

The double-bubble problem on the square lattice

Manuel Friedrich, Wojciech Górný, and Ulisse Stefanelli

Abstract. We investigate the minimal-perimeter configurations of two finite sets of points on the square lattice. This corresponds to a lattice version of the classical double-bubble problem. We give a detailed description of the fine geometry of minimisers, and, in some parameter regime, we compute the optimal perimeter as a function of the size of the point sets. Moreover, we provide a sharp bound on the difference between two minimisers, which are generally not unique, and use it to rigorously identify their Wulff shape as the size of the point sets scales up.

1. Introduction

The classical double-bubble problem is concerned with the shape of two sets of given volume under minimisation of their surface area. In the Euclidean space, minimisers are enclosed by three spherical caps, intersecting at an angle of $2\pi/3$. The proof of this fact in \mathbb{R}^2 dates back to [23] and has then been extended to \mathbb{R}^3 [31] and \mathbb{R}^n for $n \geq 4$ [43]. See also [15] for a quantitative stability analysis in two dimensions. A number of variants of the problem have also been tackled, including double bubbles in spherical and hyperbolic spaces [16, 17, 19, 36], hyperbolic surfaces [9], cones [32, 39], the 3-torus [11, 18], the Gauß space [16, 38], and in the anisotropic Grushin plane [24].

The aim of this paper is to tackle a lattice version of the double-bubble problem. We restrict our attention to the square lattice \mathbb{Z}^2 and define the *lattice length* of the interface separating two disjoint sets $C, D \subset \mathbb{Z}^2$ as

$$Q(C, D) = \#\{(c, d) \in C \times D : |c - d| = 1\},$$

where $|\cdot|$ is the Euclidean norm. The *lattice double-bubble problem* consists in finding two distinct lattice subsets A and B of fixed sizes $N_A, N_B \in \mathbb{N}$ solving

$$\min\{P(A, B) : A, B \subset \mathbb{Z}^2, A \cap B = \emptyset, \#A = N_A, \#B = N_B\}, \quad (1.1)$$

where the *lattice perimeter* $P(A, B)$ is defined by

$$\begin{aligned} P(A, B) &= Q(A, A^c) + Q(B, B^c) - 2\beta Q(A, B) \\ &= Q(A, A^c \setminus B) + Q(B, B^c \setminus A) + (2 - 2\beta)Q(A, B). \end{aligned} \quad (1.2)$$

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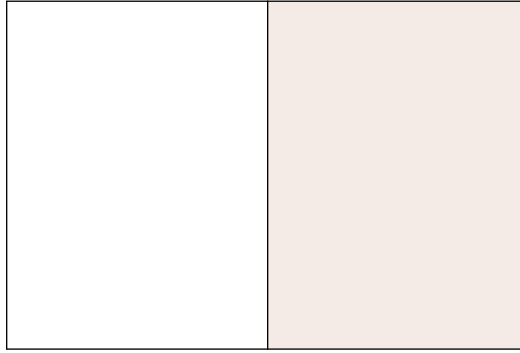


Figure 1. A minimiser for $\beta = 1/2$.

The latter definition features the parameter $\beta \in (0, 1)$. Note that the classical double-bubble case corresponds to the choice $\beta = 1/2$. In the following, we allow for the more general $\beta \in (0, 1)$, for this will be relevant in connection with applications, see Section 2. In particular, β models the interaction between the two sets. The reader is referred to [28] where cost-minimising networks featuring different interaction costs are considered.

Analogously to the Euclidean case, we prove that minimisers (A, B) of (1.1) are connected (A , B , and $A \cup B$ are connected in the usual lattice sense, see below). We call *isoperimetric* those subsets of the lattice which minimise $C \mapsto Q(C, C^c)$ under given cardinality. Without claiming completeness, the reader is referred to the monograph [29] and to [4, 6–8, 46] for a minimal collection of results on discrete isoperimetric inequalities, to [14, 34, 35] for sharp fluctuation estimates, and to [2] for some numerical approximation. A second analogy with the Euclidean setting is that optimal pairs (A, B) *do not* consist of the mere union of two isoperimetric sets A and B , for the onset of an interface between A and B influences their shape.

Differently from the Euclidean case, the existence of minimisers for (1.1) is here obvious, for the minimisation problem is finite. Moreover, the geometry of the intersection of interfaces is much simplified, as effect of the discrete geometry of the underlying lattice. In particular, all interfaces meet at multiples of $\pi/2$ angles.

At finite sizes N_A, N_B , boundary effects are relevant and a whole menagerie of minimisers of (1.1) may arise, depending on the specific values of N_A, N_B , and β . Indeed, although uniqueness holds in some special cases, it cannot be expected in general. We are however able to prove an a priori estimate on the symmetric distance of two minimisers, which differ at most by $N_A^{1/2} = N_B^{1/2}$ points for β irrational or by $N_A^{3/4} = N_B^{3/4}$ points for β rational.

As size scales up, whereas properly rescaled isoperimetric sets approach the square, A and B converge to suitable rectangles. In the limit $N_A = N_B \rightarrow \infty$ (and for $\beta = 1/2$), we prove that minimisers of (1.1) converge to the *Wulff shape* configuration of Figure 1.

That is, uniqueness is restored in the Wulff shape limit. In fact, in the crystalline-perimeter case, the double-bubble problem for $\beta = 1/2$ has been already tackled in [40], see also the recent [22] for an elementary proof of the existence of minimisers. The case $\beta \neq 1/2$ is addressed in [47] instead. In particular, the different possible geometries of the Wulff shape, corresponding to different volume fractions of the two phases, have been identified.

Let us now present our main results. We start by associating to each $\mathcal{V} \subset \mathbb{Z}^2$ the corresponding *unit-disk graph*, namely, the undirected simple graph $G = (\mathcal{V}, \mathcal{E})$, where vertices are identified with the points in \mathcal{V} , and the set $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ of edges contains one edge for each pair of points in \mathcal{V} at distance 1. We say that a subset $\mathcal{V} \subset \mathbb{Z}^2$ is *connected* if the corresponding unit-disk graph is connected. Moreover, we indicate by $R_z := \mathbb{Z} \times \{z\}$ and $C_z = \{z\} \times \mathbb{Z}$ rows and columns for all $z \in \mathbb{Z}$.

Our main findings read as follows.

Theorem 1.1. *Let (A, B) solve the double-bubble problem (1.1). Then,*

- (i) *Connectedness. The sets A , B , and $A \cup B$ are connected. Moreover, the sets $A \cap R_z$, $B \cap R_z$, $(A \cup B) \cap R_z$, $A \cap C_z$, $B \cap C_z$, and $(A \cup B) \cap C_z$ are connected (possibly being empty) for all $z \in \mathbb{Z}$.*
- (ii) *Separation. If $\max\{x : (x, z) \in A\} \leq \min\{x : (x, z) \in B\} - 1$ for some $z \in \mathbb{Z}$, then the same holds with equality for all $z \in \mathbb{Z}$ (whenever not empty). An analogous statement is valid for columns, possibly after exchanging the role of A and B .*
- (iii) *Interface. Let $I \subset \mathbb{R}^2$ be the set of midpoints of segments connecting points in A with points in B at distance 1. Then, for all $x \in I$ there exists $y \in I \setminus \{x\}$ with $|x - y| \in \{1/\sqrt{2}, 1\}$ and I can be included in the image of a piecewise-affine curve $\iota: [0, 1] \rightarrow \mathbb{R}^2$ with monotone components.*

If $N_A = N_B = N$ and $\beta \leq 1/2$, we additionally have that

- (iv) *Minimal perimeter:*

$$P(A, B) = \min_{h \in \mathbb{N}} (4\lceil N/h \rceil + 2h(2 - \beta)), \quad (1.3)$$

where all minimisers h satisfy

$$|h - \sqrt{2N/(2 - \beta)}| \leq C_\beta N^{1/4}$$

for some constant C_β only depending on β . For $\beta \in \mathbb{R} \setminus \mathbb{Q}$, there exists a unique minimiser of (1.3).

- (v) *Explicit solution. Let h minimise (1.3) and $\ell \in \mathbb{N}$ and $0 \leq r < h$ be given with $N = h\ell + r$. Then, letting*

$$A' := \{(x, y) \in \mathbb{Z}^2 : x \in [-\ell + 1, 0], y \in [1, h] \text{ or } x = -\ell, y \in [1, r]\},$$

$$B' := \{(x, y) \in \mathbb{Z}^2 : x \in [1, \ell], y \in [1, h] \text{ or } x = \ell + 1, y \in [1, r]\},$$

the pair (A', B') solves the double-bubble problem (1.1).

(vi) *Fluctuations.* There exists a constant C_β only depending on β and an isometry T of \mathbb{Z}^2 such that

$$\begin{aligned} \#(A \Delta T(A')) + \#(B \Delta T(B')) &\leq C_\beta N^{1/2} && \text{if } \beta \in \mathbb{R} \setminus \mathbb{Q}, \\ \#(A \Delta T(A')) + \#(B \Delta T(B')) &\leq C_\beta N^{3/4} && \text{if } \beta \in \mathbb{Q}, \end{aligned} \quad (1.4)$$

where the pair (A', B') is defined in (v). (See the beginning of Section 9 for the definition of isometry.)

Theorem 1.1 is proved in subsequent steps along the paper, by carefully characterising the geometry of optimal pairs (A, B) . In fact, our analysis reveals additional geometrical details so that the statements in the coming sections are often more precise and more general in terms of conditions on the parameters N_A , N_B , and β with respect to Theorem 1.1. We prefer to postpone these details in order not to overburden the introduction.

The connectedness of optimal pairs (A, B) is discussed in Section 4 and Theorem 1.1 (i) is proved in Theorem 4.5 and Proposition 4.6. The separation property of Theorem 1.1 (ii) follows from Proposition 4.4 and Propositions 4.7–4.8. The geometry of the interface between A and B , namely, Theorem 1.1 (iii), is described by Corollary 4.10.

