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

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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

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

be the internal, respectively, external boundary of Λ , and put $\Lambda^- = \Lambda \setminus \partial^- \Lambda$ 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 $\eta = \{\eta(x) : x \in \Lambda\}$ 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 $\Lambda^{*, -} = \{(x, y) : x, y \in \Lambda^-, |x - y| = 1; |x - z| > 2, |y - z| > 2 \forall z \in \partial^- \Lambda\}$ 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 $\Delta_1 > 0$

4 Critical configurations

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

$$\Delta_1 \leq \Delta_2. \quad (4.3)$$

The Gibbs measure associated with H is

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

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

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

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:

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

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-neighbor attraction between different types. We may think of

$\mathbb{Z}^2 \setminus \Lambda$ 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) $\omega: \eta \rightarrow \eta'$ 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

$$\Phi(\eta, \eta') = \min_{\omega: \eta \rightarrow \eta'} \max_{\xi \in \omega} H(\xi), \quad (4.7)$$

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

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

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

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

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

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

4 Critical configurations

where $\mathcal{I}_\eta = \{\xi \in \mathcal{X} : H(\xi) < H(\eta)\}$ is the set of configurations with energy lower than η .

(g) $\mathcal{X}_{\text{stab}} = \{\eta \in \mathcal{X} : H(\eta) = \min_{\xi \in \mathcal{X}} H(\xi)\}$ is the set of stable configurations, i.e., the set of configurations with minimal energy.

(h) $\mathcal{X}_{\text{meta}} = \{\eta \in \mathcal{X} : V_\eta = \max_{\xi \in \mathcal{X} \setminus \mathcal{X}_{\text{stab}}} V_\xi\}$ is the set of metastable configurations, i.e., the set of non-stable configurations with maximal stability level.

(i) $\Gamma = V_\eta$ for $\eta \in \mathcal{X}_{\text{meta}}$ (note that $\eta \mapsto V_\eta$ is constant on $\mathcal{X}_{\text{meta}}$), $\Gamma^* = \Phi(\square, \boxplus) - H(\square)$ (note that $H(\square) = 0$).

Definition 4.2 (a) $(\eta \rightarrow \eta')_{\text{opt}}$ 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 $\eta \rightarrow \eta'$ if $\mathcal{W} \subset \mathcal{S}(\eta, \eta')$ and $\omega \cap \mathcal{W} \neq \emptyset$ for all $\omega \in (\eta \rightarrow \eta')_{\text{opt}}$.

(c) A set $\mathcal{W} \subset \mathcal{X}$ is called a minimal gate for $\eta \rightarrow \eta'$ if it is a gate for $\eta \rightarrow \eta'$ and for any $\mathcal{W}' \subsetneq \mathcal{W}$ there exists an $\omega' \in (\eta \rightarrow \eta')_{\text{opt}}$ 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 $(\eta \rightarrow \eta')_{\text{opt}}$. The configurations in $\mathcal{S}(\eta, \eta') \setminus \mathcal{G}(\eta, \eta')$ 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 $\omega \in (\eta \rightarrow \eta')_{\text{opt}}$ such that $\omega \ni \zeta$ the following holds: $S(\omega) \setminus \{\zeta\} \neq \emptyset$ and there exists an $\omega' \in (\eta \rightarrow \eta')_{\text{opt}}$ such that $S(\omega') \subseteq S(\omega) \setminus \{\zeta\}$.

(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 $\omega \in (\eta \rightarrow \eta')_{\text{opt}}$ such that $S(\omega) = \{\zeta\}$.

(f2) There exists an $\omega \in (\eta \rightarrow \eta')_{\text{opt}}$ such that $S(\omega) \supseteq \{\zeta\}$ and $S(\omega') \not\subseteq S(\omega) \setminus \{\zeta\}$ for all $\omega' \in (\eta \rightarrow \eta')_{\text{opt}}$.

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 $\beta \rightarrow \infty$. 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 $\mathcal{C}^*$ of the essential gate $\mathcal{G}(\square, \boxplus)$, and all have energy Γ^* (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 $\beta \rightarrow \infty$. These results, which are typical for metastable behavior, were proved under *three hypotheses*:

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

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

(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) $\mathcal{C}_{\text{bd}}^*$ is the minimal set of configurations in $\mathcal{G}(\square, \boxplus)$ such that all paths in $(\square \rightarrow \boxplus)_{\text{opt}}$ enter $\mathcal{G}(\square, \boxplus)$ through $\mathcal{C}_{\text{bd}}^*$.

(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 $L^* \times L^*$ square somewhere in Λ^- for some $L^* \in \mathbb{N}$ large enough that is independent of $\hat{\eta}$ and Λ . Every $\eta \in \mathcal{C}_{\text{bd}}^*$ 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) $\mathcal{C}_{\text{att}}^*$ is the set of configurations obtained from $\mathcal{C}_{\text{bd}}^*$ 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 $\mathcal{C}_{\text{att}}^* = \cup_{\hat{\eta} \in \mathcal{P}} \mathcal{C}_{\text{att}}^*(\hat{\eta})$.

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

Note that $\Gamma^* = H(\mathcal{C}^*) = H(\mathcal{P}) + \Delta_2$, and that $\mathcal{C}^*$ consists of precisely those configurations “interpolating” between $\mathcal{P}$ and $\mathcal{C}_{\text{att}}^*$: 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 $\mathcal{C}^*$ 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 $\mathcal{C}^*$ are referred to as the *protocritical droplets*, respectively, the *critical droplets*.

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

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

4 Critical configurations

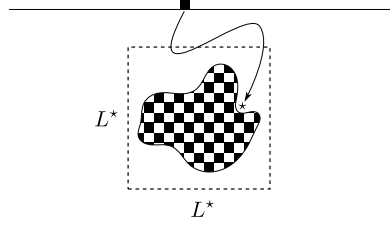


Figure 4.1: A qualitative representation of a configuration in $\mathcal{C}_{\text{bd}}^*$. If the free particle of type 2 reaches the site marked as $\star$, then the dynamics has entered the “basin of attraction” $\boxplus$.

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 Γ^* of critical droplets. In this Chapter (H3), identify the set $\mathcal{C}^*$ of critical droplets, and compute the cardinality N^* of the set $\mathcal{P}$ of protocritical droplets modulo shifts, thereby completing our analysis.

Hypotheses (H1–H2) imply that $(\mathcal{X}_{\text{meta}}, \mathcal{X}_{\text{stab}}) = (\square, \boxplus)$, 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 $\Lambda \rightarrow \mathbb{Z}^2$ 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 (Γ^*) was identified in Chapter 3, the second ($\mathcal{C}^*$) and the third (N^*) 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

$$0 < \Delta_1 \leq \Delta_2, \quad \Delta_1 + \Delta_2 < 4U, \quad \Delta_2 \geq U, \quad (4.11)$$

as indicated in Fig. 4.2.

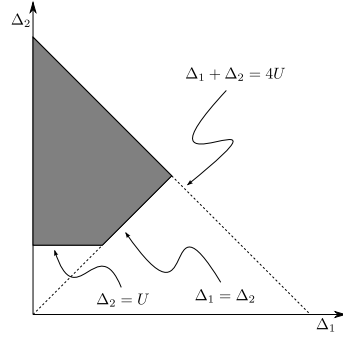


Figure 4.2: Proper metastable region.

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

$$\Delta_1 < U, \quad \Delta_2 - \Delta_1 > 2U, \quad \Delta_1 + \Delta_2 < 4U, \quad (4.12)$$

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.)

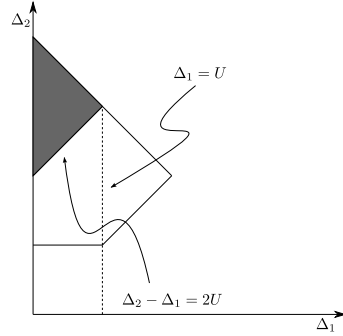


Figure 4.3: Subregion of the proper metastable region given by (4.12).

Hypothesis (H3) involves additional characterizations of the sets $\mathcal{P}$ and $\mathcal{C}^*$. 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, $\Gamma^* = 4\Delta_1 + 2\Delta_2 - 4U$ and $N^* = 1$. 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 $\mathcal{P}$, $\mathcal{C}^*$ and $\mathcal{C}_{\text{bd}}^*$, prove (H3), and compute N^* , namely,

4 Critical configurations

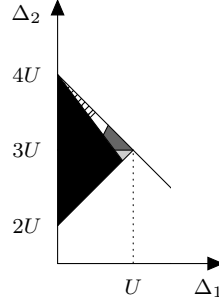


Figure 4.4: Subregions of the parameter space. In the black region $\ell^* \leq 3$; **RA**, **RB** and **RC** are, respectively, the light gray, the dark grey and the dashed region.

