_1 to the cluster. The configuration that is reached in this way is again a configuration that can be reached with a single heavy-step completed by moving a corner particle of type 2 belonging to a 12–bar of dual length $m = 2$ (see Fig. 4.24(d)).



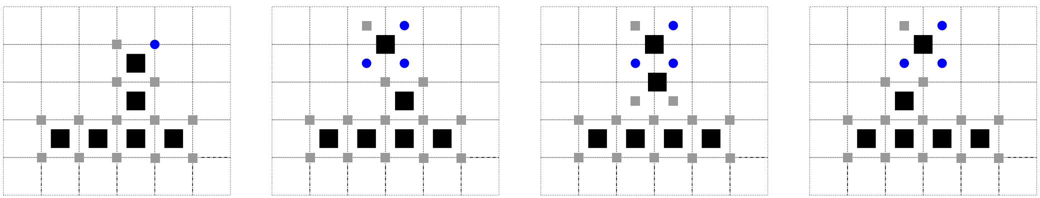
(a) η_0 (b) η_1 (c) η_d (d) η_2

Figure 4.24: First heavy-step from a bar of length 2.

Let p_1 be the Western-most particle of type 2 in the bar of length 2 in configuration η_0, and p_2 the particle of type 1 East of p_1 (see Fig.4.24(a)). Let the first heavy-step from η_0 be completed by moving p_1 North-West. Suppose that p_1 is not re-attached to the cluster before the next heavy-step is completed. As in Step 3, we can consider the path from η_1 obtained by saturating p_1 with two extra particles of type 1 and by moving the particle North-West of p_2 one step South-West (see Fig. 4.24(b)). Note that η_1 can be reached within energy barrier $U + 3\Delta_1$.

Since from η_1 it is not allowed to break another bond, the only possible heavy-step is the one obtained by moving p_2 North-West after an extra particle of type 1 has entered Λ and has reached a site adjacent to the destination of p_2. After that, since it is not possible to further increase the energy, before the next heavy-step is completed it is necessary to move a particle of type 1 to the empty site adjacent to p_2, reaching configuration η_d. The first heavy-step from η_d, since it contains three extra particles of type 1, must be completed breaking at most one bond. This means that a particle of type 1 must be moved from a good dual corner to another. This is only possible, without backtracking, by moving p_1 one step South-West to site x after the particle of type 1 sitting at x in η_d has been moved one step North-West. Particle p_1 can be saturated with a free particle of type 1, to reach configuration η_2 of Fig. 4.24(d). Note that η_2 is the "mirror image" of η_1, and hence the same arguments can be repeated.

For further reference, let us consider also a configuration with a vertical 12–bar of length 2. Such a configuration η_v does not belong to $\mathcal{D}_B$, but could be reached by a modifying path below energy level $\Gamma^\star$ (see Fig. 4.25(a)).



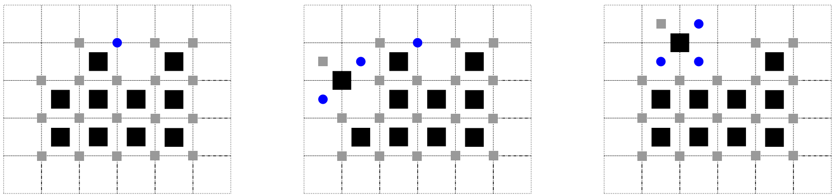
(a) η_v (b) η_w (c) η_x (d) η_y

Figure 4.25: Protuberances attached to 12–bars can be treated as 12–bars of length 2.

The analysis is completely analogous to the case of a horizontal 12–bar of length 2, and the claim is that if the first heavy-step is completed by moving the particle p_1 of type 2 on top of the vertical 12–bar and the path does not exceed the energy level $\Gamma^\star$, then either p_1 is re-attached to the cluster before the next heavy-step is completed, or after p_1 has been saturated (configuration η_w; see Fig. 4.25(b)) the next heavy-step must be completed by moving the other particle p_2 of type 2 originally in the 12–bar to reach a 2–tiled configuration η_x with three extra particles of type 1 where the 12–bar is "floating" on a side of the cluster (see Fig. 4.25(c)). From η_x, the only heavy-step that can be completed is the one obtained by re-attaching p_2 to the cluster. Then p_2 can be saturated to obtain configuration η_y (see Fig. 4.25(d)). Note that η_y is the mirror image of η_w and the same argument can be repeated. Note that when p_1 is re-attached, either a configuration with again a vertical 12–bar of length 2 is reached, or the path visits a configuration where p_1, after being saturated, belongs to a hanging protuberance. We will see below that in this case the next heavy-step must be completed by moving p_1 again.

Thus, after the first heavy-step from a configuration η_0 in $\mathcal{D}_B$ is completed by moving a particle p_1 of type 2, this particle must be re-attached to the cluster. This particle can be saturated to reach a configuration η_1 in which p_1 belongs to a (possibly hanging) protuberance. Note that η_1 contains one extra particle of type 1, and therefore $H(\eta_1) = H(\eta_0) + \Delta_1$. Note that in the case p_1 belonged to a bar of length 2, and configuration η_1 contains two protuberances.