In Section 5, we present a collection of examples, illustrating the variety of optimal geometries. In particular, we show that optimal pairs may be not unique and, in some specific parameter range, present quite distinguished shapes. We then classify different admissible pairs in Section 6 by introducing five distinct classes of configurations.

The first of these classes, called Class \mathcal{I} and corresponding to Figure 1, is indeed the reference one and is studied in detail in Section 7. In Proposition 7.3, we prove the existence of optimal pairs in Class \mathcal{I} , among which there is the explicit one of Theorem 1.1 (v). The minimal perimeter in Theorem 1.1 (iv) is then computed by referring to this specific class in Theorem 7.4. The remaining classes are studied in Section 8. We show that some of the classes cannot be optimal in the case $N_A = N_B$, and that the other ones can be modified to a configuration in Class \mathcal{I} by an explicit regularisation procedure. We also observe that for arbitrarily large N solutions may appear which are not in Class \mathcal{I} , see Proposition 8.16.

Although optimal pairs (A, B) are not unique, by carefully inspecting our constructions, we are able to prove that, in some specific parameter regime, two optimal pairs differ by at most $C_\beta N^{1/2}$ or $C_\beta N^{3/4}$ points, respectively, depending on the irrationality or rationality of β and up to isometries. This is studied in Section 9, see Theorem 9.1 which proves Theorem 1.1 (vi). If β is irrational, an output of our construction is that the fluctuation bound $C_\beta N^{1/2}$ is sharp. In the case of a rational β , the sharpness of the fluctuation bound will be proved in some future work. The $N^{1/2}$ -scaling in fluctuations is specifically related to the presence of an interface between the two sets A and B . In fact, in case of a single set A , optimal configurations show fluctuations of order $N^{3/4}$, see Section 2.1 for details.

Although the setting of our paper is discrete, our results deliver some understanding of the continuous case as well. This results by considering the so-called *thermodynamic*

limit as $N \rightarrow \infty$. For all $V = \{x_1, \dots, x_N\} \subset \mathbb{Z}^2$, let

$$\mu_V = \left(\sum_{i=1}^N \delta_{x_i/\sqrt{N}} \right) / N$$

be the corresponding empirical measure on the plane and denote by \mathcal{L} the two-dimensional Lebesgue measure. We indicate by

$$\mathcal{A} := \left(-\sqrt{\frac{2-\beta}{2}}, 0 \right) \times \left(0, \sqrt{\frac{2}{2-\beta}} \right) \quad \text{and} \quad \mathcal{B} := \left(0, \sqrt{\frac{2-\beta}{2}} \right) \times \left(0, \sqrt{\frac{2}{2-\beta}} \right) \quad (1.5)$$

the continuous Wulff shapes, see Figure 1. Note that

$$\mathcal{L}(\mathcal{A}) = \mathcal{L}(\mathcal{B}) = 1.$$

By combining the explicit construction of Theorem 1.1 (v) and the fluctuation estimate (1.4), we have the following.

Corollary 1.2 (Wulff shapes). *Let $\beta \leq 1/2$ and (A_N, B_N) be solutions of (1.1) with $N_{A_N} = N_{B_N} = N$ for all $N \in \mathbb{N}$. Then, there exist isometries T_N of \mathbb{Z}^2 such that*

$$\mu_{T_N A_N} \xrightarrow{*} \mathcal{L} \llcorner \mathcal{A} \quad \text{and} \quad \mu_{T_N B_N} \xrightarrow{*} \mathcal{L} \llcorner \mathcal{B}$$

as $N \rightarrow \infty$, where the symbol $\xrightarrow{*}$ indicates the weak-* convergence of measures.

Note that, by taking $\beta = 1$ in (1.5) (not covered by the corollary though), we have that $\mathcal{A} \cup \mathcal{B}$ form a single square with side $\sqrt{2}$, whereas for $\beta = 0$, the Wulff shapes \mathcal{A} and \mathcal{B} are two squares of side 1.

Our results also allow to solve the double-bubble problem in the continuous setting of \mathbb{R}^2 with respect to a crystalline perimeter notion. More precisely, for every set $D \subset \mathbb{R}^2$ of finite perimeter, we denote by $\partial^* D$ its reduced boundary [1, 33] and define the crystalline perimeter and the crystalline length as

$$\text{Per}(D) = \int_{\partial^* D} \|v\|_1 d\mathcal{H}^1, \quad \text{L}(\gamma) = \int_{\gamma} \|v\|_1 d\mathcal{H}^1,$$

where v is the outward pointing unit normal to $\partial^* D$, $\|v\|_1 = |v_x| + |v_y|$, \mathcal{H}^1 is the one-dimensional Hausdorff measure, and $\gamma \subset \partial^* D$ is measurable.

The continuous analogue of (1.1) is the *crystalline double-bubble problem*

$$\min \left\{ \text{Per}(A) + \text{Per}(B) - 2\beta \text{L}(\partial^* A \cap \partial^* B) : A, B \subset \mathbb{R}^2 \text{ of finite perimeter, } A \cap B = \emptyset, \mathcal{L}(A) = \mathcal{L}(B) = 1 \right\}. \quad (1.6)$$

By combining Theorem 1.1 (v) and 1.1 (vi), we obtain the following.

Corollary 1.3 (Crystalline double bubble). *For all $\beta \leq 1/2$, the pair $(\mathcal{A}, \mathcal{B})$ is a solution of (1.6). The minimal energy is given by $4\sqrt{4 - 2\beta}$.*

For the reference choice $\beta = 1/2$, the solution of the crystalline double-bubble problem (1.6) is depicted in Figure 1, see also [21, 40]. Corollaries 1.2 and 1.3 are proved in Section 10.

In the recent work [21], the difference in energy between any properly rescaled optimal discrete configuration and the Wulff shape is estimated. In case $N_A = N_B$ and $\beta \leq 1/2$, such an estimate can be recovered from the exact expressions in Theorem 1.1 (iv) and Corollary 1.3. Note however that the analysis in [21] covers the case $N_A \neq N_B$ as well, although for $\beta = 1/2$ only.

2. Equivalent formulations of the double-bubble problem

2.1. Optimal particle configurations

The double-bubble problem (1.1) can be equivalently recasted in terms of ground states of configurations of particles of two different types. Let $A = \{x_1, \dots, x_{N_A}\}$ and $B = \{x_{N_A+1}, \dots, x_{N_A+N_B}\}$ indicate the mutually distinct positions of particles of two different particle species, and assume that $A, B \subset \mathbb{Z}^2$, which in turn restricts the model to the description of zero-temperature situations. To the particle configuration (A, B) we associate the *configurational energy*

$$E(A, B) = \frac{1}{2} \sum_{i,j=1}^{N_A+N_B} V_{\text{sticky}}(x_i, x_j), \quad (2.1)$$

where

$$V_{\text{sticky}}(x_i, x_j) = \begin{cases} -1 & \text{if } |x_i - x_j| = 1 \text{ and } x_i, x_j \in A \text{ or } x_i, x_j \in B, \\ -\beta & \text{if } |x_i - x_j| = 1 \text{ and } x_i \in A, x_j \in B \text{ or } x_i \in B, x_j \in A, \\ 0 & \text{if } |x_i - x_j| \neq 1. \end{cases}$$

The interaction density $V_{\text{sticky}}(x_i, x_j)$ corresponds to the so-called *sticky* or *Heitmann–Radin-type* potential [30] and models the binding energy of the two particles x_i and x_j . In particular, only first-neighbour interactions contribute to the energy, and *intraspecific* (namely, of type $A - A$ or $B - B$) and *interspecific* (type $A - B$) interactions are quantified differently, with interspecific interactions being weaker as $\beta < 1$.

The relation between the minimisation of E and the double-bubble problem (1.1) is revealed by the equality

$$E(A, B) + 2N_A + 2N_B = \frac{1}{2}P(A, B). \quad (2.2)$$

This follows by analysing the contribution to E and P of each point. In fact, one could decompose

$$E(A, B) = \sum_{i=1}^{N_A+N_B} e(x_i),$$

$$P(A, B) = \sum_{i=1}^{N_A+N_B} p(x_i),$$

where the single-point contribution to energy and perimeter is quantified via

$$e(x) = -\frac{1}{2}\#\{\text{same-species neighbours of } x\} - \frac{\beta}{2}\#\{\text{other-species neighbours of } x\},$$

$$p(x) = 4 - \#\{\text{same-species neighbours of } x\} - \beta\#\{\text{other-species neighbours of } x\}.$$

These definitions entail (2.2), which in turn ensures that ground states of E and minimisers of P coincide, for all given sizes N_A and N_B of the sets A and B .

The geometry of ground states of E results from the competition between intraspecific and interspecific interaction. In the extremal case $\beta = 1$, intra- and interspecific interaction are indistinguishable, and one can consider the whole system (A, B) as a single species. The minimisation of E is then the classical *edge-isoperimetric problem* [5, 29], namely, the minimisation of $C \mapsto Q(C, C^c)$ under prescribed size $\#C$. Ground states are isoperimetric sets, the ground-state energy is known, the possible distance between two ground states scales as $N^{3/4}$ where $N = \#C$, and one could even directly prove crystallisation, i.e., the periodicity of ground states, under some stronger assumptions on the interaction potentials [34].

In the other extremal case $\beta = 0$, no interspecific interaction is accounted for, and both phases A and B are independent isoperimetric sets. In particular, if N_A and N_B are perfect squares (or for $N_A, N_B \rightarrow \infty$ and up to rescaling), the phases A and B are squares.