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

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

and put

$$\ell^* = \left\lceil \frac{\Delta_1}{\varepsilon} \right\rceil \in \mathbb{N} \setminus \{1\}. \quad (4.14)$$

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 $\mathcal{D}^{\text{bd}2}$ 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 $\ell^*(\ell^* - 1) + 1$ particles of type 2 whose dual tile support is a rectangle of side lengths $\ell^*, \ell^* - 1$ 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 $\ell^*(\ell^* - 1) + 1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing rectangle has side lengths either ℓ^*, ℓ^* or $\ell^* + 1, \ell^* - 1$ (see Fig. 4.20).

(c) $\mathcal{D}_C$ is the set of 2-tiled configurations with $\ell^*(\ell^*-1)+1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing rectangle has perimeter $4\ell^*$ (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**, $\mathcal{P} = \mathcal{D}_A$, $\mathcal{C}_{\text{bd}}^* = \mathcal{D}_A^{\text{bd}2}$, and $N^* = 8\ell^* - 4$.

Theorem 4.9 In subregion **RB**, $\mathcal{P} = \mathcal{D}_B$, $\mathcal{C}_{\text{bd}}^* = \mathcal{D}_B^{\text{bd}2}$, and $N^* = 8[q_{\ell^*-1} + r_{\ell^*-1-1}]$.

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

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 $\ell^* \geq 4$ only. For $\ell^* = 2, 3$, 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 $\mathcal{C}^*$ and N^* , 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 Γ^* the motion

4 Critical configurations

of the particles becomes more restricted. 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*

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

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 $L > 2\ell^*$ (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).

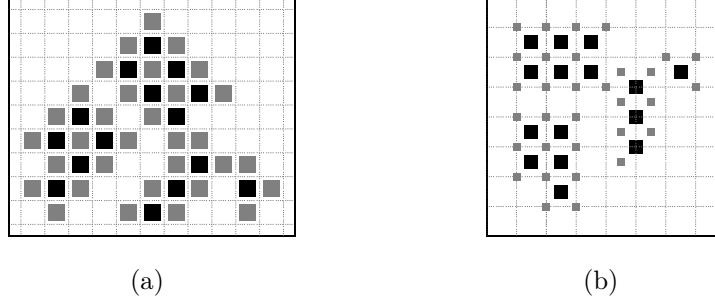


Figure 4.5: A configuration represented in: (a) standard coordinates; (b) dual coordinates. Light-shaded squares are particles of type 1, dark-shaded squares are particles of type 2. In dual coordinates, particles of type 2 are represented by larger squares than particles of type 1 to exhibit the “tiled 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 $\text{supp}(\eta)$. 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

4 Critical configurations

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 $t(i)$, 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 $t(i)$ is alternatively denoted by $t(p)$ 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 ℓ^* belongs to $\mathcal{X}_{\boxplus}$.

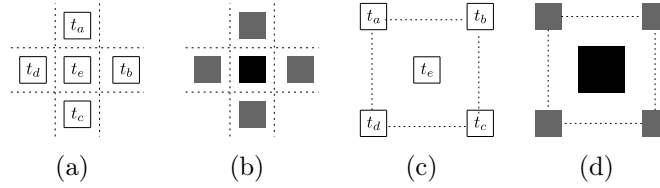


Figure 4.6: Tiles: (a) standard representation of the labels of a tile; (b) standard representation of a 2-tile; (c) dual representation of the labels of a tile; (d) dual representation of a 2-tile.

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

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

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 $\mathcal{V}_{\star, n_2}^{4n_2}$ 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 $\eta \in \mathcal{V}_{\star, n_2}^{4n_2}$ 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:

$$\mathcal{X} = \bigcup_{n_2=0}^{|\Lambda|} \mathcal{V}_{\star, n_2}. \quad (4.17)$$

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 $\partial^- \Lambda$ ($\mathcal{V}_{\star, n} \rightarrow \mathcal{V}_{\star, n+1}$) or removing a particle of type 2 from $\partial^- \Lambda$ ($\mathcal{V}_{\star, n} \rightarrow \mathcal{V}_{\star, n-1}$). Note further that $\square \in \mathcal{V}_{\star, 0}$ and $\boxplus \in \mathcal{V}_{\star, (L-1)^2}$. Therefore, to realize the transition $\square \rightarrow \boxplus$, the dynamics must visit all manifolds $\mathcal{V}_{\star, n}$ with $n = 1, \dots, (L-1)^2$. Abbreviate $\mathcal{V}_{\star, \leq m} = \bigcup_{n=0}^m \mathcal{V}_{\star, n}$ and $\mathcal{V}_{\star, \geq m} = \bigcup_{n=m}^{|\Lambda|} \mathcal{V}_{\star, n}$.

9. For $\mathcal{Y} \subset \mathcal{X}$, $\hat{\eta} \in \mathcal{Y}$ and $x \in \Lambda \setminus \text{supp}[\hat{\eta}]$, 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 $\mathcal{Y}^{\text{bd}2}$ 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., $\mathcal{Y}^{\text{bd}2} = \bigcup_{\hat{\eta} \in \mathcal{Y}} \bigcup_{x \in \partial^- \Lambda} (\hat{\eta}, x)$. For $\omega: \square \rightarrow \boxplus$, let $\sigma_{\mathcal{Y}}(\omega)$ be the configuration in $\mathcal{Y}$ that is first visited by ω . Define

$$\begin{aligned} \bar{\mathcal{r}}\mathcal{Y} &= \bigcup_{\omega: \square \rightarrow \boxplus} \sigma_{\mathcal{Y}}(\omega), \\ \bar{\mathcal{r}}\mathcal{Y} &= \bigcup_{\substack{\omega: \square \rightarrow \boxplus \\ \text{optimal}}} \sigma_{\mathcal{Y}}(\omega), \end{aligned} \quad (4.18)$$

4 Critical configurations

called the *entrance*, respectively, the *optimal entrance* of $\mathcal{Y}$. With this notation we have $\mathcal{C}_{\text{bd}}^* = \bar{\Gamma}\mathcal{G}(\square, \boxplus)$.

10. For $\mathcal{A}, \mathcal{B} \subset \mathcal{X}$, define

$$\begin{aligned} g(\mathcal{A}, \mathcal{B}) &= \{\eta \in \mathcal{B} : \exists \zeta \in \mathcal{A} \text{ and } \omega : \zeta \rightarrow \eta : n_2(\eta) \leq n_2(\xi) \leq n_2(\zeta), H(\xi) < \Gamma^* \forall \xi \in \omega\}, \\ \bar{g}(\mathcal{A}, \mathcal{B}) &= \{\eta \in \mathcal{B} : \exists \zeta \in \mathcal{A} \text{ and } \omega : \zeta \rightarrow \eta : n_2(\eta) \leq n_2(\xi) \leq n_2(\zeta), H(\xi) \leq \Gamma^* \forall \xi \in \omega\}. \end{aligned} \quad (4.19)$$

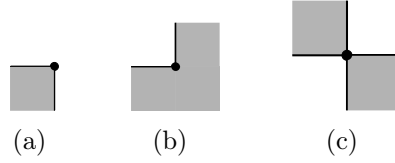


Figure 4.7: Corners of polyominoes: (a) one convex corner; (b) one concave corner; (c) two concave corners. Shaded mean occupied by a unit square.

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

$$F(\eta) = \{x \in \Lambda : \exists y \sim x : \eta(y) = 1\}. \quad (4.20)$$

For $\eta \in \mathcal{X}$, let

$$\mathcal{T}(\eta) = 2P(\eta) + [\psi(\eta) - \phi(\eta)] = 2P(\eta) + 4[C(\eta) - Q(\eta)], \quad (4.21)$$

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 $\bar{\Gamma}\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ (Lemmas 4.14–4.15 below), in Section 4.3.2 we characterize $g(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ and $\bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ (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 $\ell^*(\ell^* - 1) + 1 \leq n_2 \leq (\ell^*)^2$, then η is 2-tiled and its dual perimeter is equal to $4\ell^*$.*

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 $\bar{\Gamma}\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$

Lemma 4.14 *Let ρ be a 2-tiled configuration with $\ell^*(\ell^* - 1)$ particles of type 2 and with dual tile support equal to a rectangle of side lengths $\ell^*, (\ell^* - 1)$ (i.e., ρ is a standard configuration).*

- (1) *If $\eta \neq \rho$ is a 2-tiled configuration with $\ell^*(\ell^* - 1)$ particles of type 2, then $H(\eta) > \Gamma^* - \Delta_2$.*
- (2) *If $\eta \neq \rho$ is a configuration with $\ell^*(\ell^* - 1)$ particles of type 2 such that $[\eta] \neq [\rho]$, then $H(\eta) > \Gamma^* - \Delta_2$.*
- (3) *If $\eta \neq \rho$ is a configuration with $\ell^*(\ell^* - 1)$ 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 $H(\eta) > \Gamma^* - \Delta_2$.*