We claim that, from η_1, the first heavy-step must be completed by moving a particle of type 1 in one of the protuberances. This can be seen as follows.



(a) η_1 (b) η_2 (c) η_2'

Figure 4.26: Heavy-step from a configuration with protuberances non in $\mathcal{D}_A$

1. Let η_1 be a configuration like the one in Fig. 4.26(a), and let the first heavy-step from η_1 be completed by moving the particle p_2 of type 2 sitting at the Northern-most site of the West bar of η_1 one step North-West. Let η_2 be the configuration that is reached when this heavy-step is completed (see Fig. 4.26(b)). Since η_p has already one extra particle of type 1, it is not possible to have $B(p_2, \eta_2) = 1$ (i.e., three broken bonds). Similarly, if we consider the case $B(p_2, \eta_2) = 2$, then we must require one extra particle of type 1, but this is incompatible with a configuration with two broken bonds. Therefore the only possibility is $B(p_2, \eta_2) = 1$, where the three bonds of p_1 in η_2 are obtained with the help of two extra particles of type 1. From η_2 it is not possible to increase the energy further. Since in η_2 all configurations have at least three active bonds, the next heavy-step must be completed by moving a particle of type 2 from a good dual corner to another without increasing the number of broken bonds. But this is impossible from configuration η_2.

2. Clearly the same conclusion can be reached also if p_1 belongs to a hanging protuberance (see Step 2). Note that, by completing a heavy-step from η_1 by moving p_1, the configuration that is reached is either one heavy-step away from being attached in a good dual corner to form a bar of length $m \geq 2$ (and we know that it must be re-attached by Step 3 and 4), or it is far from good dual corners. In this case, if we assume that the next heavy-step is not completed by moving again p_1, then we can consider the path from the configuration η_2' obtained by saturating p_1 (see Fig.4.26(c)). This configuration has three extra particles of type 1, and hence no heavy-step can be completed without exceeding energy level $\Gamma^\star$ by moving a particle of type 2 different from p_1. It is straightforward to see in the next heavy-step p_1 must indeed be re-attached to the cluster.

Step 5: It follows from Steps 1–4 that the set of single cluster configurations (and, consequently, the set of configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$) that can be visited by a modifying path that does not exceed energy level $\Gamma^\star$ coincides with the set of configurations that can be reached by a modifying path whose configurations do not have more than one particle of type 2 not belonging to the main cluster such that if a configuration has a particle of type 2 that is not connected to the cluster, then this particle is re-attached to the cluster in the next heavy-step, and afterwards is saturated. This means that the configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ that are reached without exceeding energy level $\Gamma^\star$ are obtained by iteratively moving a corner 2–tile around the cluster (with the help of one or two extra particles of type 1 used to saturate the particle of type 2). We already saw in Steps 1–2 that a modifying path starting from a configuration in $\mathcal{D}_A$ with a heavy-step involving the particles of type 2 in the protuberance cannot leave the set $\mathcal{D}_A$. In the other cases, if the 2–tile that is moved reaches a corner, then a new configuration in $\mathcal{D}_B$ is reached. Otherwise, a configuration with one or two protuberances not belonging to $\mathcal{D}_A$ is reached. But in this case, the path can only proceed by moving one of the protuberances, which eventually reach a corner and again producing a configuration in $\mathcal{D}_B$.

Step 6: From what has been seen so far it follows that the set of single cluster 2–tiled configurations that can be visited by a modifying path starting from a standard configuration $\bar{\eta}$ without exceeding energy level $\Gamma^\star$ consists of those configurations that can be reached by either moving the protuberance of a configuration in $\mathcal{D}_A$, or by iteratively moving corner 2–tile to some other corner possibly created by adding an extra particle of type 1. This observation implies that $\bar{g}(\Box, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) \subset \mathcal{D}_B$. Furthermore, if $\eta \in \mathcal{D}_B$ and has support far enough from $\partial^-\Lambda$, then $\eta \in g(\Box, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. It is straightforward to see that lattice distance 2 from the annulus where no interaction is present is already far enough. In order to prove that $g(\Box, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \bar{g}(\Box, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$, we will show that the set $\bar{g}(\Box, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) \backslash g(\Box, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ indeed is empty.

Remark: Note that variations in the energy are only possible when a particle of type 1 enters or leaves Λ or when the number of active bonds changes as a consequence of the motion of a particle inside Λ. This implies that, for all $\eta \in \mathcal{D}_B$, $\Phi(\bar{\eta}, \eta)$ for some standard configuration $\bar{\eta} \in \mathcal{V}_{\star,\ell^\star(\ell^\star-1)+1}$ can take only a discrete set of values. In region **RB**, $\Phi(\bar{\eta}, \eta) = \Gamma^\star$ can only happen when $\Phi(\bar{\eta}, \eta) = H(\bar{\eta}) + U + 3\Delta_1$ and $\Delta_2 = U + 3\Delta_1$.