In the intermediate case $\beta \in (0, 1)$, which is hence the interesting one, intraspecific and interspecific interaction compete, and neither A or B nor $A \cup B$ end up being isoperimetric sets. The presence of interspecific interactions adds some level of rigidity. This is revealed by the fact, which we prove, that the distance between different ground states scales like $N^{1/2}$ for β irrational and like $N^{3/4}$ for β rational. Note that in the purely edge-isoperimetric case fluctuations are of order $N^{3/4}$ [34], see also [14, 20, 35, 44].

Although we do not directly deal with crystallisation here, for the points A and B are *assumed* to be subset of the lattice \mathbb{Z}^2 , let us mention that a few rigorous crystallisation results in multispecies systems are available. At first, the existence of quasiperiodic ground states in a specific multicomponent two-dimensional system has been shown by Radin [42]. One-dimensional crystallisation of *alternating* configurations of two-species has been investigated by Bétermin, Knüpfer, and Nolte [3], see also [27] for some related crystallisation and noncrystallisation results. In the two-dimensional, sticky interaction case, two crystallisation results in hexagonal and square geometries are given in [25, 26]. Here, however, interspecific interactions favour the onset of alternating phases.

2.2. Finite Ising model

The double-bubble problem (1.1) can also be equivalently seen as the ground-state problem for a *finite* Ising model with ferromagnetic interactions. In particular, given $C = A \cup B \subset \mathbb{Z}^2$, one describes the state of the system by $u: C \rightarrow \pm 1$, distinguishing the $+1$ and the -1 phase. The Ising-type energy of the system is then given by

$$F(C, u) = -\frac{1-\beta}{4} \sum_{\substack{x, y \in C \\ |x-y|=1}} u(x)u(y) - \frac{1+\beta}{4} \sum_{\substack{x, y \in C \\ |x-y|=1}} |u(x)u(y)|.$$

The first term above is the classical ferromagnetic interaction contribution, while the second sum gives the total number of interactions, irrespective of the phase. This second term is required since in our model same-phase and different-phase interactions are both assumed to give negative contributions to the energy.

Under the above provisions, minimisers of the problem

$$\min\{F(C, u) : C \subset \mathbb{Z}^2, u : C \rightarrow \pm 1, \\ \#\{x \in C : u(x) = 1\} = N_A, \#\{x \in C : u(x) = -1\} = N_B\}$$

corresponds to solutions (A, B) of the double-bubble problem (1.1), under the equivalence

$$A \equiv \{x \in C : u(x) = 1\} \quad \text{and} \quad B \equiv \{x \in C : u(x) = -1\}.$$

In fact, each pair of first neighbours contributes -1 to F if it belongs to the same phase and $-\beta$ if it belongs to different phases, namely,

$$F(C, u) = E(A, B).$$

The literature on the Ising model is vast, and the reader is referred to [12, 37] for a comprehensive collection of results. Ising models are usually investigated from the point of view of their thermodynamic limit $\#C \rightarrow \infty$ and at positive temperature. In particular, models are usually formulated on the whole lattice or on a large box with constant boundary states. Correspondingly, the analysis of Wulff shapes is concerned with the study of a droplet of one phase in a sea of the other one [13].

Our setting is much different, for our system is finite and boundary effects matter. To the best of our knowledge, we contribute here the first characterisation of ferromagnetic Ising ground states, where the location C of the system is also unknown and results from minimisation.

Alternatively to the finite two-state setting above, one could equivalently formulate the minimisation problem in the whole \mathbb{Z}^2 by allowing a third state, to be interpreted as interaction-neutral. In particular, we could equivalently consider the minimisation problem

$$\min\{F(\mathbb{Z}^2, v) : v : \mathbb{Z}^2 \rightarrow \{-1, 0, 1\}, \\ \#\{x \in \mathbb{Z}^2 : v(x) = 1\} = N_A, \#\{x \in \mathbb{Z}^2 : v(x) = -1\} = N_B\}.$$

The equivalence is of course given by setting $u = v$ on

$$C := \{x \in \mathbb{Z}^2 : v(x) \neq 0\}.$$

2.3. Finite Heisenberg model

The three-state formulation of the previous section can be easily reconciled within the frame of the classical Heisenberg model [45]. In particular, we will define the vector-valued state function $s: M \rightarrow \{s_{-1}, s_0, s_1\}$ where the box M is given as

$$M := [0, m]^2 \cap \mathbb{Z}^2$$

for m large. We choose the three possible spins as

$$s_0 = (-1, 0), \quad s_1 = \left(\beta, \sqrt{1 - \beta^2} \right), \quad s_{-1} = \left(\beta, -\sqrt{1 - \beta^2} \right).$$

The energy of the system is defined as

$$H(s) = - \sum_{\substack{x, y \in M \\ |x-y|=1}} s(x) \cdot s(y).$$

For all $s: M \rightarrow \{s_{-1}, s_0, s_1\}$, let $A := \{x \in M : s(x) = s_1\}$ and $B := \{x \in M : s(x) = s_{-1}\}$. We are interested in the minimisation problem

$$\min \{H(s) : s: M \rightarrow \{s_{-1}, s_0, s_1\}, \#A = N_A, \#B = N_B\}.$$

By letting m be very large compared with N_A and N_B , we can with no loss of generality, assume that $s = s_0$ close to the boundary ∂M .

Let us now show that the latter minimisation problem is indeed equivalent to the double-bubble problem (1.1). To this aim, we start by noting that the total number of first-neighbour interactions in M is $2m^2 + 2m$. First-neighbour interactions between identical states contribute -1 to the energy, $s_0 - s_1$ and $s_0 - s_{-1}$ interactions contribute $-s_1 \cdot s_0 = -s_{-1} \cdot s_0 = \beta$, and $s_1 - s_{-1}$ interactions contribute $-s_1 \cdot s_{-1} = 1 - 2\beta^2$. We hence have that

$$\begin{aligned} H(s) + (2m^2 + 2m) &= (\beta + 1)(Q(A, A^c \setminus B) + Q(B, B^c \setminus A)) + (2 - 2\beta^2)Q(A, B) \\ &= (\beta + 1)(Q(A, A^c \setminus B) + Q(B, B^c \setminus A) + (2 - 2\beta)Q(A, B)) \\ &= (\beta + 1)P(A, B) \end{aligned}$$

so that minimising H is actually equivalent to solving (1.1).

2.4. Minimum balanced-separator problem

One can rephrase the double-bubble problem (1.1) as a minimum balanced-separator problem on an unknown graph as well. Indeed, as interspecific contributions are energetically less favoured with respect to intraspecific ones, given the common occupancy $\mathcal{V} = A \cup B$ of the two phases, one is asked to part \mathcal{V} into two regions A and B with given size in

such a way that the interface between A and B is minimal. This corresponds to a minimum balanced-separator problem on the *unit-disk graph* corresponding to \mathcal{V} , i.e., finding a disjunct partition $\mathcal{V} = A \cup B$ solving

$$\min\{Q(A, B) : \#A = N_A, \#B = N_B\}.$$

This is indeed a classical problem with relevant applications in operations research and computer science [41].

Here, we generalise the above minimum balanced-separator problem by letting the underlying graph also vary and by simultaneously optimising its perimeter. In particular, we consider

$$\min\{P(A, B) : V = A \cup B, A \cap B = \emptyset, \#A = N_A, \#B = N_B\},$$

where $(\mathcal{V}, \mathcal{E})$ is again the unit graph related to $A \cup B \subset \mathbb{Z}^2$.

Also, in this setting, the competition between minimisation of the interface and of the perimeter is evident. Recall

$$P(A, B) = Q(A, A^c \setminus B) + Q(B, B^c \setminus A) + (2 - 2\beta)Q(A, B).$$

On the one hand, a graph with few edges between A and B would give a short cut $Q(A, B)$, while necessarily having large $Q(A, A^c \setminus B) + Q(B, B^c \setminus A)$. On the other hand, a graph with small $Q(A, A^c \setminus B) + Q(B, B^c \setminus A)$ has $A \cup B$ close to be a square, and for $N_A = N_B$, all possible cuts partitioning it in two are approximately as long as its side.

3. Notation

Let us collect here some notation, to be used throughout the paper. For each pair of disjoint sets $A, B \subset \mathbb{Z}^2$, we call the elements of A and B the *A-points* and *B-points*, respectively. We let $N_A = \#A$ and $N_B = \#B$. For any point $p \in A \cup B$, we denote its first and second coordinate by $p = (p_x, p_y)$. We say that two points are *connected by an edge* if their distance is equal to one. (Equivalently, we sometimes use the words *bond* or *connection* in place of *edge*.) We say that a set $S \subset A \cup B$ is *connected* if it is connected as a graph with edges described above, or equivalently if the corresponding unit-disk graph is connected.

For the sake of definiteness, from here on, our notation is adapted to the setting of Section 2.1. In particular, we say that a configuration is *minimal* (or *optimal*) if it minimises the energy E given in (2.1) in the class of configurations with the same number of A - and B -points. Recall once more that minimisers of E and solutions of the double-bubble problem (1.1) coincide.

Since the number of points is finite, any configuration lies in a bounded square. Suppose that a configuration (A, B) has N_{row} rows (i.e., there are N_{row} rows in \mathbb{Z}^2 with at least one point from $A \cup B$). For $k = 1, \dots, N_{\text{row}}$, denote by R_k the k th row (counting from the top). In a similar fashion, N_{col} denotes the number of columns, and C_k indicates the

k th column (counting from the left). To simplify the notation, given a finite set $X \subset \mathbb{Z}^2$, we denote

$$X_k^{\text{row}} = X \cap R_k \quad \text{and} \quad X_k^{\text{col}} = X \cap C_k.$$

We will typically apply this to the sets A , B , their union or some of their subsets. Moreover, denote by n_k^{row} the number of A -points in the row R_k and by m_k^{row} the number of B -points in the row R_k . In a similar fashion, n_k^{col} and m_k^{col} denote the number of A - and B -points in column C_k , respectively. In the following, we will frequently modify configurations. Not to overburden the notation, when we use the notation n_k^{row} and m_k^{row} (and similarly for columns), we always refer to the configuration in the same sentence, unless otherwise specified.