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 $\mathcal{T}(\eta) - \mathcal{T}(\rho) \geq 4$, and so $H(\eta) - H(\rho) \geq \Delta_1$. The claim now follows by observing that $H(\rho) = \Gamma^* + \varepsilon - \Delta_1 - \Delta_2$ 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 $H(\eta') \leq H(\eta)$ with equality if and only if $\eta' = \eta$. Clearly, $[\eta] = [\eta']$. By part (1), we

4 Critical configurations

have $H(\eta) \geq H(\eta') > \Gamma^* - \Delta_2$. If η consists of clusters $c_1, \dots, c_m$ with $m \in \mathbb{N} \setminus \{1\}$, 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 $H(\eta) \geq \Gamma^* - \Delta_1 - \Delta_2 + \varepsilon + 2U - \Delta_1$. The claim follows by observing that $\Delta_1 < U$. ★

Lemma 4.15 (1) All paths in $(\square \rightarrow \boxplus)_{\text{opt}}$ enter the set $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ via a configuration $(\hat{\eta}, x)$ with $\hat{\eta} \in \mathcal{V}_{\star, \ell^*(\ell^*-1)}$ a quasi-standard configuration and $x \in \partial^- \Lambda$.
(2) All paths in $(\square \rightarrow \boxplus)_{\text{opt}}$ enter the set $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ via a configuration $(\hat{\eta}, x)$ with $\hat{\eta} \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ such that $\Phi(\square, \hat{\eta}) \leq \Gamma^*$, i.e., $\hat{\eta} \in \bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, and $x \in \partial^- \Lambda$. Consequently, $\bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ is a gate for the transition $\square \rightarrow \boxplus$.

Proof. (1) This is immediate from Lemma 4.14.

(2) By Theorem 3.5 in Chapter 3 (which identifies Γ^*) 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 $\eta \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$, then $H(\eta) = \Gamma^* - \Delta_2$. We argue by contradiction. Suppose that $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ enters $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ via a configuration $\zeta = (\hat{\zeta}, x)$ with $\zeta \in \mathcal{V}_{\star, \ell^*(\ell^*-1)+1} \setminus \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ and $x \in \partial^- \Lambda$. Then $H(\zeta) = H(\hat{\zeta}) + \Delta_2 > \Gamma^*$, because $H(\hat{\zeta}) > \Gamma^* - \Delta_2$. Hence ω is not optimal. ★

4.3.2 Characterization of $g(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ and $\bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$

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 $\omega: \square \rightarrow \boxplus = (\square, \dots, \xi, \eta, \zeta, \dots, \boxplus)$. 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

4.3 Preparatory lemmas

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 $\zeta \in \bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ there is a standard configuration $\bar{\eta} \in \hat{\mathcal{S}}_{\ell^*(\ell^*-1)+1}$ such that $\zeta \in \bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$.

(2) For every $\zeta \in g(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ there is a standard configuration $\bar{\eta} \in \hat{\mathcal{S}}_{\ell^*(\ell^*-1)+1}$ such that $\zeta \in g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. Consequently,

$$g(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \bigcup_{\bar{\eta} \in \hat{\mathcal{S}}_{\ell^*(\ell^*-1)+1}} g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}). \quad (4.22)$$

Proof. (1) Pick $\zeta \in \bar{g}(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. Let $\omega: \square \rightarrow \zeta$ be such that $\max_{\xi \in \omega} H(\xi) \leq \Gamma^*$. Let η be the configuration visited by ω when it enters the set $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ 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 $\mathcal{V}_{\star, \ell^*(\ell^*-1)}$ and $x \in \partial^- \Lambda$, otherwise $H(\eta) > \Gamma^*$. We will show that there is a standard configuration $\bar{\eta} \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ and a path $\omega_3: \eta \rightarrow \bar{\eta}$ such that $H(\xi) \leq H(\eta)$ and $n_2(\xi) = \ell^*(\ell^* - 1) + 1$ for all $\xi \in \omega_3$.

Let $\tilde{\eta}$ be the standard configuration in $\mathcal{V}_{\star, \ell^*(\ell^*-1)}$ 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 $\ell^*(\ell^* - 1)$ 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 $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ obtained from $\tilde{\eta}$ by adding a protuberance, with the particle of type 2 in this protuberance located at a site y^* 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 $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ is entered for the last time before visiting ζ , all configurations in $S_{\omega_2}(\eta)$ have at least $\ell^*(\ell^* - 1) + 1$ 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 $H(\eta) \geq \Gamma^* + \varepsilon - \Delta_1$, 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 $L > 2\ell^*$ (and hence the sides of $\hat{\eta}$ are smaller than the sides of Λ), it follows that all sites $y \in \Lambda^-$ such that $y \notin \text{supp}(\hat{\eta})$ are lattice-connecting. In particular, there exists a lattice path $\lambda = x_0, x_1, \dots, x_m$ in Λ for some $m \in \mathbb{N}$ with $x_0 = x$ and $x_m = y^*$.

4 Critical configurations

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^* and then saturating all the particles of type 2 in $(\hat{\eta}, y^*)$. Note that $H(\hat{\eta}, y^*) \leq H(\eta) - U$ 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 $H(\xi) \leq \Gamma^*$ and $n_2(\xi) \geq \ell^*(\ell^* - 1) + 1$ for all $\xi \in \tilde{\omega}$.

(2) Same as part (1).

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4.3.3 Characterization of $\mathcal{G}(\square, \boxplus)$

Lemma 4.18 (1) *All saddles in $\mathcal{V}_{\star, \leq \ell^*(\ell^*-1)}$ are unessential.*

(2) *Let $\zeta \in \mathcal{V}_{\star, \leq \ell^*(\ell^*-1)+1}$ be such that $H(\zeta) = \Gamma^*$. Let $\mathcal{O}(\zeta) = \{\omega \in (\square \rightarrow \boxplus)_{\text{opt}} : \omega \ni \zeta\}$ be the set of optimal paths visiting ζ . If all paths in $\mathcal{O}(\zeta)$ visit $g(\{\square\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ after visiting ζ , then ζ is unessential.*

Proof. (1) Let $\zeta \in \mathcal{V}_{\star, \leq \ell^*(\ell^*-1)}$ be a configuration such that $H(\zeta) = \Gamma^*$. By Lemma 4.15(2), we have (recall Definition 4.2(e)) $S(\omega) \setminus \{\zeta\} \neq \emptyset$ for all $\omega \in \mathcal{O}(\zeta)$, i.e., all paths in $\mathcal{O}(\zeta)$ visit at least one other saddle configuration. Pick $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$. By Lemma 4.15(1), ω (last) enters the set $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ via a configuration (ρ_i, x) with ρ_i a quasi-standard configuration obtained from the standard configuration $\rho_0 \in \mathcal{V}_{\star, \ell^*(\ell^*-1)}$ 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, $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ implies that $H(\rho_i, x) \leq \Gamma^*$ and, consequently, $H(\rho_i) \leq \Gamma^* - \Delta_2$. Furthermore, $H(\rho_j) < H(\rho_i)$ for $j < i$. Let $\omega_3: \square \rightarrow \rho_0$ be a path from $\square$ to ρ_0 such that $H(\xi) < \Gamma^*$ for all $\xi \in \omega_3$ (e.g. follow the construction of the “reference path” in Chapter 3), and let $\omega_4: \rho_0 \rightarrow \rho_i$ 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 $\max_{\xi \in \omega_4} H(\xi) < \Gamma^*$. Consider the path $\hat{\omega} = \omega_3 + \omega_4 + \omega_2$. By construction, $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ and $S(\hat{\omega}) \subset S(\omega) \setminus \{\zeta\}$. Finally, observe that the same argument holds for any $\omega \in \mathcal{O}(\zeta)$.