Consider the set of 2–tiled configurations consisting of a single cluster that can be reached with the moves considered at the various stages of the previous analysis. Clearly, this set contains $\bar{g}(\bar{\eta}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$. Let η' belong to this set, and let $\omega : \bar{\eta} \to \eta'$. Assume that $\max_{\xi\in\omega} H(\xi) = U + 3\Delta_1$ and let $\mathrm{supp}(\omega) = \cup_{\xi\in\omega}\mathrm{supp}(\xi)$. Then, from the previous analysis, it follows that there is a path $\omega' : \bar{\eta} \to \eta'$ such that $\max \xi \in \omega' H(\xi) = H(\bar{\eta} + 3U$ and $\mathrm{supp}(\omega') \subset \mathrm{supp}(\omega)$. In words, if a configuration in $\mathcal{D}_B$ can be reached within energy barrier $U + 3\Delta_1$, then it can also be reached within energy barrier $3U$, irrespective of the distance from the boundary of Λ. ★

Remark 4.36 *Let η be a 2–tiled conconfiguration of minimal energy with a fixed number of particles of type 2, and let $R(\eta)$ be the rectangle circumscribing its dual support. Then the 2–tiled configuration η' with dual support equal to $R(\eta)$ can be obtained by iteratively bringing a particle of type 2 to a good dual corner and saturating it with a particle of type 1 within energy barrier Δ_2. Clearly, $H(\eta') < H(\eta)$. We say that η' is obtained by filling the rectangle circumscribing the dual support of η.*

Existence of a good site

Lemma 4.37 *For all $\hat{\eta} \in \mathcal{D}_B$, there exists an $x \in F(\hat{\eta})$ such that $\Phi((\hat{\eta}, x), \boxplus) < \Gamma^\star$.*

Proof. The dual support of $\hat{\eta} \in \mathcal{D}_B$ is either a square of side length $\ell^\star$ or a rectangle of side lengths $\ell^\star + 1, \ell^\star - 1$. Let x be a site in a good dual corner of $\hat{\eta}$. After a particle of type 2 has reached site x $(H((\hat{\eta}, x)), \Gamma^\star - 3U)$, it is possible to saturate this particle with an extra particle of type 1 within energy barrier Δ_1, reaching the configuration η' with energy $H(\eta') = \Gamma^\star - \Delta_2 - \varepsilon$. Note that the dual support of η' has the same circumscribing rectangle as $\hat{\eta}$. If the rectangle circumscribing the dual support of η' is a square, then by filling this rectangle we obtain a dual 2–tiled square of side length $\ell^\star$. By Remark 4.11 this is enough. If, on the other hand, the rectangle circumscribing the dual support of η' has side length $\ell^\star + 1, \ell^\star - 1$, then by filling this rectangle we obtain a dual 2–tiled rectangle of side lengths $\ell^\star + 1, \ell^\star - 1$. From this point on, it is possible to argue as in the final part of the proof of Lemma 4.33. ★

Identification of $\mathcal{P}$ and $\mathcal{C}^\star_{\mathrm{bd}}$

Lemma 4.38 $\mathcal{P} = \mathcal{D}_B$ *and* $\mathcal{C}^\star_{\mathrm{bd}} = \mathcal{D}_B^{\mathrm{bd2}}$.

Proof. Same as the proof of Lemma 4.34. ★

4.5.3 Region RC

In this section we prove Theorem 4.10.

Let $\mathcal{D}_C$ be the set of 2–tiled configurations with $\ell^\star(\ell^\star - 1) + 1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing rectangle has perimeter $4\ell^\star$ (see Fig. 4.27).

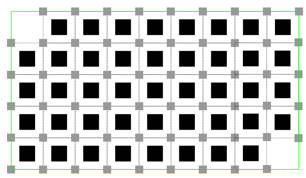


Figure 4.27: An example of configuration in $\mathcal{D}_C$ for $\ell^\star = 7$.

Identification of $g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$ and $\bar g(\{\bar\eta\}, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1})$

Lemma 4.39 $g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \bar g(\square, \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}) = \mathcal{D}_C$.

Proof. First observe that the sets $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ and $\mathcal{D}_C$ coincide by Lemma 4.13. Therefore it remains to prove that for any configuration $\eta \in \mathcal{D}_C$ there exist a standard configuration $\bar\eta$ and a path $\omega : \bar\eta \to \eta$ such that $\max_{\xi\in\omega} H(\xi) < \Gamma^\star$ or, equivalently, a path $\omega'\colon\ \eta \to \bar\eta$ such that $\max_{\xi\in\omega'} H(\xi) < \Gamma^\star$.

1. We know from Remark 4.25 that, starting from a 2–tiled configuration $\eta' \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ whose dual tile support has a circumscribing rectangle of side lengths L, l with $L \geq l$ and $L\times l > \ell^\star(\ell^\star-1)+1$, it is possible to reach below energy level $\Gamma^\star$ all configurations in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ whose dual support has the same circumscribing rectangle (provided that the cluster is sufficiently far from $\partial^-\Lambda$). We next show that, from η', it is also possible to reach a configuration $\eta'' \in \bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ whose dual support has a circumscribing rectangle with side lengths $L+1, l-1$ (whenever $(L+1) \times (l-1) \geq \ell^\star(\ell^\star-1)+1$).