For two points $p, q \in A \cup B$, we say that p lies to the left (respectively, right) of q if $p_y = q_y$ and $p_x < q_x$ (respectively, $p_x > q_x$). In other words, they are in the same row, and the first coordinate of p is smaller (respectively, larger) than the first coordinate of q . We say that p lies directly to the left (respectively, right) of q if additionally p and q are connected by an edge. Similarly, we say that p lies above (respectively, below) q if $p_x = q_x$ and $p_y > q_y$ (respectively, $p_y < q_y$). Again, we say that p lies directly above (respectively, below) q if additionally these two points are connected by an edge.

We will also say that the set A_k^{row} lies to the left (respectively, right) of B_k^{row} if for every $p \in A_k^{\text{row}}$ and $q \in B_k^{\text{row}}$ the point p lies to the left (respectively, right) of q . (Note that by definition A_k^{row} and B_k^{row} are in the same row.) We also say that A_k^{row} lies directly to the left of B_k^{row} if additionally there is a connection between one of the points in A_k^{row} and one of the points in B_k^{row} . An analogous notion is used for columns.

Furthermore, we say that a number of points from different rows are *aligned* if their first coordinates are equal. We also say that two sets are *aligned to the right* (or *left*) if their rightmost (leftmost) points are aligned. The same notion is also used for columns.

Finally, given a finite set $X \subset \mathbb{Z}^2$, we denote by $X + (a, b)$ the set consisting of all points of X shifted by the vector $(a, b) \in \mathbb{Z}^2$.

4. Connectedness, separation, and interface

In this section, we introduce a procedure in order to modify an arbitrary configuration (A, B) into another configuration (\hat{A}, \hat{B}) with specific additional properties, without increasing the energy. In particular, this will prove that for a minimal configuration the sets A , B , and $A \cup B$ are connected.

4.1. Description of the procedure

The goal of this section is to present a procedure allowing to modify a configuration, making it more regular in the following sense: not only the sets A and B are connected, but also for any $k = 1, \dots, N_{\text{row}}$ and any $l = 1, \dots, N_{\text{col}}$ the sets A_k^{row} , B_k^{row} , $(A \cup B)_k^{\text{row}}$, A_l^{col} , B_l^{col} , and $(A \cup B)_l^{\text{col}}$ are connected. We start with the following preliminary result.

Proposition 4.1. *Let (A, B) be a configuration in the sense described above. If there are any empty rows (or columns) between any two rows (or columns) in (A, B) , then there exists a configuration (\hat{A}, \hat{B}) with strictly smaller energy.*

Proof. Without restriction we present the argument for rows. Suppose that between rows R_k and R_{k+1} for some $k \in \{1, \dots, N_{\text{row}} - 1\}$ there are l empty rows. Then, we can reduce the energy in the following way: denote by (A', B') the configuration consisting of the top k rows and by (A'', B'') the configuration consisting of the bottom $N_{\text{row}} - k$ rows. Then, we remove the empty rows, i.e., replace (A'', B'') with $(A'', B'') + (0, l)$. Clearly, this does not increase the energy of the configuration (A, B) . If after this shift there is at least one connection between $A_k^{\text{row}} \cup B_k^{\text{row}}$ and $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$, the energy even decreases by at least β . Otherwise, if after this shift there are no connections between $A_k^{\text{row}} \cup B_k^{\text{row}}$ and $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$, we shift the configuration (A', B') horizontally to make at least one connection. Again, the energy is decreased by at least β . ■

Hence, in studying minimal configurations, we may assume that there are no empty rows and columns. Now, we are ready to describe a modification procedure making the configuration more regular. Notice that we may write the energy in the following way:

$$E(A, B) = \sum_{k=1}^{N_{\text{row}}} E_k^{\text{row}}(A, B) + \sum_{k=1}^{N_{\text{row}}-1} E_k^{\text{inter}}(A, B).$$

Here, $E_k^{\text{row}}(A, B)$ is the part of the energy given by interactions in the row R_k , namely

$$E_k^{\text{row}}(A, B) = \frac{1}{2} \sum_{x_i, x_j \in A_k^{\text{row}} \cup B_k^{\text{row}}} V_{\text{sticky}}(x_i, x_j), \quad (4.1)$$

and $E_k^{\text{inter}}(A, B)$ is the part of the energy given by interactions between rows R_k and R_{k+1} , namely

$$E_k^{\text{inter}}(A, B) = \sum_{x_i \in A_k^{\text{row}} \cup B_k^{\text{row}}, x_j \in A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}} V_{\text{sticky}}(x_i, x_j).$$

Now, let us see that we may bound E_k^{row} and E_k^{inter} by expressions depending on n_k^{row} and m_k^{row} . First, we estimate E_k^{row} .

Lemma 4.2. *We have*

$$E_k^{\text{row}}(A, B) \geq \begin{cases} -(n_k^{\text{row}} + m_k^{\text{row}}) + 2 - \beta & \text{if } n_k^{\text{row}} > 0, m_k^{\text{row}} > 0, \\ -(n_k^{\text{row}} + m_k^{\text{row}}) + 1 & \text{else.} \end{cases}$$

Moreover, this inequality is an equality if and only if the sets A_k^{row} , B_k^{row} , and $A_k^{\text{row}} \cup B_k^{\text{row}}$ are connected.

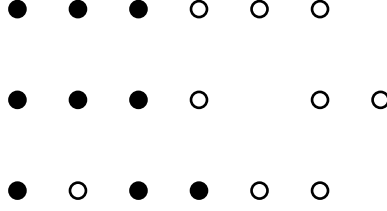


Figure 2. Different configurations inside a single row.

This result is illustrated in Figure 2; assuming that both A_k^{row} and B_k^{row} consist of three points, we present three possible configurations. The configuration on top is optimal and is exactly of the form given in the statement of the lemma, while the other two configurations do not have the optimal energy.

Proof. We consider two cases. In the first case, we suppose that $m_k^{\text{row}} = 0$ (a similar argument works if $n_k^{\text{row}} = 0$): then, the desired inequality takes the form $E_k^{\text{row}}(A, B) \geq -n_k^{\text{row}} + 1$. Since A_k^{row} is a subset of a single row, $n_k^{\text{row}} - 1$ is the maximum number of connections between points in A_k^{row} and it is achieved only if A_k^{row} is connected.

In the second case, we have $n_k^{\text{row}} > 0$ and $m_k^{\text{row}} > 0$. Since $A_k^{\text{row}} \cup B_k^{\text{row}}$ is a subset of a single row, the maximum number of connections (regardless of their type) is $n_k^{\text{row}} + m_k^{\text{row}} - 1$. It is achieved only if $(A \cup B)_k^{\text{row}}$ is connected. Among these, at most $n_k^{\text{row}} - 1$ are connections between points in A_k^{row} and at most $m_k^{\text{row}} - 1$ are connections between points in B_k^{row} . These numbers are achieved if and only if A_k^{row} and B_k^{row} are connected. Each of these connections contributes -1 to the energy and there can be at most $n_k^{\text{row}} + m_k^{\text{row}} - 2$ of them. The remaining connections are between A_k^{row} and B_k^{row} contributing $-\beta$ to the energy. The fact that $\beta < 1$ yields the statement. ■

Now, we make a similar computation for E_k^{inter} .

Lemma 4.3. *We have*

$$E_k^{\text{inter}}(A, B) \geq -(1 - \beta) \left(\min\{n_k^{\text{row}}, n_{k+1}^{\text{row}}\} + \min\{m_k^{\text{row}}, m_{k+1}^{\text{row}}\} \right) - \beta \min\{n_k^{\text{row}} + m_k^{\text{row}}, n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}\}.$$

Moreover, equality is achieved if and only if the following conditions hold:

- (1) There are $\min\{n_k^{\text{row}}, n_{k+1}^{\text{row}}\}$ points in A_k^{row} directly above points in A_{k+1}^{row} .
- (2) There are $\min\{m_k^{\text{row}}, m_{k+1}^{\text{row}}\}$ points in B_k^{row} directly above points in B_{k+1}^{row} .
- (3) Supposing that $n_k^{\text{row}} + m_k^{\text{row}} \geq n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}$, there is a point in $A_k^{\text{row}} \cup B_k^{\text{row}}$ directly above every point in $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$. Otherwise, if $n_k^{\text{row}} + m_k^{\text{row}} < n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}$, there is a point in $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$ directly below every point in $A_k^{\text{row}} \cup B_k^{\text{row}}$.

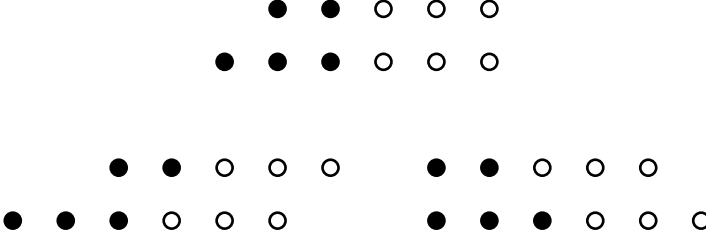


Figure 3. Different alignments of adjacent rows.

This result is illustrated in Figure 3. We present three configurations consisting of two rows; each of them has the form prescribed by Lemma 4.2 inside both rows, but the alignment of the two rows is different. Only the top configuration is optimal.