(2) Since $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) \subset \mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$, all optimal paths from $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ to $\boxplus$ must visit the set $\bar{\Gamma} \mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$. Therefore $S(\omega) \setminus \{\zeta\} \neq \emptyset$ for all $\omega \in \mathcal{O}(\zeta)$, since all configurations in $\bar{\Gamma} \mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ have energy Γ^* . Pick $\omega \in \mathcal{O}(\zeta)$, and let η be the first configuration in $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ 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 $\eta \in g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, there is a path ω_3 from $\square$ to η such that

$H(\sigma) < \Gamma^*$ for all $\sigma \in \omega_3$. Let $\hat{\omega} = \omega_3 + \omega_2$. By construction, $\hat{\omega} \in (\square \rightarrow \boxplus)_{\text{opt}}$ and $S(\hat{\omega}) \subseteq S(\omega) \setminus \{\zeta\}$. Finally, observe that the same argument holds for all $\omega \in \mathcal{O}(\zeta)$. ★

Lemma 4.19 *If $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, then $\mathcal{C}_{\text{bd}}^* \subset g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ and $\mathcal{P} \subset g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$.*

Proof. By Lemma 4.15(2), if $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, then $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ is a gate for the transition $\square \rightarrow \boxplus$. Since $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ is a gate, there exists a $\mathcal{W} \subset g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ that is a minimal gate for the transition $\square \rightarrow \boxplus$. Let $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$. Since $\mathcal{W} \subset \mathcal{G}(\square, \boxplus)$ and $\omega \cap \mathcal{W} \neq \emptyset$, it follows that $\omega \cap \mathcal{G}(\square, \boxplus) \cap g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2} \neq \emptyset$. Combining Lemmas 4.15 and 4.18, it follows that if $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, then all saddles in $\mathcal{V}_{\star, \leq \ell^*(\ell^*-1)+1}$ 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 $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$. Since the choice of $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ is arbitrary, we conclude that $\mathcal{C}_{\text{bd}}^* \subset g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$.

It remains to show that $\mathcal{P} \subset g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. The proof is by contradiction. Pick $\hat{\eta} \in \mathcal{P} \setminus g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. Since $\mathcal{C}_{\text{bd}}^* \subset g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$, there is a configuration $\eta \in g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ obtained in a single step from $\hat{\eta}$. Clearly, $\hat{\eta} \in \mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+1}$, 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 $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, all paths in $(\square \rightarrow \boxplus)_{\text{opt}}$ enter $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ by adding a particle of type 2 in $\partial^- \Lambda$ to a configuration in $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, it follows that $\hat{\eta} \in \mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+2}$ 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 ℓ^* , namely, $\ell^* = 2, 3$.

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 $\omega: \eta \rightarrow \eta'$ (possibly of length zero) such that all configuration in ω have the same tile support and $\Phi(\eta, \eta') < \Gamma^*$. In words,*

4 Critical configurations

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 Γ^* .

(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 $H(\eta') \leq H(\eta)$. 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 .

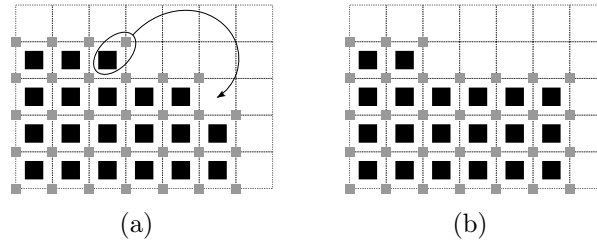


Figure 4.8: Motion of a 2-tile.

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.

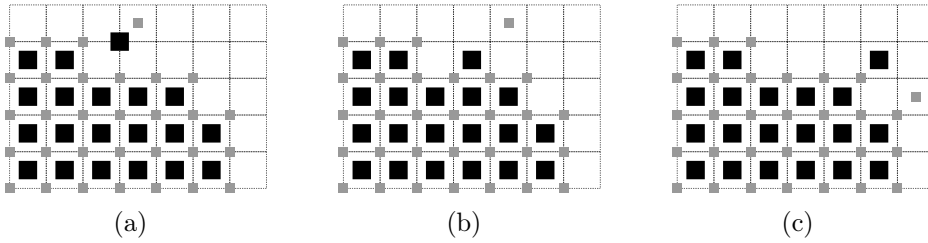


Figure 4.9: A dimer is moved to a corner within energy barrier $3U$.

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

4 Critical configurations

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)).

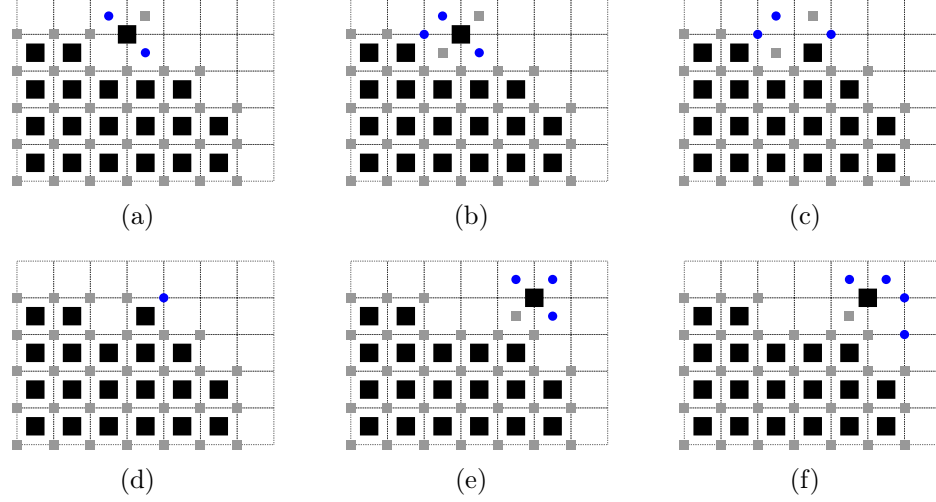


Figure 4.10: A dimer is moved to a corner within energy barrier $U + 4\Delta_1$. The small circles represent the extra particles of type 1 with respect to those in the starting configuration.

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 South-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 $(\square \rightarrow \boxplus)_{\text{opt}}$ enters the set $\mathcal{V}_{*,\ell^*(\ell^*-1)+2}$ when a particle of type 2 is added in $\partial^-\Lambda$ to a configuration in $\bar{g}(\square, \bar{\mathcal{V}}_{*,\ell^*(\ell^*-1)+1})$. By Lemma 4.17, we know that $\bar{g}(\square, \bar{\mathcal{V}}_{*,\ell^*(\ell^*-1)+1})$ can be determined by looking at all the configurations that can be reached starting from the standard configurations in $\mathcal{V}_{*,\ell^*(\ell^*-1)+1}$ 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 .*

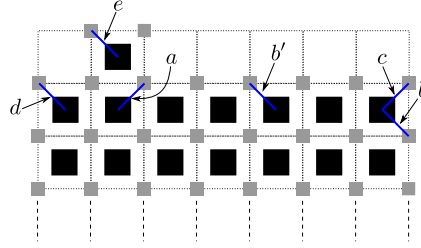


Figure 4.11: Types of edges for the first possible heavy-step starting from a standard configuration.

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

4 Critical configurations

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 $\eta_1 \notin \bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$ 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 their 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 $\eta_1 \notin \bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$ 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 $\eta_2 \notin \bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$ 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.

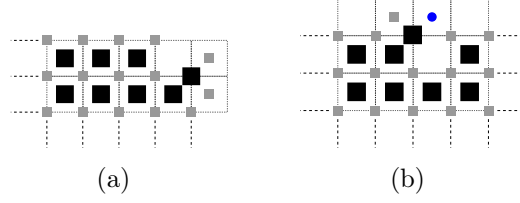


Figure 4.12: Two choices for the first heavy-step that are too costly.

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 $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})^{\text{bd}2}$ is a good candidate for $\mathcal{C}_{\text{bd}}^*$.

4.4.3 Small values of ℓ^*

In Section 4.5 we will identify the geometry of the protocritical and critical configurations for $\ell^* \geq 4$, i.e., for the subregion $\Delta_2 > 4U - \frac{4}{3}\Delta_1$. The analysis will show that the set $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ consists of all the configurations in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$. The region $\Delta_2 \leq 4U - \frac{4}{3}\Delta_1$ is denoted by **RT**.

For $\ell^* = 2$ 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 $\ell^* = 3$ 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).

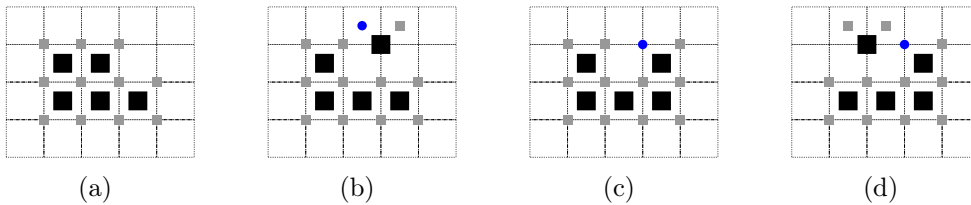


Figure 4.13: Sliding a 12-bar of length 2.