2. From η' it is possible to reach below energy level $\Gamma^\star$ a configuration $\tilde{\eta}$ whose tile support, in dual coordinates, is a rectangle of side lengths $L-1, l$ plus a bar of length $k = \ell^\star(\ell^\star - 1) + 1 - (L-1)l$ on top of the longest side of the rectangle. There are two cases. Either $k > l$ or $k \leq l$. If $k > l$, then $(L+1)(l-1) < \ell^\star(\ell^\star - 1) + 1$. If $k \leq l$, then we will show that it is possible to obtain within energy barrier Δ_2 the configuration η'' whose dual tile support is obtained from the dual tile support of $\tilde{\eta}$ by moving the bar of length k from the top of the rectangle to one of its sides as follows.

3. Suppose we want to move the bar onto the East side of the rectangle. Let a particle of type 1 enter Λ and reach the site at dual distance 1 in the East direction from the Southern-most particle of type 1 on the East side of the rectangle (configuration $\tilde{\eta}'$) in order to create a good dual corner (see Fig. 4.28). Note that $H(\tilde{\eta}') = H(\tilde{\eta}) + \Delta_1$. From $\tilde{\eta}'$, using the mechanism described in Section 4.4.1, we can iteratively move all the 2–tiles originally on the top 12–bar to the East side of the rectangle within energy barrier $3U$. The free particle of type 1 that is left afterwards is removed from Λ. Therefore the task can be achieved within energy barrier $3U + \Delta_1$. Note that it is sufficient that only the North side and the East side of the dual rectangle circumscribing the cluster of $\tilde{\eta}$ are far from $\partial^-\Lambda$.

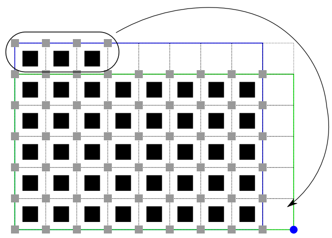
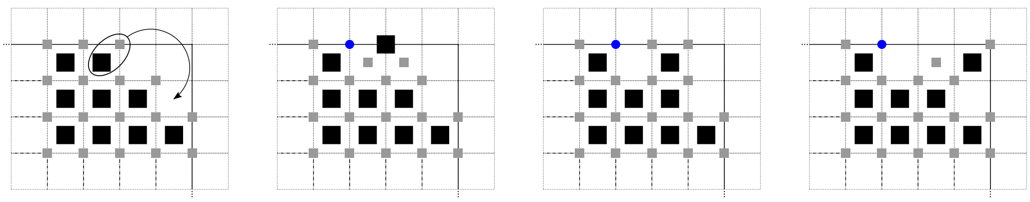


Figure 4.28: The top bar can be moved to the East side of the rectangle within a energy barrier $3U + \Delta_1$.

4. It is clear that this argument is sufficient to show that from a 2–tiled configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$ with a dual support consisting of a rectangle of side lengths $L, (l-1)$ plus a bar attached to one of the shortest sides far from $\partial^-\Lambda$ (note that at least one of the shortest side is far from $\partial^-\Lambda$) it is possible to return to a configuration of minimal energy with a dual tile support an $L \times l$ rectangle and, eventually, to some standard configuration $\bar{\eta}$ strictly below energy level $\Gamma^\star$. This implies (see Lemma 4.17) that $\Phi(\square, \eta) < \Gamma^\star$ for all $\eta \in \mathcal{D}_F$ whose dual support is far from $\partial^-\Lambda$. To complete the proof we will have to consider those configurations in $\mathcal{D}_F$ with a dual tile support consisting of an $L \times l$ rectangle that is close to $\partial^-\Lambda$ and see that also for these configurations it is possible to reach below energy level $\Gamma^\star$ some standard configuration in $\bar{\mathcal{V}}_{\star,\ell^\star(\ell^\star-1)+1}$. A particle is said to be close to

$\partial^- \Lambda$ if it is adjacent to a site in the region of Λ where interaction between particles is not possible. Dimers, 2–tiles, 12–bars and cluster are said to be close to $\partial^- \Lambda$ if they contain at least one particle that is close to $\partial^- \Lambda$.



(a) (b) (c) (d)

Figure 4.29: Dimers that are close to $\partial^- \Lambda$ can be moved within a $3U + \Delta_1$ energy barrier. A particle that is "beyond" the black linec an not have active bonds.