Proof. First, as there are $n_k^{\text{row}} + m_k^{\text{row}}$ points in $A_k^{\text{row}} \cup B_k^{\text{row}}$ and $n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}$ points in $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$, there are at most $\min\{n_k^{\text{row}} + m_k^{\text{row}}, n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}\}$ connections between points in $A_k^{\text{row}} \cup B_k^{\text{row}}$ and $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$, regardless of their type. Among these, we denote the number of connections between points in A_k^{row} and A_{k+1}^{row} by \tilde{n}_k and the number of connections between points in B_k^{row} and B_{k+1}^{row} by \tilde{m}_k . We have $\tilde{n}_k \leq \min\{n_k^{\text{row}}, n_{k+1}^{\text{row}}\}$ and $\tilde{m}_k \leq \min\{m_k^{\text{row}}, m_{k+1}^{\text{row}}\}$ with equality if these many points in A_{k+1}^{row} are placed directly under points in A_k^{row} (and similarly for B_k^{row} and B_{k+1}^{row}). Each of these connections contributes -1 to the energy, i.e., a total contribution of $-\tilde{n}_k - \tilde{m}_k$. Then, there are at most $\min\{n_k^{\text{row}} + m_k^{\text{row}}, n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}\} - (\tilde{n}_k + \tilde{m}_k)$ possible connections which need to be either connections between points in A_k^{row} and B_{k+1}^{row} or between points in B_k^{row} and A_{k+1}^{row} . Either way, each of these connections contributes $-\beta$ to the energy. In conclusion, we obtain the desired inequality, with equality only if

$$\tilde{n}_k = \min\{n_k^{\text{row}}, n_{k+1}^{\text{row}}\}, \quad \tilde{m}_k = \min\{m_k^{\text{row}}, m_{k+1}^{\text{row}}\},$$

and if there are $\min\{n_k^{\text{row}} + m_k^{\text{row}}, n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}\}$ connections between $A_k^{\text{row}} \cup B_k^{\text{row}}$ and $A_{k+1}^{\text{row}} \cup B_{k+1}^{\text{row}}$. ■

In light of these estimates, we describe a simple modification procedure making any configuration more regular. For any configuration (A, B) , we construct a configuration (\hat{A}, \hat{B}) having the same number of A - and B -points in each row as (A, B) such that the energy is lower or equal and (\hat{A}, \hat{B}) has some additional structure properties.

Step 0. We start with the first row from the top. We let \hat{A}_1 be a connected set in a single row consisting of n_1^{row} atoms and let \hat{B}_1 be the connected set in the same row with m_1^{row} points right of \hat{A}_1 , in such a way that there is a connection between \hat{A}_1 and \hat{B}_1 . By Lemma 4.2, we have

$$E_1^{\text{row}}(\hat{A}, \hat{B}) \leq E_1^{\text{row}}(A, B).$$

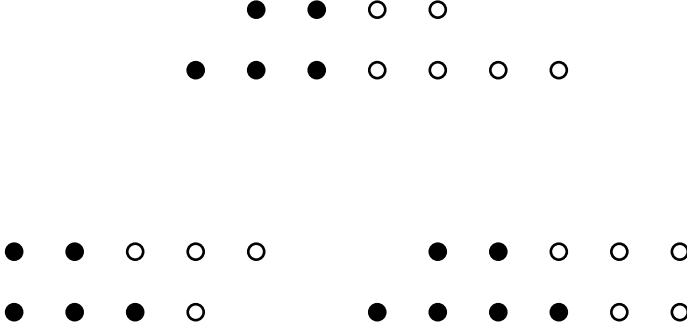


Figure 4. Different cases of the regularisation procedure.

Step k (for $k = 1, \dots, N_{\text{row}} - 1$). We suppose that the sets in the previous steps have been constructed in such a way that \hat{A}_k , \hat{B}_k , and $\hat{A}_k \cup \hat{B}_k$ are connected, and \hat{A}_k lies on the left of \hat{B}_k . We will now define \hat{A}_{k+1} and \hat{B}_{k+1} . To this end, we distinguish four cases.

Case 1. $n_k^{\text{row}} \leq n_{k+1}^{\text{row}}$ and $m_k^{\text{row}} \leq m_{k+1}^{\text{row}}$. We place n_k^{row} points of \hat{A}_{k+1} directly below \hat{A}_k . Then, we put the remaining $n_{k+1}^{\text{row}} - n_k^{\text{row}}$ points to the left of the previously placed points so that \hat{A}_{k+1} is connected. Similarly, we place m_k^{row} points from \hat{B}_{k+1} directly below \hat{B}_k and the remaining $m_{k+1}^{\text{row}} - m_k^{\text{row}}$ points to the right of the previously placed points so that \hat{B}_{k+1} is connected. By Lemma 4.2, we have $E_{k+1}^{\text{row}}(\hat{A}, \hat{B}) \leq E_{k+1}^{\text{row}}(A, B)$, and by Lemma 4.3, we have $E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B)$. The situation is presented in Figure 4 (the top configuration).

Case 2. $n_k^{\text{row}} > n_{k+1}^{\text{row}}$ and $m_k^{\text{row}} > m_{k+1}^{\text{row}}$. We place all the points of \hat{A}_{k+1} directly below \hat{A}_k , starting from the right. Then, we place all the points of \hat{B}_{k+1} directly below \hat{B}_k , starting from the left. In this way, the sets \hat{A}_{k+1} , \hat{B}_{k+1} and $\hat{A}_{k+1} \cup \hat{B}_{k+1}$ are connected. Again, by Lemma 4.2, we have $E_{k+1}^{\text{row}}(\hat{A}, \hat{B}) \leq E_{k+1}^{\text{row}}(A, B)$, and by Lemma 4.3, we have $E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B)$. The situation (after exchanging the roles of the two rows) is presented in the top configuration in Figure 4.

Case 3. $n_k^{\text{row}} \leq n_{k+1}^{\text{row}}$ and $m_k^{\text{row}} > m_{k+1}^{\text{row}}$. First, we put n_k^{row} points of \hat{A}_{k+1} directly below \hat{A}_k . Then, we consider two possibilities:

- If $n_k^{\text{row}} + m_k^{\text{row}} \geq n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}$, we place the remaining $n_{k+1}^{\text{row}} - n_k^{\text{row}}$ points of \hat{A}_{k+1} under \hat{B}_k , starting from the left so that \hat{A}_{k+1} is connected. Then, we place the m_{k+1}^{row} points of \hat{B}_{k+1} to the right of the previously placed points so that \hat{B}_{k+1} and $\hat{A}_{k+1} \cup \hat{B}_{k+1}$ are connected. The situation is presented in Figure 4 (the left configuration).
- If $n_k^{\text{row}} + m_k^{\text{row}} < n_{k+1}^{\text{row}} + m_{k+1}^{\text{row}}$, we place the m_{k+1}^{row} points of \hat{B}_{k+1} below points in \hat{B}_k , starting from the right, so that \hat{B}_{k+1} is connected. Then, we place $m_k^{\text{row}} - m_{k+1}^{\text{row}}$

points of \hat{A}_{k+1} between the two sets of previously placed points. Finally, we place the remaining points of \hat{A}_{k+1} to the left of all points placed so far so that $\hat{A}_{k+1} \cup \hat{B}_{k+1}$ is connected. The situation is presented in Figure 4 (the right configuration).

In both cases, by Lemma 4.2, we have $E_{k+1}^{\text{row}}(\hat{A}, \hat{B}) \leq E_{k+1}^{\text{row}}(A, B)$, and by Lemma 4.3, we get $E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B)$.

Case 4. $n_k^{\text{row}} > n_{k+1}^{\text{row}}$ and $m_k^{\text{row}} \leq m_{k+1}^{\text{row}}$. We proceed as in Case 3 with the roles of A and B interchanged, with “left” and “right” also interchanged. Again, by Lemma 4.2 we have $E_{k+1}^{\text{row}}(\hat{A}, \hat{B}) \leq E_{k+1}^{\text{row}}(A, B)$ and by Lemma 4.3, we have $E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B)$. The situation is presented in Figure 4 (the two bottom configurations) after exchanging the roles of the two colours.

Proposition 4.4. *The procedure described above modifies a configuration (A, B) into a configuration (\hat{A}, \hat{B}) with $E(\hat{A}, \hat{B}) \leq E(A, B)$. Moreover, if one of the sets A_k^{row} , B_k^{row} , or $(A \cup B)_k^{\text{row}}$ for $k = 1, \dots, N_{\text{row}}$ is not connected, or one of the properties (1)–(3) in Lemma 4.3 is violated, then $E(\hat{A}, \hat{B}) < E(A, B)$.*

Proof. The construction ensures that the configuration (\hat{A}, \hat{B}) has the same number of rows as (A, B) . Hence, we compute

$$\begin{aligned} E(\hat{A}, \hat{B}) &= \sum_{k=1}^{N_{\text{row}}} E_k^{\text{row}}(\hat{A}, \hat{B}) + \sum_{k=1}^{N_{\text{row}}-1} E_k^{\text{inter}}(\hat{A}, \hat{B}) \\ &\leq \sum_{k=1}^{N_{\text{row}}} E_k^{\text{row}}(A, B) + \sum_{k=1}^{N_{\text{row}}-1} E_k^{\text{inter}}(A, B) \\ &= E(A, B). \end{aligned}$$

In view of Lemma 4.2, we obtain strict inequality if one of the sets A_k^{row} , B_k^{row} , or $(A \cup B)_k^{\text{row}}$ is not connected. In a similar fashion, we get strict inequality whenever one of the properties (1)–(3) in Lemma 4.3 does not hold. ■

In particular, for optimal configurations (A, B) , all sets A_k^{row} , B_k^{row} , and $(A \cup B)_k^{\text{row}}$ are connected. In other words, inside any row we have first all points of one type and then all points of the other type without any gaps in between. Moreover, we may make use of this procedure (and prove an analogue of Lemma 4.2–Proposition 4.4) for columns in place of rows. Hence, the sets A_k^{col} , B_k^{col} , and $(A \cup B)_k^{\text{col}}$ are connected. In other words, given an optimal configuration, in each column, there are first all points of one type and then all points of the other type without any gaps in between. In particular, as a consequence, we get an important property of any minimising configuration.