4 Critical configurations

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 $\mathcal{P} = \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ and $\mathcal{C}_{\text{bd}}^* = \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}^{\text{bd}2}$. 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 $\mathcal{C}_{\text{bd}}^*$ for the subregions **RA**, **RB** and **RC**, respectively. Once the structure of the configurations in $\mathcal{P}$ and $\mathcal{C}_{\text{bd}}^*$ are identified, (H3-a) and (H3-b) will follow immediately. To prove (H3-c), we will show the existence of a $\zeta \in \mathcal{C}_{\text{att}}^*(\hat{\eta})$ such that $\Phi(\zeta, \boxplus) < \Gamma^*$ (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 $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ pass through $\mathcal{C}_{\text{att}}^*$, we observe that, as long as the free particle of type 2 does not attach itself to the cluster, the energy cannot drop below Γ^* and hence no other particle is allowed to enter Λ . In particular, this implies that the set $\mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+2} \ni \boxplus$ 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 $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ and $\bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ 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 Γ^* ; (3) identification of $\mathcal{P}$ and $\mathcal{C}_{\text{bd}}^*$.

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 $\ell^*(\ell^* - 1) + 1$ particles of type 2 whose dual tile support is a rectangle of side lengths $\ell^*, \ell^* - 1$ plus a protuberance on one of the four side of the rectangle (see Fig. 4.14).

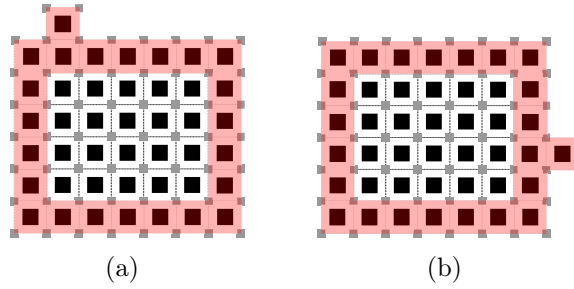


Figure 4.14: Two examples of configurations in $\mathcal{D}_A$ for $\ell^* = 7$. The external particles of type 2 are those lying in the shaded area.

Definition 4.27 A path ω from $\eta \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ to $\eta' \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ 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 $\eta' \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ belongs to $\bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ (respectively, $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$) with $\bar{\eta}$ a standard configuration in $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ if and only if there is a modifying path from $\bar{\eta}$ to η' that does not exceed (respectively, stays below) energy level Γ^* .

Remark 4.28 Note that if there is a path $\omega: \eta \rightarrow \eta'$ that does not exceed (stay below) Γ^* , then there is also a path $\omega': \eta \rightarrow \eta'$ 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 $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ and $\bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$

Lemma 4.29 $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \mathcal{D}_A$.

Proof. Let ρ be a configuration consisting of 2-tiled dual rectangle with horizontal side length ℓ^* and vertical side length $\ell^* - 1$ whose top-rightmost 2-tile is centered

4 Critical configurations

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 $H(\bar{\eta}) = \Gamma^* - \Delta_2$. 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 $\mathcal{D}_A \subseteq g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1})$. 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 $\Phi((\rho, y), \eta) < \Gamma^*$ 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 Γ^* . Note that we are interested only in those modifying paths consisting of at least one heavy-step, otherwise the only configuration in $\bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$ 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 Γ^* , i.e., within energy barrier Δ_2 , the only configurations in $\bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$ that can be reached via a path consisting of configurations with $\ell^*(\ell^*-1) + 1$ particles of type 2 are obtained by “moving” the 2-tiled protuberance.

Let $\eta \in \bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1})$, and let ω be a modifying path from $\bar{\eta}$ to η such that $H(\xi) \leq \Gamma^* = H(\bar{\eta}) + \Delta_2$ for all $\xi \in \omega$. Note that, since $\Delta_2 < 3U$, we have $B^-(\xi) \leq 2$ for all $\xi \in \omega$. Furthermore, in $\mathcal{D}_A \setminus (\mathcal{D}_A \cap \mathbf{RT})$ we have $\Delta_1 > \frac{1}{2}U$ and $\Delta_2 > U + 3\Delta_1$. This implies that, for $\xi \in \omega$,

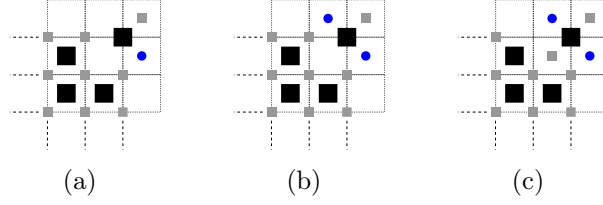
- (i) if $B^-(\xi) = 1$, then $n_1^+(\xi) \leq 2$;
- (ii) if $B^-(\xi) = 2$, then $n_1^+(\xi) \leq 1$.

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 $\mathbf{RA}$ 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 Γ^* .*

Proof. **1.** Assume that the 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


 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 Γ^* .
- $B(p_1, \eta_1) = 1$: $H(\eta_1) - H(\bar{\eta}) = 3U > \Delta_2$.
- $B(p_1, \eta_1) = 2$. 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 $\bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$, 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 of 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 Γ^* 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 Γ^* .

2. Assume that the first heavy-step is along edge d . Let x be the site where

4 Critical configurations

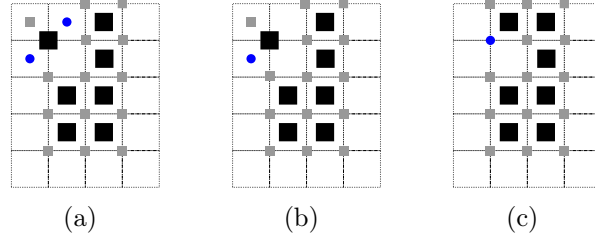


Figure 4.16: Region **RA**, first heavy-step along edge d .

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 $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ 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 Γ^* from η_2 are the same as those that

4.5 Geometry of critical configurations

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 Γ^* 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 Γ^* before reaching a configuration in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$.*

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.

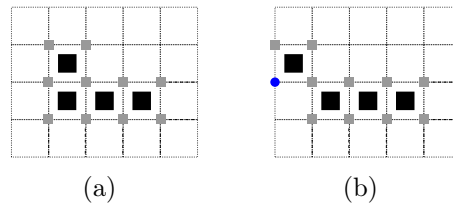


Figure 4.17: Modifying paths may create hanging protuberances.

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.

4 Critical configurations

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 $\bar{\mathcal{V}}_{\star, \ell^{\star}(\ell^{\star}-1)+1} \setminus \mathcal{D}_A$ 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 or 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 from Λ ($\Delta H = -\Delta_1$).

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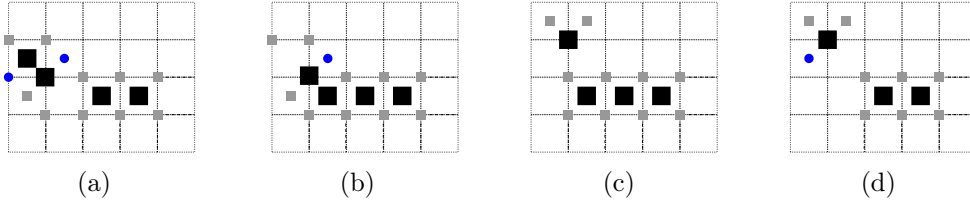


Figure 4.18: Region **RA**, first heavy-step along edge e .

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 $\Phi((\hat{\eta}, x), \boxplus) < \Gamma^*$.*

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 ℓ^* . Conversely, if the protuberance is on one of the shortest sides, then the rectangle circumscribing the cluster has side lengths $\ell^* - 1, \ell^* + 1$. 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 $\Gamma^* - 3U$ is reached. The particle at site x can be saturated within the energy barrier Δ_1 , to reach a configuration with energy $\Gamma^* - \Delta_2 - \varepsilon < H(\eta)$ for all $\eta \in \mathcal{D}_A$, consisting of a rectangle of side lengths $\ell^*, \ell^* - 1$ 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 ℓ^* . The claim in the lemma follows from Remark 4.11. Such a configuration is

4 Critical configurations

supercritical (and has energy smaller than the standard configuration with $\ell^*(\ell^* - 1)$ particles of type 2). Therefore it can grow until $\boxplus$ is reached while staying below energy level Γ^* .

- 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 $\Gamma^* - 3U$ is reached. The particle at site x can be saturated within energy barrier Δ_1 , to reach a configuration with energy $\Gamma^* - \Delta_2 - \varepsilon < H(\eta)$ for all $\eta \in \mathcal{D}_A$, consisting of a rectangle of side lengths $\ell^*, \ell^* - 1$ plus a 12-bar of length 2 on its shortest (see Fig. 4.19(a)).

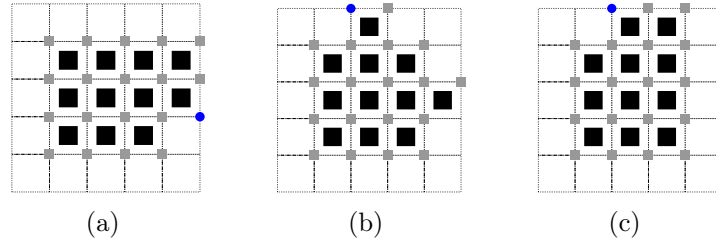


Figure 4.19: Region **RA**, first heavy-step along edge e .