5. We will show how it is possible to move those dimers that are close to $\partial^- \Lambda$ within energy barrier $3U + \Delta_1$ using a modification of the argument presented in Section 4.4.1. For this purpose, we refer to Fig. 4.29. Let p and q_1 be the particle of type 2, respectively, type 1 of the dimer that is encircled in configuration η in Fig. 4.29(a), and let q_2 be the particle of type 1 adjacent to p in the North-East direction. We will construct a path ω that moves the dimer to a different 12–bar, as follows. Move q_1 one step South-East ($\Delta H(\omega) = U$), and p one step North-East ($\Delta H(\omega) = 3U$). Then move q_2 one step South-East ($\Delta H(\omega) = 3U$), and let a new particle of type 1 enter Λ ($\Delta H(\omega) = 3U + \Delta_1$) and reach the site originally occupied by q_2 ($\Delta H(\omega) = 2U + \Delta_1$; see Fig. 4.29(b)). Afterwards, move q_1 one step North-East ($\Delta H(\omega) = 3U + \Delta_1$), p one step South-East ($\Delta H(\omega) = 3U + \Delta_1$), and q_2 one step North-East ($\Delta H(\omega) = 2U + \Delta_1$; see Fig. 4.29(c)). The same procedure described so far can be repeated (now it is not necessary to let a new particle of type 1 enter Λ, since p is adjacent to two corner particles of type 1), to reach the configuration represented in Fig. 4.29(d) (as in the case of Section 4.4.1), which is the key configuration to see that the dimer can moved to a corner without further increasing the energy difference with the original configuration.

6. Let $\eta \in \mathcal{D}_C$ consist of a cluster close to $\partial^- \Lambda$, and let L, l be the side lengths of the rectangle circumscribing its dual tile support. Using the mechanism described above, we see that also from η it is possible to reach a configuration η' with a dual support consisting of a rectangle of side lengths $L - 1, (l)$ plus a 12–bar (possibly still close to $\partial^- \Lambda$) attached to one of its sides.

- If $L = l = \ell^\star$, then we can reach a standard configuration and we are done.

- If $L = \ell^\star + 1$ and $l = \ell^\star - 1$ (and hence $L - l = 2$), then the same procedure can be used to reach a configuration with a protuberance that can be easily moved below energy level $\Gamma^\star$ to obtain a standard configuration (detach and remove the two particles of type 1, detach and move the particle of type 2, and saturate the particle of type 2 with two new particles of type 1).
- If $L - l > 2$, then it is possible to proceed as follows. Move the short external 12–bar that is far from $\partial^- \Lambda$ onto the longest side of the dual rectangle far from $\partial^- \Lambda$, as described above within energy barrier $3U + \Delta_1$, to obtain a configuration η' such that $H(\eta') = H(\eta)$ and with a dual tile support that has a circumscribing rectangle of side lengths $L - 1, l + 1$. From η' it is possible to iterate the above procedure until a configuration with dual support with a circumscribing rectangle of side lengths $\ell^\star + 1, \ell^\star - 1$ is reached. But this case has already been treated.

★

Existence of a good site

Lemma 4.40 *For all $\hat{\eta} \in \mathcal{D}_C$, there exists an $x \in F(\hat{\eta})$ such that $\Phi((\hat{\eta}, x), \boxplus) < \Gamma^\star$.*

Proof. If $\hat{\eta} \in \mathcal{D}_B$, then the claim follows from the proof of Lemma 4.37. We will show that, for all $\hat{\eta}$ whose dual support has a circumscribing rectangle with side lengths L, l, there is a site x such that from configuration $(\hat{\eta}, x)$ there is a path ω to a configuration $\tilde{\eta}'$ whose dual support has a circumscribing rectangle of side lengths $L - 1, l + 1$ such that $H(\tilde{\eta}') \leq H(\hat{\eta})$ and $H(\xi) < \Gamma^\star$ for all $\xi \in \omega$. The procedures that we present only require that two sides of the circumscribing rectangle of the dual support of η are far from $\partial^- \Lambda$, which is always the case. Without loss of generality we may assume that these two sides are the North side and the East side.

- $Ll > \ell^\star(\ell^\star - 1) + 1$. In this case, configuration $\hat{\eta}$ contains at least one good dual corner. Let x be one of these dual corners. From $\hat{\eta}$, first saturate the particle of type 2 at x with a new particle of type 2, to obtain configuration η'. Let η'' be the configuration obtained from η' by filling $R(\hat{\eta})$ (note that $\eta' = \eta''$ is possible). Clearly, $H(\eta'') < H(\hat{\eta})$ and $\Phi(\hat{\eta}, \eta'') < \Gamma^\star$. Let $\tilde{\eta}$ be the configuration obtained from η'' within energy barrier Δ_2 by adding a 2–tile on the North side of the 2–tiled dual rectangle with side lengths L, l. $H(\tilde{\eta}) \leq \Gamma^\star - 4U + 2\Delta_1$. As in the proof of Lemma 4.39, all the tiles of the Eastern-most 12–bar of $\tilde{\eta}$ can be itereatively moved to a corner on

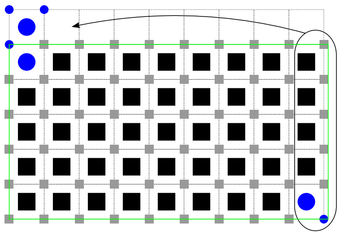


Figure 4.30: The configuration obtained from $\hat{\eta}$ by first filling the rectangle circumscribing its dual support and then adding a 2–tiled on the North side; circles represent particles added to $\hat{\eta}$.

the North side of the cluster within energy barrier $3U$ (see Fig. 4.30), to obtain a 2–tiled configuration $\tilde{\eta}'$ whose dual support has a circumscribing rectangle with side lengths $L-1, l+1$ and such that $\tilde{\eta}' = H(\eta'')$. Hence $\Phi((\hat{\eta}, x), \tilde{\eta}') le \Gamma^\star - 4U + 2\Delta_1 + 3U < \Gamma^\star$ as soon as $\Delta_1 < \frac{1}{2}$, which is satisfied in **RF**.