Theorem 4.5. *Suppose that (A, B) is an optimal configuration. Then, A and B are connected.*

Proof. Suppose by contradiction that A is not connected (we proceed similarly for B). First of all, let us notice that for each $k = 1, \dots, N_{\text{row}}$ the set A_k^{row} is connected. Otherwise, by Proposition 4.4, we find that (A, B) was not an optimal configuration.

Let us first suppose that $n_k^{\text{row}} > 0$ for all $k \in 1, \dots, N_{\text{row}}$ (i.e., $A_k^{\text{row}} \neq \emptyset$). Since every A_k^{row} is connected, if A is not connected, it means that there is no connection between A_k^{row} and A_{k+1}^{row} for some choice of k . In this case, by Lemma 4.3 and by Proposition 4.4, we find that (A, B) was not an optimal configuration.

Hence, the only remaining possibility that A is not connected is that there exist $k_1 < k_2 < k_3$ such that $n_{k_1}^{\text{row}}, n_{k_3}^{\text{row}} > 0$ and $n_{k_2}^{\text{row}} = 0$ (i.e., $A_{k_1}^{\text{row}}, A_{k_3}^{\text{row}} \neq \emptyset$ and $A_{k_2}^{\text{row}} = \emptyset$). Without loss of generality, we may require that for every $k = k_1 + 1, \dots, k_3 - 1$ the set A_k^{row} is empty. Let us apply the reorganisation $(A, B) \rightarrow (\hat{A}, \hat{B})$ using the procedure described above. Clearly, (\hat{A}, \hat{B}) is still optimal by Proposition 4.4. Then, for $k = k_1$, we are either in Case 2 or in Case 4 of the procedure. We distinguish these two cases.

In the first one, suppose that for $k = k_1$ Case 2 of the procedure applies. Then, the leftmost point of \hat{B}_{k_1+1} lies directly below the leftmost point of \hat{B}_{k_1} . Then, since for every $k = k_1 + 1, \dots, k_3 - 1$ the set A_k^{row} is empty, Case 1 or 3 of the procedure shows that also the leftmost point of \hat{B}_k lies below the leftmost point of \hat{B}_{k_1+1} (hence below the leftmost point of \hat{B}_{k_1}). Now, for $k = k_3 - 1$, when we place the sets \hat{A}_{k_3} and \hat{B}_{k_3} , we either fall into Case 1 or Case 3 in the description of the procedure. In Case 1, the leftmost point of \hat{B}_{k_3} is again placed below the leftmost point of \hat{B}_{k_1} . Then, the rightmost point of \hat{A}_{k_3} is placed below the rightmost point of \hat{A}_{k_1} . Now, one reaches a contradiction by following the same construction of Proposition 4.4, by exchanging the role of rows and columns. In Case 3, we either have that a point of \hat{A}_{k_3} is placed below a point of \hat{A}_{k_1} , which as above is a contradiction to Proposition 4.4, or the leftmost point of \hat{A}_{k_3} is placed below the leftmost point of \hat{B}_{k_1} . In particular, the leftmost point of \hat{A}_{k_3} is placed one point to the right of the rightmost point of \hat{A}_{k_1} . Then, by Lemma 4.3 (1) and Proposition 4.4 for columns in place of rows, we again see that the energy of (\hat{A}, \hat{B}) was not minimal, a contradiction. The situation is presented in the top line of Figure 5 in a simplified setting with $k_1 = 1$ and $k_3 = 3$.

In the second case, we have that for $k = k_1$ Case 4 of the algorithm applies. Then, the leftmost point of \hat{B}_{k_1+1} does not lie directly below the leftmost point of \hat{B}_{k_1} , but it lies to its left (but no further than the leftmost point of \hat{A}_{k_1}). Again, for every $k = k_1 + 1, \dots, k_3 - 1$ the leftmost point of \hat{B}_k lies below the leftmost point of \hat{B}_{k_1+1} . Again, when we place the sets \hat{A}_{k_3} and \hat{B}_{k_3} , Case 1 or Case 3 of the procedure applies. In Case 1, the leftmost point of \hat{B}_{k_3} is again placed below the leftmost point of \hat{B}_{k_1+1} . Hence, the rightmost point of \hat{A}_{k_3} is placed either below a point in \hat{A}_{k_1} or, in view of the definition of \hat{B}_{k_1+1} , one point to the left from the leftmost point of \hat{A}_{k_1} . As before, by Lemma 4.3 (1) and Proposition 4.4 for columns in place of rows, we see that the energy of (\hat{A}, \hat{B}) was not minimal, a contradiction. In Case 3, a point of \hat{A}_{k_3} is placed below the leftmost point of \hat{B}_{k_3-1} . This shows that the leftmost point of \hat{A}_{k_3} is placed either below a point in \hat{A}_{k_1} or one point to the right from the rightmost point of \hat{A}_{k_1} . The situation is presented in the

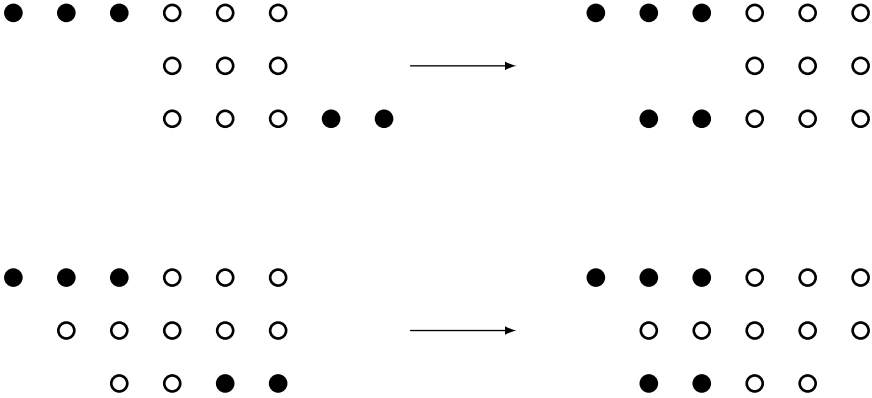


Figure 5. Different cases of the regularisation procedure.

bottom line of Figure 5 in a simplified setting with $k_1 = 1$ and $k_3 = 3$. As before, we obtain a contradiction to the minimality of (\hat{A}, \hat{B}) , and the proof is concluded. ■

A careful inspection of the proofs of Proposition 4.4 and Theorem 4.5 provides some more information about the structure of any minimising configuration, collected in the following statements.

Proposition 4.6. *Let (A, B) be an optimal configuration. Then, for any row R_k , the sets $A_k^{\text{row}}, B_k^{\text{row}}$ and $(A \cup B)_k^{\text{row}}$ are connected. The same claim holds for columns.* ■

Proposition 4.7. *Let (A, B) be an optimal configuration. If for some $1 \leq k_1 < k_2 \leq N_{\text{row}}$ we have $A_{k_1}^{\text{row}}, A_{k_2}^{\text{row}} \neq \emptyset$, then also $A_k^{\text{row}} \neq \emptyset$ for all $k_1 \leq k \leq k_2$. The same claim holds for columns and the set B .* ■

Proposition 4.8. *Let (A, B) be an optimal configuration. Suppose that there exists a row R_{k_0} such that $A_{k_0}^{\text{row}}, B_{k_0}^{\text{row}} \neq \emptyset$ and $A_{k_0}^{\text{row}}$ lies to the left of $B_{k_0}^{\text{row}}$. Then, for every row R_k either A_k^{row} lies to the left of B_k^{row} or one of these sets is empty. The same claim holds for columns and if we interchange the roles of A and B .* ■

We observe that Theorem 4.5 and Proposition 4.6 imply Theorem 1.1 (i) and that Theorem 1.1 (ii) follows from Proposition 4.4 and Propositions 4.7–4.8. Corollary 4.10 below implies Theorem 1.1 (iii) and will be crucial for our later considerations. To this end, we introduce the following definition.

Definition 4.9. The interface I_{AB} (between A and B) is the set of midpoints of edges connecting a point in A with a point in B . We say that there is an edge between two points $p, q \in I_{AB}$ if $|p - q| \in \{1/\sqrt{2}, 1\}$ and the line segment between p and q does not intersect any point in \mathbb{Z}^2 . We say that the interface is connected if it is connected as a graph.

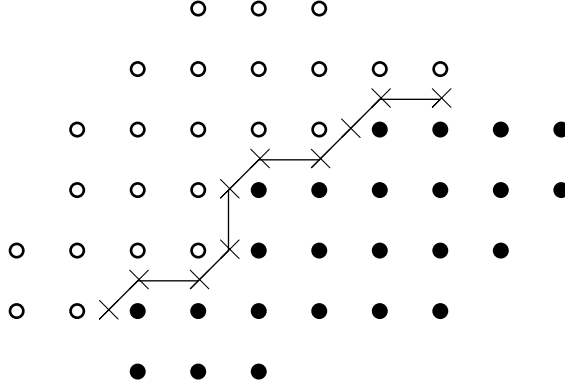


Figure 6. Definition of the interface.

In other words, a point $p \in \mathbb{R}^2$ lies in the interface I_{AB} between A and B if there exist points $p_1 \in A$ and $p_2 \in B$ such that

$$|p - p_1| = |p - p_2| = 1/2.$$

Necessarily, the interface is a subset of the lattice

$$\left\{ \left(k + \frac{1}{2}, l \right) : k, l \in \mathbb{Z} \right\} \cup \left\{ \left(k, l + \frac{1}{2} \right) : k, l \in \mathbb{Z} \right\}.$$

An example is presented in Figure 6.