Let y be the central site of a tile adjacent to the North side of the rectangle of side lengths $\ell^*, \ell^* - 1$. 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 $\Gamma^* - \Delta_2 - \varepsilon + U$. 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 $\Gamma^* - \Delta_2 - \varepsilon + U$ (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 $\ell^*, \ell^* - 1$ 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 Γ^* and obtain a 2-tiled rectangle of side lengths $\ell^* + 1, \ell^* - 1$. From this configuration it is possible to iteratively remove $\ell^* - 3$ 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 Γ^* . 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 $\mathcal{C}_{\text{bd}}^*$

Lemma 4.34 $\mathcal{P} = \mathcal{D}_A$ and $\mathcal{C}_{\text{bd}}^* = \mathcal{D}_A^{\text{bd}2}$.

Proof. All configurations in $\mathcal{D}_A^{\text{bd}2}$ have energy Γ^* . We will show that all configurations in $\mathcal{D}_A^{\text{bd}2}$ are essential saddles, and therefore belong to $\mathcal{G}(\square, \boxplus)$ by Lemma 4.3. Pick $\eta = (\hat{\eta}, x)$ in $\mathcal{D}_A^{\text{bd}2}$.

Let $\mathcal{U}(\eta)$ be the set of optimal paths entering $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ via configuration η . Pick $\omega \in \mathcal{U}(\eta)$ such that $H(\xi) < \Gamma^*$ 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 $H(\xi) < \Gamma^*$ for all $\xi \in S_\omega((\hat{\eta}, y_m))$. Note that such a path ω exists because:

- (i) $\hat{\eta} \in g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ by Lemma 4.29;
- (ii) there exists an $y_m \in F(\hat{\eta})$ such that $\Phi((\hat{\eta}, y_m)) < \Gamma^*$ 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 not 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 $S(\omega') \not\subseteq S(\omega) \setminus \{\eta\}$ for all $\omega' \in (\eta, \eta')_{\text{opt}}$. Consider the partition $(\square \rightarrow \boxplus)_{\text{opt}} = (\mathcal{U}(\eta), \mathcal{U}^c(\eta))$ with $\mathcal{U}^c(\eta) = (\square \rightarrow \boxplus)_{\text{opt}} \setminus \mathcal{U}(\eta)$. If $\omega' \in \mathcal{U}(\eta)$, then $S(\omega') \not\subseteq S(\omega) \setminus \{\eta\}$ 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 $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ via some configuration $\zeta = (\hat{\zeta}, z)$ with $H(\zeta) = \Gamma^*$ and $z \in \partial^-\Lambda$ that does not belong to $S(\omega)$ (by the construction of ω). Since the choice of $\eta \in \mathcal{D}_A^{\text{bd}2}$ was arbitrary, we conclude that all configurations in $\mathcal{D}_A^{\text{bd}2}$ are essential saddles, and hence that $\mathcal{D}_A^{\text{bd}2} \subset \mathcal{G}(\square, \boxplus)$.

4 Critical configurations

To prove that $\mathcal{D}_A^{\text{bd}2} = \mathcal{C}_{\text{bd}}^*$, i.e., $\mathcal{D}_A^{\text{bd}2}$ is the entrance of the essential gate, we will show that, for any path $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$, any configuration $\zeta \in \mathcal{S}(\square, \boxplus)$ that is visited by ω before some configuration in $\mathcal{D}_A^{\text{bd}2}$ is an unessential saddle and therefore does not belong to $\mathcal{G}(\square, \boxplus)$.

- We show that all saddles in $\mathcal{V}_{\star, \leq \ell^*(\ell^*-1)+1}$ are unessential. To that end, we pick $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ and we let $\zeta \in \omega$ be such that $H(\zeta) = \Gamma^*$ and $n_2(\zeta) \leq \ell^*(\ell^* - 1) + 1$. By Lemma 4.15(1), all optimal paths enter $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ via a configuration in $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+2})^{\text{bd}2}$. Hence, after visiting ζ , ω must visit $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+2})$ before entering $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$. By Lemma 4.29, combined with Lemma 4.17, we have $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+2}) = g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+2})$. The claim now follows via Lemma 4.18(1).
- For all $\omega \in (\square \rightarrow \boxplus)_{\text{opt}}$ such that $\xi \in S(\omega)$ and $\xi \in \mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+2} \setminus \mathcal{D}_A^{\text{bd}2}$, there exists an $\eta \in \mathcal{D}_A^{\text{bd}2}$ such that $\eta \in P_\omega(\xi)$. Indeed, by Lemmas 4.15(1) and 4.29, all optimal paths enter $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ via a configuration in $\mathcal{D}_A^{\text{bd}2}$.
- To conclude, we need to show that $\mathcal{P} = \mathcal{D}_A$. The inclusion $\mathcal{P} \supseteq \mathcal{D}_A$ is immediate, since all $\eta = (\hat{\eta}, x) \in \mathcal{D}_A^{\text{bd}2} = \mathcal{C}_{\text{bd}}^*$ are obtained, in a single step, by adding a particle of type 2 at the boundary of Λ to a configuration $\hat{\eta} \in g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \mathcal{D}_A$. To see that $\mathcal{P} \subseteq \mathcal{D}_A$, suppose that there is a configuration $\hat{\eta} \in \mathcal{P} \setminus \mathcal{D}_A$. Let $\hat{\eta}'$ be the configuration in $\mathcal{C}_{\text{bd}}^* = \mathcal{D}_A^{\text{bd}2}$ obtained in a single step from $\hat{\eta}$. Observe that $\mathcal{D}_A^{\text{bd}2} \subset \uparrow \mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$. Since, by Lemma 4.15(1), all optimal paths enter $\mathcal{V}_{\star, \ell^*(\ell^*-1)+2}$ by adding a particle of type 2 at $\partial^- \Lambda$ to a configuration in $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \mathcal{D}_A$, it follows that $\hat{\eta} \in \mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+2}$. Indeed, by assumption, this configuration cannot be in $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \mathcal{D}_A$. In particular, it follows that $\hat{\eta} \in \mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+2} \setminus \mathcal{D}_A^{\text{bd}2}$. But this means that there is a path $\hat{\omega} \in (\square \rightarrow \boxplus)_{\text{opt}}$ that reaches $\hat{\eta} \in \mathcal{V}_{\star, \geq \ell^*(\ell^*-1)+2} \setminus \mathcal{D}_A^{\text{bd}2}$ and does not contain any configuration in $\mathcal{G}(\square, \boxplus)$. In particular, $\hat{\omega}$ does not contain any configuration in $\mathcal{D}_A^{\text{bd}2}$. But this is a contradiction, since by Lemmas 4.15(1) and 4.29, all optimal paths enter $\mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ via a configuration in $\mathcal{D}_A^{\text{bd}2}$.

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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 $\ell^*(\ell^* - 1) + 1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing

4.5 Geometry of critical configurations

rectangle has side lengths either ℓ^*, ℓ^* or $\ell^* + 1, \ell^* - 1$ (see Fig. 4.20). Note that $\mathcal{D}_B \supseteq \mathcal{D}_A$.

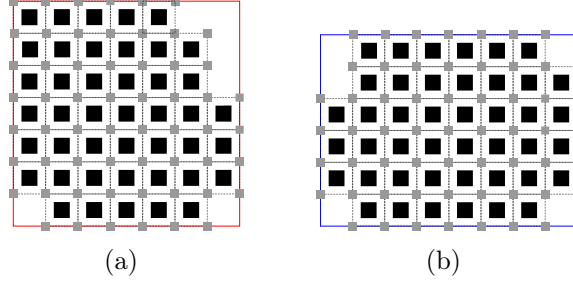


Figure 4.20: Two examples of configurations in $\mathcal{D}_B$ for $\ell^* = 7$.

Identification of $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ and $\bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$

There are configurations in $\mathcal{D}_B$ that cannot be reached within energy level Γ^* . These configurations have support near the boundary of Λ and for $\Lambda \rightarrow \mathbb{Z}^2$ form a negligible fraction of $\mathcal{D}_B$.

Lemma 4.35 $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) \subseteq \mathcal{D}_B$.

Proof. Note that in $\mathcal{D}_B$, for $\xi \in \mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ the following conditions are satisfied

- (i) $B^-(\sigma) = 1$: $n_1^+(\sigma) \leq 3$;
- (ii) $B^-(\sigma) = 2$: $n_1^+(\sigma) \leq 1$.
- (iii) $B^-(\sigma) = 3$: $n_1^+(\sigma) \leq 0$.