- $Ll > \ell^\star(\ell^\star - 1) + 1$. In this case the dual support of $\hat{\eta}$ is already a rectangle with side lengths L, l. Let x be the central site of a tile adjacent to the North side of the rectangle. We have $H((\hat{\eta}, x)) = \Gamma^\star - 2U$. Let $\tilde{\eta}$ be the configuration obtained within energy barrier Δ_1 by saturating the particle of type 2 at x. $H(\tilde{\eta}) = \Gamma^\star - 4U + 2\Delta_1$. From $\tilde{\eta}$ proceed as in the previous case.

★

Identification of $\mathcal{P}$ and $\mathcal{C}^\star_{\mathrm{bd}}$

Lemma 4.41 $\mathcal{P} = \mathcal{D}_C$ *and* $\mathcal{C}^\star_{\mathrm{bd}} = \mathcal{D}_C^{\mathrm{bd2}}$.

Proof. Same as the proof of Lemma 4.34. ★

Appendix: Computation of $N^\star$

Kurz [Kur08] shows how to construct all polyominoes of minimal perimeter with fixed area, and gives an expression for their number in terms of generating functions. Two basic generating functions

$$s(x) = 1 + \sum_{k=1}^{\infty} x^{k^2} \prod_{j=1}^{k} \frac{1}{1-x^{2j}}, \qquad a(x) = \prod_{j=1}^{\infty} \frac{1}{1-x^j} \tag{4.23}$$

are used to define two composite generating functions

$$r(x) = \tfrac{1}{4}\left[a(x)^4 + 3a(x^2)^2\right], \qquad q(x) = \tfrac{1}{8}\left[a(x)^4 + 3a(x^2)^2 + 2s(x)^2 a(x^2) + 2a(x^4)\right], \tag{4.24}$$

whose coefficients r_k, q_k of x^k count the polyominoes as follows. The number of polyominoes of minimal perimeter with area n equals

$$e(n) = \begin{cases} 1 & \text{if } n = s^2, \\ \sum_{c=0}^{\left\lfloor -\frac{1}{2}+\frac{1}{2}\sqrt{1+4s-4t}\right\rfloor} r_{s-c-c^2-t} & \text{if } n = s^2+t \text{ with } 0<t<s, \\ 1 & \text{if } n = s^2+s+t, \\ q_{s+1-t} + \sum_{c=1}^{\left\lfloor\sqrt{s+1-t}\right\rfloor} r_{s+1-c^2-t} & \text{if } n = s^2+s+t \text{ with } 0<t\le s, \end{cases} \tag{4.25}$$

where $s = \lfloor\sqrt{n}\rfloor$.

We need to count the number of polyominoes of minimal perimeter with area $n = \ell^\star(\ell^\star-1)+1$ for $\ell^\star \geq 4$, i.e., we are only interested in n of the form s^2+s+t with $s = \ell^\star - 1$ and $t = 1$. Kurz [Kur08] counts polyominoes modulo translations, rotations and reflections. We need the number modulo translations only. Therefore we must put in correction factors: 4 for the rotations and 2 for the reflections.

In region **RC** we retain all c-terms. In region **RB** we only retain the term with $c = 1$. Indeed, $q_{\ell^\star-1}$ is the number of polyominoes of minimal perimeter when the circumscribing rectangle is a square of side length $\ell^\star$, and $r_{\ell^\star-c^2-1}$ is the number of polyominoes of minimal perimeter when the circumscribing rectangle has side lengths $\ell^\star+1, \ell^\star-1$. Thus, modulo rotations and reflections, we have

$$N^\star = \begin{cases} 8\left[q_{\ell^\star-1} + r_{\ell^\star-1-1}\right] & \text{in region } \mathbf{RB}, \\ 8\left[q_{\ell^\star-1} + \sum_{c=1}^{\left\lfloor\sqrt{\ell^\star-1}\right\rfloor} r_{\ell^\star-c^2-1}\right] & \text{in region } \mathbf{RC}. \end{cases} \tag{4.26}$$

Bibliography

[AC96] Laurent Alonso and Raphael Cerf. The three dimensional polyominoes of minimal area. *Electronic Journal of Combinatorics*, 3, 1996.

[BAC96] G. Ben Arous and R. Cerf. Metastability of the three dimensional ising model on a torus at very low temperatures. *Electronic Journal of Probability*, 1:1–55, 1996.

[BdH] A. Bovier and F. den Hollander. Metastability - a potential-theoretic approach. *manuscript in preparation.*

[BdHS10] Anton Bovier, Frank den Hollander, and Cristian Spitoni. Homogeneous nucleation for Glauber and Kawasaki dynamics in large volumes at low temperatures. *Ann. Probab.*, 38(2):661–713, 2010.