Notice that Proposition 4.6 implies that there is at most one point in I_{AB} which is a midpoint of an edge between a point in A_k^{row} and a point in B_k^{row} . Similarly, there is at most one point in I_{AB} which is a midpoint of an edge between a point in A_k^{col} and a point in B_k^{col} . Hence, we get the following result.

Corollary 4.10. *For any optimal configuration (A, B) , the interface I_{AB} is connected. Moreover, it is monotone: up to reflections, it goes only upwards and to the right, i.e., given $p, q \in I_{AB}$, if $p_1 > q_1$, then $p_2 \geq q_2$. ■*

We will use this result to study the minimal configurations in the following way: we will identify all possible shapes of the interface, collected in different classes. Analysing the different classes in detail, we will show that there always exists an optimal configuration in the most natural class (called Class \mathcal{I}). For this class, we are able to directly compute the minimal energy, explicitly exhibit a minimiser, and provide a sharp estimate of the possible mismatch of ground states in terms of their size, see (1.4).

Let us also note that the introduction of I_{AB} enables us to write a convenient formula for the energy associated to an optimal configuration (A, B) . Namely, denote by E_A the energy inside A , i.e., minus the number of bonds between A -points. In a similar fashion,



Figure 7. Minimisers for $N_A = 2$, $N_B = 1$.

we define E_B . Eventually, by

$$E_{AB} := -\#I_{AB}\beta$$

we denote the interfacial energy, i.e., minus the number of bonds between A - and B -points weighted by the coefficient β . Then,

$$E(A, B) = E_A + E_B + E_{AB}. \quad (4.2)$$

This simple formula has a very important consequence. Namely, if we separate the sets A and B and reattach them in a different way (i.e., apply an isometry to one or both sets), then E_A and E_B do not change, but E_{AB} possibly might. Therefore, if a configuration is optimal, it has the longest possible interface with respect to this operation. We will use variants of this argument on multiple occasions in Section 8.

5. A collection of examples

In this short section, we consider a few examples of minimisers that will serve as a motivation for the discussion about possible shapes of the interface in the next section. By Theorem 4.5, for any optimal configuration, both sets A and B are connected. The properties of an optimal configuration are further restricted by Propositions 4.6–4.8 and Corollary 4.10. For different choices of $N_A, N_B > 0$ and $\beta \in (0, 1)$, we provide here a complete account of optimal configurations. Note that the limited number of points involved allows a direct exhaustive analysis. Even though some optimal configuration is irregular, the main effort in this paper will be to prove that actually for $N_A = N_B$ and $\beta \leq 1/2$ one may find an optimal configuration which is very regular, in the sense that they roughly consist of two rectangles as given in Theorem 1.1 (v).

The first example consists of only three points: we have $N_A = 2$, $N_B = 1$, for any $\beta \in (0, 1)$. Even then, the minimiser may fail to be unique: up to isometries, we have two minimisers, both presented in Figure 7.

The second example consists of six points: we have $N_A = N_B = 3$ for any $\beta \in (0, 1)$. The numbers of A - and B -points are equal. The minimiser may fail to be unique: up to isometries, we have two minimisers, both presented in Figure 8. Note that the interface is not necessarily straight. However, there is a minimiser which has a straight interface.

The third example consists of eight points: we have $N_A = N_B = 4$ for any $\beta \in (0, 1)$. In this case, the minimiser is unique. Up to isometries, the only solution is presented in



Figure 8. Minimisers for $N_A = 3, N_B = 3$.

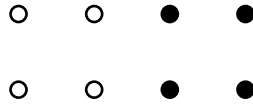


Figure 9. Unique minimiser for $N_A = 4, N_B = 4$.

Figure 9. Note that the interface is straight and both rectangles are “full”. This situation is very special, and in a generic case, we do not expect uniqueness.

The fourth example consists of seven points: we have $N_A = 3, N_B = 4$, for any $\beta \in (0, 1)$. Up to isometries, we have three minimisers, presented in Figure 10. As in the second example of Figure 8, in the configuration on the right, the interface is “L-shaped”.

The fifth example consists of ten points: we have $N_A = N_B = 5$ for any $\beta \in (0, 1)$. Up to isometries, we have five possible minimisers, presented in Figure 11. Notice that the heights of the two types may differ and that the interface may fail to be straight. Furthermore, the two configurations on the left differ even though the interface is straight.

The final example consists of sixteen points: we have $N_A = 12$ and $N_B = 4$. Then, the situation may differ with β . For $\beta \in (1/2, 1)$, up to isometries, we have two possible minimisers (with energy $-20 - 4\beta$), presented in Figure 12. In one case, we have a straight interface, while in the other it is L-shaped.

For $\beta \in (0, 1/2)$, up to isometries, we have three possible minimisers (with energy $-21 - 2\beta$), presented in Figure 13. Here, the structure of sets A and B is fixed, but we may attach them in a few different ways.

For $\beta = 1/2$, all configurations presented in Figures 12 and 13 are minimal.

6. Classification of admissible configurations

For simplicity, we will call the configurations which satisfy the statement of Theorem 4.5 and of the corollaries below it *admissible*. In particular, these results show that optimal configurations are admissible. In this section, we collect admissible configurations in different classes. These classes will be analysed in more detail in the subsequent sections.

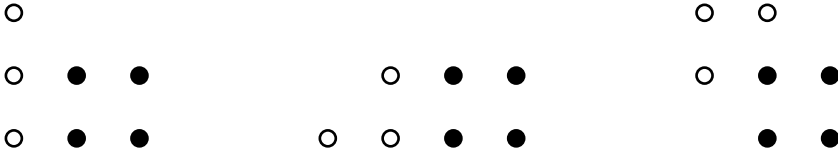


Figure 10. Minimisers for $N_A = 3, N_B = 4$.

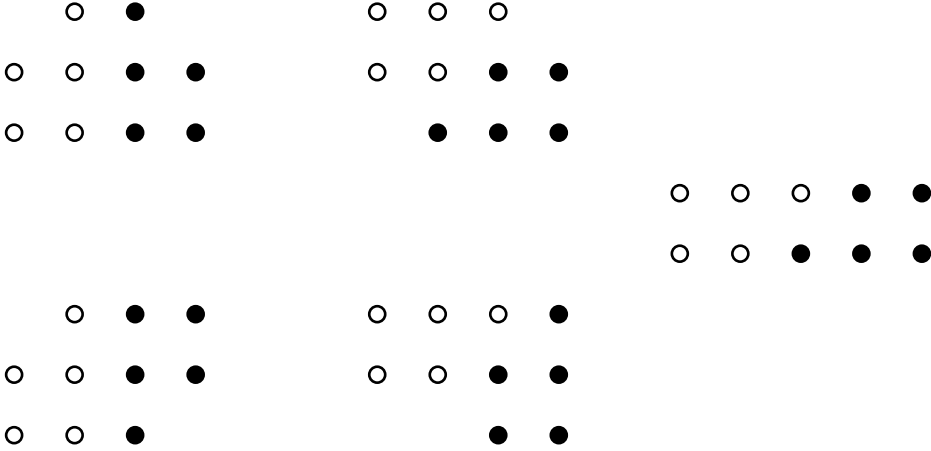


Figure 11. Minimisers for $N_A = 5, N_B = 5$.

The starting point is the observation that by Proposition 4.7 we have that there cannot be a row R_{k_0} such that $n_k^{\text{row}} > 0$ above and below this row (for some $k > k_0$ and some other $k < k_0$), while $n_{k_0}^{\text{row}} = 0$. The same result holds for columns. Therefore, we may cluster the minimisers into several classes which are easier to handle and are described using this property.

Let us start from the top and suppose that $n_1^{\text{row}} > 0$ (otherwise, we exchange the roles of the two types). Denote by R_{k_0} the last row such that $n_{k_0}^{\text{row}} > 0$. Then, we have the two possibilities

$$k_0 = N_{\text{row}}, \tag{6.1a}$$

$$k_0 < N_{\text{row}}. \tag{6.1b}$$

In eq. (6.1a), we distinguish three possibilities, depending on whether B_1^{row} and $B_{N_{\text{row}}}^{\text{row}}$ are empty or not, if $m_1^{\text{row}}, m_{N_{\text{row}}}^{\text{row}} > 0$, then each row contains points from both types. This case corresponds to class \mathcal{I} . If m_1^{row} or $m_{N_{\text{row}}}^{\text{row}}$ equals zero, then the B -part of the configuration



Figure 12. Minimisers for $N_A = 12, N_B = 4$, large β .

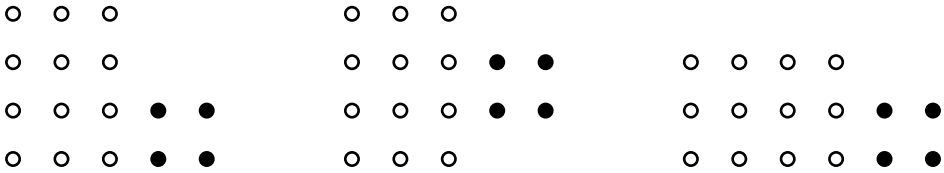


Figure 13. Minimisers for $N_A = 12, N_B = 4$, small β .

has a smaller height. This corresponds to either class $\mathcal{I}\mathcal{I}$ or $\mathcal{I}\mathcal{I}\mathcal{I}$. In eq. (6.1b), we have

$$n_{N_{\text{row}}}^{\text{row}} = 0 \quad \text{and} \quad m_{N_{\text{row}}}^{\text{row}} > 0.$$

We distinguish two possibilities, if the last column $B_{N_{\text{row}}}^{\text{col}}$ is not empty, i.e., $m_{N_{\text{col}}}^{\text{col}} > 0$, the configuration is in class $\mathcal{I}\mathcal{V}$. The case $m_{N_{\text{col}}}^{\text{col}} = 0$ instead corresponds to class \mathcal{V} .