Observe that $\Delta_2 \leq 3U + \Delta_1$ throughout region **RB**, and therefore Lemma 4.26 applies. This means that any heavy-step, completed without exceeding energy level Γ^* and starting from a configuration in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$, 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 (ℓ^*, ℓ^*) or $(\ell^* - 1, \ell^* + 1)$, and with a fixed lower left corner far enough from $\partial^- \Lambda$, belong to $g(\bar{\eta}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. It remains to show that all other configurations in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ cannot be reached without exceeding energy level Γ^* . 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

4 Critical configurations

the main cluster before the next heavy-step is completed, then the path exceeds energy level Γ^* before reaching a configuration in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$. Therefore we may consider a path whose first heavy-step involves the protuberance and whose second heavy-step does not.

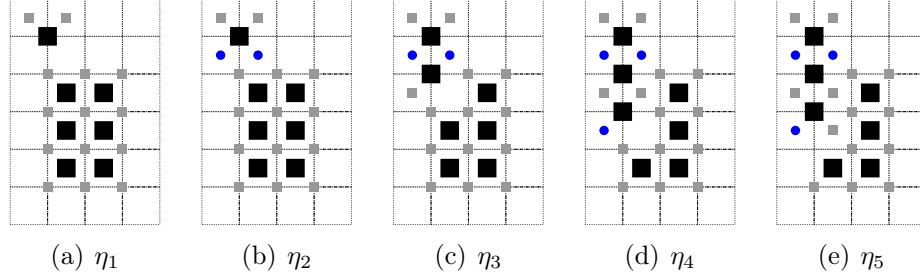


Figure 4.21: The presence of a detached 2-tile precludes the motion of other 2-tiles.

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 Γ^* . 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

4.5 Geometry of critical configurations

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 Γ^* .

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 Γ^* before reaching a configuration in $\bar{\mathcal{V}}_{\star, \ell^* (\ell^* - 1) + 1}$. 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 Γ^* 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 energy level Γ^* , and it is immediate that no other heavy-step is allowed.

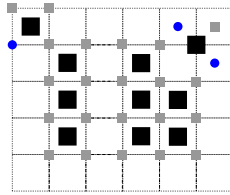


Figure 4.22: The presence of a hanging protuberance precludes the motion of other 2-tiles.

Step 1 and 2 imply the following. A modifying path that does not exceed energy level Γ^* and starts with any heavy-step involving the particle of the protuberance

4 Critical configurations

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 Γ^* before reaching a configuration in $\bar{\mathcal{V}}_{*, \ell^*(\ell^*-1)+1}$.

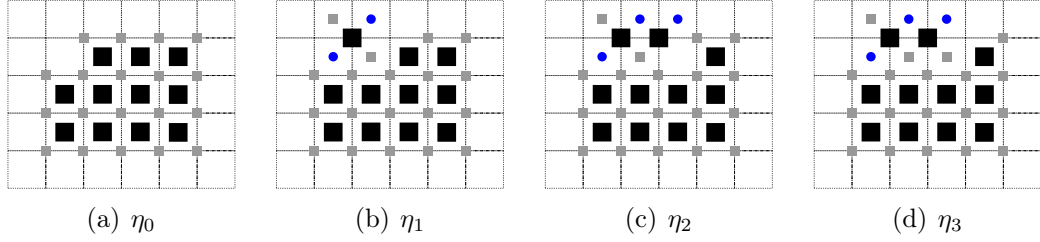


Figure 4.23: First heavy-step from a bar of length ≥ 3 .

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 Γ^* , 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

4.5 Geometry of critical configurations

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 Γ^* .

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 Γ^* , 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)).

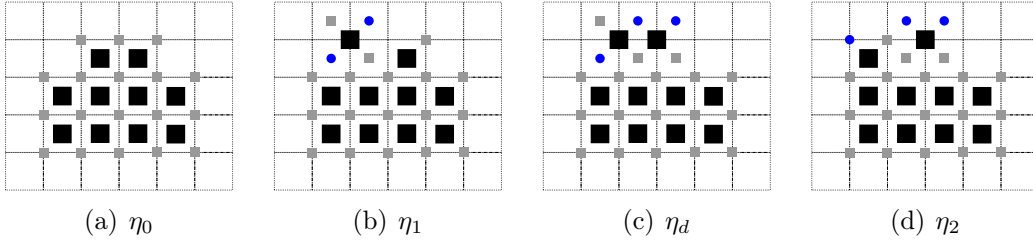


Figure 4.24: First heavy-step from a bar of length 2.

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 $U + 3\Delta_1$.

4 Critical configurations

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 Γ^* (see Fig. 4.25(a)).

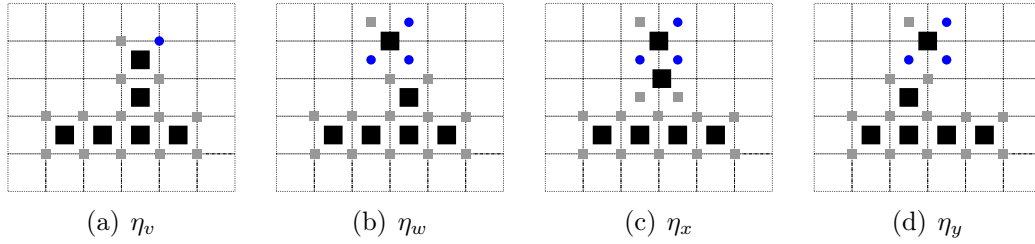


Figure 4.25: Protuberances attached to 12-bars can be treated as 12-bars of length 2.

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 Γ^* , 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

4.5 Geometry of critical configurations

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.

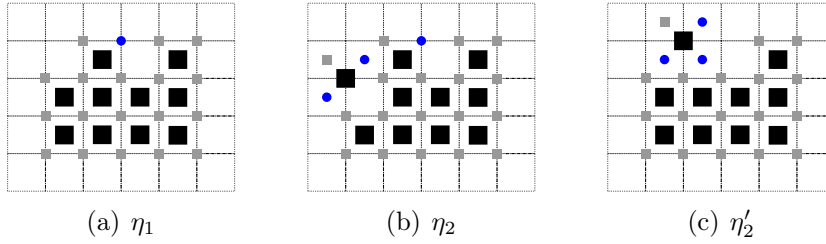


Figure 4.26: Heavy-step from a configuration with protuberances non in $\mathcal{D}_A$

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 Northernmost 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

4 Critical configurations

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 Γ^* 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 $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$) that can be visited by a modifying path that does not exceed energy level Γ^* 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 $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ that are reached without exceeding energy level Γ^* 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–tilled configurations that can be visited by a modifying path starting from a standard configuration $\bar{\eta}$ without exceeding energy level Γ^* 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 $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) \subset \mathcal{D}_B$. Furthermore, if $\eta \in \mathcal{D}_B$ and has support far enough from $\partial^-\Lambda$, then $\eta \in g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. 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 $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$, we will show that the set $\bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) \setminus g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ 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

4.5 Geometry of critical configurations

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 $\bar{\eta} \in \mathcal{V}_{\star, \ell^*(\ell^*-1)+1}$ can take only a discrete set of values. In region **RB**, $\Phi(\bar{\eta}, \eta) = \Gamma^*$ 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 $\bar{g}(\bar{\eta}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$. Let η' belong to this set, and let $\omega : \bar{\eta} \rightarrow \eta'$. Assume that $\max_{\xi \in \omega} H(\xi) = U + 3\Delta_1$ and let $\text{supp}(\omega) = \cup_{\xi \in \omega} \text{supp}(\xi)$. Then, from the previous analysis, it follows that there is a path $\omega' : \bar{\eta} \rightarrow \eta'$ such that $\max_{\xi \in \omega'} H(\xi) = H(\bar{\eta}) + 3U$ and $\text{supp}(\omega') \subset \text{supp}(\omega)$. 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 $\Phi((\hat{\eta}, x), \boxplus) < \Gamma^*$.*

Proof. The dual support of $\hat{\eta} \in \mathcal{D}_B$ is either a square of side length ℓ^* or a rectangle of side lengths $\ell^* + 1, \ell^* - 1$. Let x be a site in a good dual corner of $\hat{\eta}$. After a particle of type 2 has reached site x ($H((\hat{\eta}, x)), \Gamma^* - 3U$), 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 $H(\eta') = \Gamma^* - \Delta_2 - \varepsilon$. 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 ℓ^* . By Remark 4.11 this is enough. If, on the other hand, the rectangle circumscribing the dual support of η' has side length $\ell^* + 1, \ell^* - 1$, then by filling this rectangle we obtain a dual 2-tiled rectangle of side lengths $\ell^* + 1, \ell^* - 1$. From this point on, it is possible to argue as in the final part of the proof of Lemma 4.33. ★

4 Critical configurations

Identification of $\mathcal{P}$ and $\mathcal{C}_{\text{bd}}^*$

Lemma 4.38 $\mathcal{P} = \mathcal{D}_B$ and $\mathcal{C}_{\text{bd}}^* = \mathcal{D}_B^{\text{bd}2}$.