[BdN06] A. Bovier, F. den Hollander, and F. R. Nardi. Sharp asymptotics for Kawasaki dynamics on a finite box with open boundary. *Probab. Theory Related Fields*, 135(2):265–310, 2006.

[BEGK01] Anton Bovier, Michael Eckhoff, V. Gayrard, and Markus Klein. Metastability in stochastic dynamics of disordered mean-field models. *Probab. Theory Related Fields*, 119(1):99–161, 2001.

[BEGK02] Anton Bovier, Michael Eckhoff, V. Gayrard, and Markus Klein. Metastability and low lying spectra in reversible Markov chains. *Comm. Math. Phys.*, 228(2):219–255, 2002.

[BEGK04] Anton Bovier, Michael Eckhoff, V. Gayrard, and Markus Klein. Metastability in reversible diffusion processes. I. Sharp asymptotics for capacities and exit times. *J. Eur. Math. Soc. (JEMS)*, 6(4):399–424, 2004.

[BM02] A. Bovier and F. Manzo. Metastability in glauber dynamics in the low-temperature limit: beyond exponential asymptotics. *Journal of statistical physics*, 107(3):757–779, 2002.

[Bov06] Anton Bovier. Metastability: a potential theoretic approach. In

International Congress of Mathematicians. Vol. III, pages 499–518. Eur. Math. Soc., Zürich, 2006.

[Bov09] Anton Bovier. Metastability. In *Methods of contemporary mathematical statistical physics*, volume 1970 of *Lecture Notes in Math.*, pages 177–221. Springer, Berlin, 2009.

[Bov11] Anton Bovier. Metastability: from mean field modelt to spdes. In *to appear in a Festschrift on the occassion of the 60-th birthday of Jürgen Gärtner*. Springer Proceedings in Mathematics, 2011.

[CC97] O. Catoni and R. Cerf. The exit path of a markov chain with rare transitions. *ESAIM: Probability and Statistics*, 1(1):95–144, 1997.

[CGOV84] Marzio Cassandro, Antonio Galves, Enzo Olivieri, and Maria Eulalia Vares. Metastable behavior of stochastic dynamics: a pathwise approach. *J. Statist. Phys.*, 35(5-6):603–634, 1984.

[CN03] E.N.M. Cirillo and F.R. Nardi. Metastability for a stochastic dynamics with a parallel heat bath updating rule. *Journal of statistical physics*, 110(1):183–217, 2003.

[CNS08a] E.N.M. Cirillo, F.R. Nardi, and C. Spitoni. Competitive nucleation in reversible probabilistic cellular automata. *Physical Review E*, 78(4):040601, 2008.

[CNS08b] E.N.M. Cirillo, F.R. Nardi, and C. Spitoni. Metastability for reversible probabilistic cellular automata with self-interaction. *Journal of Statistical Physics*, 132(3):431–471, 2008.

[CO96] Emilio N. M. Cirillo and Enzo Olivieri. Metastability and nucleation for the Blume-Capel model. Different mechanisms of transition. *J. Statist. Phys.*, 83(3-4):473–554, 1996.

[den09] F. den Hollander. Three lectures on metastability under stochastic dynamics. In *Methods of Contemporary Mathematical Statistical Physics*, volume 1970/2009 of *Lecture Notes in Mathematics*, pages 1–24, Berlin, 2009. Springer.

[dHNOS03] F. den Hollander, FR Nardi, E. Olivieri, and E. Scoppola. Droplet growth for three-dimensional kawasaki dynamics. *Probability theory and related fields*, 125(2):153–194, 2003.

[dHNT11] F. den Hollander, F. R. Nardi, and A. Troiani. Kawasaki dynamics with two types of particles: Stable/metastable configurations and communication heights. *Journal of Statistical Physics*, 145:1423–1457, 2011. 10.1007/s10955-011-0370-0.

[dOS00] F. den Hollander, E. Olivieri, and E. Scoppola. Metastability and nucleation for conservative dynamics. *Journal of Mathematical Physics*, 41(3):1424–1498, 2000.

[DS97] P. Dehghanpour and R.H. Schonmann. Metropolis dynamics relaxation via nucleation and growth. *Communications in mathematical physics*, 188(1):89–119, 1997.

[Eyr35] H. Eyring. The acrivated complex in chemical reactions. *J. Chem. Phys.*, 3:107, 1935.

[FW84] M. I. Freidlin and A. D. Wentzell. *Random perturbations of dynamical systems*, volume 260 of *Grundlehren der Mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, New York, 1984.

[Gau09] A. Gaudilliere. Condenser physics applied to markov chains, Lecture notes for the 12th Brazilian School of Probability. *arXiv:0901.3053v1[math.PR]*, 2009.