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 $\ell^*(\ell^* - 1) + 1$ particles of type 2 whose dual tile support is a monotone polyomino and whose circumscribing rectangle has perimeter $4\ell^*$ (see Fig. 4.27).

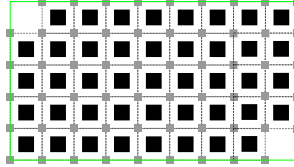


Figure 4.27: An example of configuration in $\mathcal{D}_C$ for $\ell^* = 7$.

Identification of $g(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$ and $\bar{g}(\{\bar{\eta}\}, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1})$

Lemma 4.39 $g(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \bar{g}(\square, \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}) = \mathcal{D}_C$.

Proof. First observe that the sets $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ 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 $\omega : \bar{\eta} \rightarrow \eta$ such that $\max_{\xi \in \omega} H(\xi) < \Gamma^*$ or, equivalently, a path $\omega' : \eta \rightarrow \bar{\eta}$ such that $\max_{\xi \in \omega'} H(\xi) < \Gamma^*$.

1. We know from Remark 4.25 that, starting from a 2-tiled configuration $\eta' \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ whose dual tile support has a circumscribing rectangle of side lengths L, l with $L \geq l$ and $L \times l > \ell^*(\ell^* - 1) + 1$, it is possible to reach below energy level Γ^* all configurations in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ 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 $\eta'' \in \bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ whose dual support has a circumscribing rectangle with side lengths $L+1, l-1$ (whenever $(L+1) \times (l-1) \geq \ell^*(\ell^* - 1) + 1$).

4.5 Geometry of critical configurations

2. From η' it is possible to reach below energy level Γ^* a configuration $\tilde{\eta}$ whose tile support, in dual coordinates, is a rectangle of side lengths $L-1, l$ plus a bar of length $k = \ell^*(\ell^*-1) + 1 - (L-1)l$ on top of the longest side of the rectangle. There are two cases. Either $k > l$ or $k \leq l$. If $k > l$, then $(L+1)(l-1) < \ell^*(\ell^*-1) + 1$. 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 $\partial^-\Lambda$.

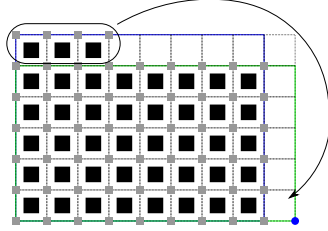


Figure 4.28: The top bar can be moved to the East side of the rectangle within a energy barrier $3U + \Delta_1$.

4. It is clear that this argument is sufficient to show that from a 2-tiled configuration in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$ 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 Γ^* . This implies (see Lemma 4.17) that $\Phi(\square, \eta) < \Gamma^*$ 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 Γ^* some standard configuration in $\bar{\mathcal{V}}_{\star, \ell^*(\ell^*-1)+1}$. A particle is said to be close to

4 Critical configurations

$\partial^- \Lambda$ 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 $\partial^- \Lambda$.

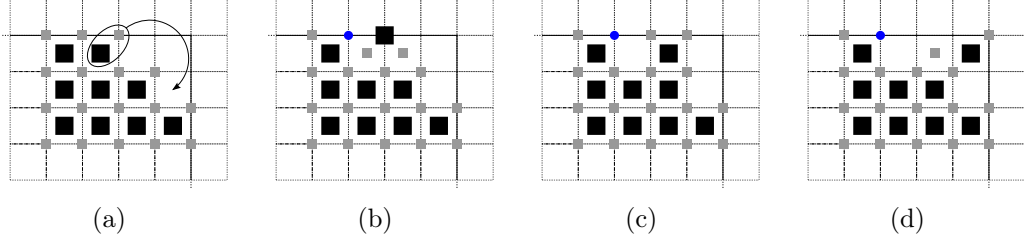


Figure 4.29: Dimers that are close to $\partial^- \Lambda$ can be moved within a $3U + \Delta_1$ energy barrier. A particle that is “beyond” the black line can not have active bonds.

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 be 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 $L = l = \ell^*$, then we can reach a standard configuration and we are done.

4.5 Geometry of critical configurations

- If $L = \ell^* + 1$ and $l = \ell^* - 1$ (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 Γ^* 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 $\ell^* + 1, \ell^* - 1$ is reached. But this case has already been treated.

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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 $\Phi((\hat{\eta}, x), \boxplus) < \Gamma^*$.*

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 $H(\xi) < \Gamma^*$ 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.

- $Ll > \ell^*(\ell^* - 1) + 1$. 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 $\Phi(\hat{\eta}, \eta'') < \Gamma^*$. 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 . $H(\tilde{\eta}) \leq \Gamma^* - 4U + 2\Delta_1$. As in the proof of Lemma 4.39, all the tiles of the Eastern-most 12-bar of $\tilde{\eta}$ can be iteratively moved to a corner on

4 Critical configurations

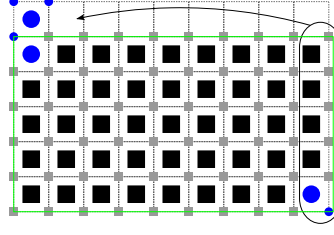


Figure 4.30: The configuration obtained from $\hat{\eta}$ by first filling the rectangle circumscribing its dual support and then adding a 2-tiled on the North side; circles represent particles added to $\hat{\eta}$.

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 $\Phi((\hat{\eta}, x), \tilde{\eta}')le\Gamma^* - 4U + 2\Delta_1 + 3U < \Gamma^*$ as soon as $\Delta_1 < \frac{1}{2}$, which is satisfied in **RF**.

- $Ll > \ell^*(\ell^* - 1) + 1$. 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 $H((\hat{\eta}, x)) = \Gamma^* - 2U$. Let $\tilde{\eta}$ be the configuration obtained within energy barrier Δ_1 by saturating the particle of type 2 at x . $H(\tilde{\eta}) = \Gamma^* - 4U + 2\Delta_1$. From $\tilde{\eta}$ proceed as in the previous case.

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Identification of $\mathcal{P}$ and $\mathcal{C}_{\text{bd}}^*$

Lemma 4.41 $\mathcal{P} = \mathcal{D}_C$ and $\mathcal{C}_{\text{bd}}^* = \mathcal{D}_C^{\text{bd}2}$.

Proof. Same as the proof of Lemma 4.34.

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Appendix: Computation of N^*

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 func-

4.5 Geometry of critical configurations

tions. Two basic generating functions

$$s(x) = 1 + \sum_{k=1}^{\infty} x^{k^2} \prod_{j=1}^k \frac{1}{1 - x^{2j}}, \quad a(x) = \prod_{j=1}^{\infty} \frac{1}{1 - x^j} \quad (4.23)$$

are used to define two composite generating functions

$$r(x) = \frac{1}{4} [a(x)^4 + 3a(x^2)^2], \quad q(x) = \frac{1}{8} [a(x)^4 + 3a(x^2)^2 + 2s(x)^2 a(x^2) + 2a(x^4)], \quad (4.24)$$

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

$$e(n) = \begin{cases} 1 & \text{if } n = s^2, \\ \sum_{c=0}^{\lfloor -\frac{1}{2} + \frac{1}{2}\sqrt{1+4s-4t} \rfloor} r_{s-c-c^2-t} & \text{if } n = s^2 + t \text{ with } 0 < t < s, \\ 1 & \text{if } n = s^2 + s + t, \\ q_{s+1-t} + \sum_{c=1}^{\lfloor \sqrt{s+1-t} \rfloor} r_{s+1-c^2-t} & \text{if } n = s^2 + s + t \text{ with } 0 < t \leq s, \end{cases} \quad (4.25)$$

where $s = \lfloor \sqrt{n} \rfloor$.

We need to count the number of polyominoes of minimal perimeter with area $n = \ell^*(\ell^* - 1) + 1$ for $\ell^* \geq 4$, i.e., we are only interested in n of the form $s^2 + s + t$ with $s = \ell^* - 1$ 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_{ℓ^*-1} is the number of polyominoes of minimal perimeter when the circumscribing rectangle is a square of side length ℓ^* , and $r_{\ell^*-c^2-1}$ is the number of polyominoes of minimal perimeter when the circumscribing rectangle has side lengths $\ell^* + 1, \ell^* - 1$. Thus, modulo rotations and reflections, we have

$$N^* = \begin{cases} 8[q_{\ell^*-1} + r_{\ell^*-1-1}] & \text{in region } \mathbf{RB}, \\ 8 \left[q_{\ell^*-1} + \sum_{c=1}^{\lfloor \sqrt{\ell^*-1} \rfloor} r_{\ell^*-c^2-1} \right] & \text{in region } \mathbf{RC}. \end{cases} \quad (4.26)$$