[GdHN+a] A. Gaudillière, F. den Hollander, F. R. Nardi, E. Olivieri, and E. Scoppola. Droplet dynamics in a two-dimensional rarified gas under kawasaki dynamics, manuscript in preparation. *manuscript in preparation.*

[GdHN+b] A. Gaudillière, F. den Hollander, F. R. Nardi, E. Olivieri, and E. Scoppola. Homogeneous nucleation for two-dimensional kawasaki dynamics. *manuscript in preparation.*

[GDHN+09] A. Gaudillière, F. Den Hollander, FR Nardi, E. Olivieri, and E. Scoppola. Ideal gas approximation for a two-dimensional rarefied gas under kawasaki dynamics. *Stochastic Processes and their Applications*, 119(3):737–774, 2009.

[GS08] A. Gaudilliere and E. Scoppola. An introduction to metastability. *Lecture notes for the 12th Brazilian School of Probability*, 2008.

[GSSV11] A. Gaudillière, B. Scoppola, E. Scoppola, and M. Viale. Phase transitions for the cavity approach to the clique problem on random graphs. *Journal of statistical physics*, 145(5):1127–1155, 2011.

[Kra40] H. A. Kramers. Brownian motion if a field of force and the diffusion model of chemical reactions. *Physica*, 3:284–304, 1940.

[Kur08] Sascha Kurz. Counting polyominoes with minimum perimeter. *Ars Combin.*, 88:161–174, 2008.

[MNOS04] F. Manzo, F. R. Nardi, E. Olivieri, and E. Scoppola. On the essential features of metastability: tunnelling time and critical configurations. *Journal of Statistical Physics*, 115(1-2):591–642, 2004.

[NO96] F.R. Nardi and E. Olivieri. Low temperature stochastic dynamics for an ising model with alternating field. *Markov Process. Relat. Fields*, 2:117–166, 1996.

[NOS05] F. R. Nardi, E. Olivieri, and E. Scoppola. Anisotropy effects in nucleation for conservative dynamics. *J. Stat. Phys.*, 119(3-4):539–595, 2005.

[NS91] E. Jordao Neves and Roberto H. Schonmann. Critical droplets and metastability for a Glauber dynamics at very low temperatures. *Comm. Math. Phys.*, 137(2):209–230, 1991.

[NS92] E.J. Neves and R.H. Schonmann. Behavior of droplets for a class of glauber dynamics at very low temperature. *Probability theory and related fields*, 91(3):331–354, 1992.

[OS95] E. Olivieri and E. Scoppola. Markov chains with exponentially small transition probabilities: first exit problem from a general domain. I. The reversible case. *J. Statist. Phys.*, 79(3-4):613–647, 1995.

[OS96] E. Olivieri and E. Scoppola. Markov chains with exponentially small transition probabilities: first exit problem from a general domain. II. The general case. *J. Statist. Phys.*, 84(5-6):987–1041, 1996.

[OS10] Enzo Olivieri and Elisabetta Scoppola. An introduction to metastability through random walks. *Braz. J. Probab. Stat.*, 24(2):361–399, 2010.

[OV05] Enzo Olivieri and Maria Eulália Vares. *Large deviations and metastability*, volume 100 of *Encyclopedia of Mathematics and its Applications*. Cambridge University Press, Cambridge, 2005.

[PL71] O. Penrose and J. L. Lebowitz. Rigorous treatment of metastable states in the van der Waals-Maxwell theory. *J. Statist. Phys.*, 3:211–236, 1971.

[Ŕ90] Pal Révész. *Random Walk in Random and Non-Random Environments,*. World Scientific, Singapore, 1990.

[SS98] R.H. Schonmann and S.B. Shlosman. Wulff droplets and the metastable relaxation of kinetic ising models. *Communications in mathematical physics*, 194(2):389–462, 1998.

[vdB05] M. van den Berg. Exit and return of a simple random walk. *Potential Analysis*, 23(1):45–53, 2005.

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Alessio Troiani was born in Tivoli on 22 May 1982. He completed his high school studies at Liceo Scientifico Statale “Cartesio” in Olevano Romano in 2001. In the same year he started a bachelor program in industrial engineering at the University of Rome “Tor Vergata”. After obtaining his bachelor degree (cum laude) in 2004, he started a master program in industrial engineering and obtained his master degree (cum laude) in 2007 under the supervision of Prof. Dr. Benedetto Scoppola with a thesis entitled “An algorithm inspired by the cavity fields method for the unconstrained binary quadratic programming”. From July to October 2007 he was visiting students at the Center for Discrete Mathematics and Theoretical Computer Science – Rutgers, The State University of New Jersey (USA) in the framework of the Special Focus on Discrete Random Systems under the supervision of Prof. Dr. Joel Lebowitz. Meanwhile, until the spring of 2007, he was a competitive swimmer who was part of the national junior team and medallist at national championships. In the Spring of 2008 he worked as a Business Analyst at Accenture in Rome. In September of 2008 he moved to the Netherlands to start a Ph. D. program in Probability theory at Leiden University under the supervision of Prof. Dr. Frank den Hollander and Dr. Francesca Romana Nardi. His doctoral research has been focused on metastability for conservative dynamics. During this period he also attended several national and international summer schools and conferences and was teaching assistant for multiple courses. In the fall of 2012 he will move to France to work at Amadeus IT Group.