By performing the same analysis for columns, and recalling the corollaries after Theorem 4.5, we end up with a number of possibilities which we list below, where without restriction we assume that $n_1^{\text{col}} > 0$. This list is complete up to isometries and changing roles of the types. For the sake of the presentation, by applying Corollary 4.10, we can without restriction (possibly up to isometry and changing the roles of the types) assume that the interface is going upwards and to the right. We divide all admissible configurations into five main *classes*, the first three being quite regular and the last two a bit more difficult to handle. In this section, we list all classes and introduce appropriate notation for each of them. In the next section we advance a regularisation procedure for all configurations. This has the aim of proving that for $N_A = N_B$ and $\beta \leq 1/2$ all minimal configurations belong to Class \mathcal{I} , $\mathcal{I}\mathcal{V}$, or \mathcal{V} , as well as checking some fine geometrical properties of such minimisers.

6.1. Class \mathcal{I}

The first possibility is the reference case: we say that an admissible configuration (A, B) belongs to Class \mathcal{I} if for each $k = 1, \dots, N_{\text{row}}$ we have $n_k^{\text{row}} > 0$ and $m_k^{\text{row}} > 0$. In other

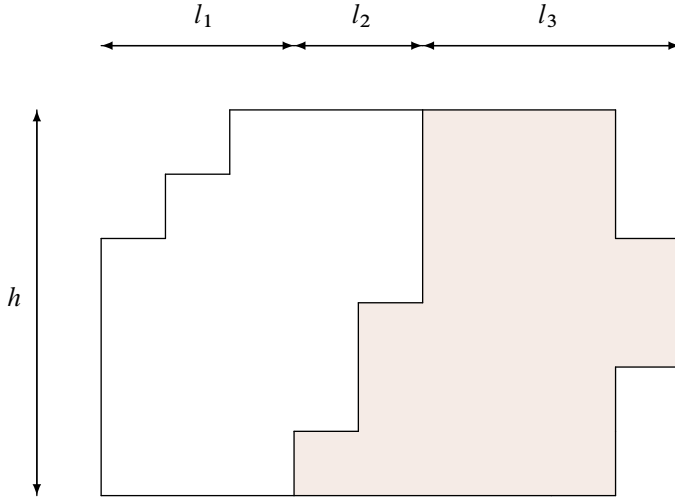


Figure 14. Class \mathcal{I} .

words, eq. (6.1a) holds with $m_1^{\text{row}}, m_{N_{\text{row}}}^{\text{row}} > 0$. The situation is presented in Figure 14. Examples of optimal configurations in Class \mathcal{I} can be found in Figure 7 (on the right), in Figure 8 (both), in Figure 9, in Figure 10 (in the middle), in Figure 11 (all but the two middle ones), and in Figure 12 (on the right). The abundance of examples in Class \mathcal{I} is in some sense expected. Indeed, we will prove that for many choices of N_A , N_B , and β existence of an optimal configuration in Class \mathcal{I} is guaranteed.

Let us introduce the following notation. Let h denote the number of rows (which in this case corresponds to the number of rows of both A and B). Let l_1 denote the number of columns such that $A_k^{\text{col}} \neq \emptyset$ and $B_k^{\text{col}} = \emptyset$. Let l_2 denote the number of columns such that $A_k^{\text{col}} \neq \emptyset$ and $B_k^{\text{col}} \neq \emptyset$. Finally, let l_3 denote the number of columns such that $A_k^{\text{col}} = \emptyset$ and $B_k^{\text{col}} \neq \emptyset$. This notation is also presented in Figure 14. Then, in view of (2.2), the energy (2.1) may be expressed as

$$E(A, B) = -2(N_A + N_B) + (l_1 + l_2 + l_3) + h + (1 - \beta)(l_2 + h). \quad (6.2)$$

In particular, the energy splits into the *bulk energy* $-2(N_A + N_B)$ and, up to a factor $1/2$, into the *lattice perimeter* introduced in (1.2). Clearly, only the latter is relevant for identifying optimal configurations. For convenience, we will frequently refer to it as the *surface energy*.

In the next section, we will simplify the structure of configurations in Class \mathcal{I} , without increasing the energy, in order to compute the minimal energy in this class. After such regularisation, it will turn out that we have two possibilities: either $l_2 = 0$ or $l_2 = 1$; i.e., either the interface is a straight line or it has one horizontal jump, see Proposition 7.1.

6.2. Class \mathcal{II}

We say that an admissible configuration (A, B) belongs to Class \mathcal{II} if there exists a column C_{k_0} such that for all $k \leq k_0$ we have $n_k^{\text{col}} > 0$ and $m_k^{\text{col}} = 0$, for all $k > k_0$ we have $n_k^{\text{col}} = 0$ and $m_k^{\text{col}} > 0$, and (A, B) does not lie in Class \mathcal{I} . In other words, the interface is a straight vertical line, and there exists at least one row which contains only one type (as otherwise $(A, B) \in \mathcal{I}$). Examples of optimal configurations in this class can be found in Figure 7 (on the left), in Figure 10 (on the left), and in Figure 13 (all of them). Notice that in all these examples we have $N_A \neq N_B$. Indeed, in Section 8, we will show that, if N_A and N_B are equal, such a configuration cannot be optimal.

A priori, this set of configurations may arise from both cases in (6.1). Up to changing the roles the two types, however, we may assume that we are in situation (6.1a), as we can see in the following simple observation.

Lemma 6.1. *Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{II}$ is a minimal configuration. Then, there exists a minimal configuration $(\hat{A}, \hat{B}) \in \mathcal{II}$ such that the last rows align, i.e., $n_{N_{\text{row}}}^{\text{row}} > 0$ and $m_{N_{\text{row}}}^{\text{row}} > 0$.*

Proof. Without loss of generality, suppose that $n_{N_{\text{row}}}^{\text{row}} > 0$ and that $r_0 < N_{\text{row}}$ is the biggest number such that $m_{r_0}^{\text{row}} > 0$. Notice that, since the interface is a straight line, we may move the set B by the vector $(0, r_0 - N_{\text{row}})$ so that the last two rows align and this procedure does not increase the energy. The resulting configuration (\hat{A}, \hat{B}) also lies in Class \mathcal{II} , if after this procedure we had also $n_1^{\text{row}} > 0$ and $m_1^{\text{row}} > 0$; i.e., (\hat{A}, \hat{B}) lies in Class \mathcal{I} , then we would have added at least one bond. This induces a drop in the energy, a contradiction to the fact that (A, B) is a minimal configuration. ■

After applying this regularisation argument, we introduce the following notation. Up to reflection along the (straight) interface and interchanging the roles of the types, we may assume that A is on the left-hand side and that it has more nonempty rows than B . Then, let h_1 denote the number of rows such that $A_k^{\text{row}} \neq \emptyset$ and $B_k^{\text{row}} = \emptyset$, and let h_2 be the number of rows such that $A_k^{\text{row}} \neq \emptyset$ and $B_k^{\text{row}} \neq \emptyset$. Moreover, let l_1 denote the number of columns such that $A_k^{\text{col}} \neq \emptyset$ and l_3 denote the number of columns such that $B_k^{\text{col}} \neq \emptyset$ (the notation l_2 is omitted on purpose to simplify some later regularisation arguments). Then, arguing as in the justification of formula (6.2), see also (2.2), the energy (2.1) may be expressed as

$$E(A, B) = -2(N_A + N_B) + (l_1 + l_3) + (h_1 + h_2) + (1 - \beta)h_2. \quad (6.3)$$

The situation is presented in Figure 15.

6.3. Class \mathcal{III}

We say that an admissible configuration (A, B) belongs to Class \mathcal{III} if for each $k = 1, \dots, N_{\text{row}}$ we have $n_k^{\text{row}} > 0$ and for each $l = 1, \dots, N_{\text{col}}$ we have $n_l^{\text{col}} > 0$. In other words, each row and each column of (A, B) contains at least one A -point (or equivalently,

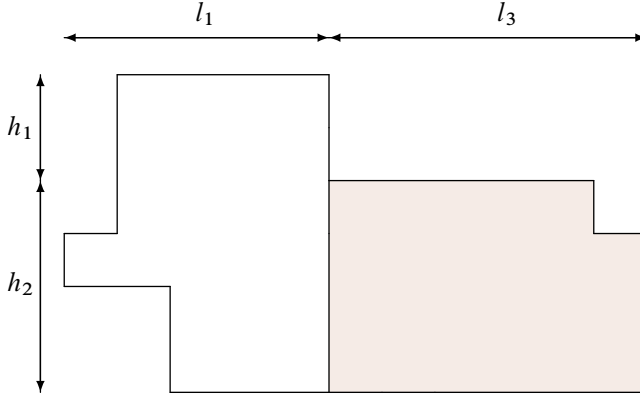


Figure 15. Class \mathcal{II} .

for every B -point there is a A -point above it and another one to its left). An example of an optimal configuration in this class can be found in Figure 12. Note that in this example the ratio N_A/N_B is far away from 1. Indeed, in Section 8, we will show that for $N_A = N_B$ configurations in this class cannot be optimal.

Counting from the left, let l_1 denote the number of columns such that $A_k^{\text{col}} \neq \emptyset$ and $B_k^{\text{col}} = \emptyset$, let l_2 denote the number of columns such that $A_k^{\text{col}} \neq \emptyset$ and $B_k^{\text{col}} \neq \emptyset$, and let l_3 be the number of columns such that $A_k^{\text{col}} \neq \emptyset$ and $B_k^{\text{col}} = \emptyset$. Similarly, counting from the top, denote by h_1 the number of rows such that $A_k^{\text{row}} \neq \emptyset$ and $B_k^{\text{row}} = \emptyset$, let h_2 be the number of rows such that $A_k^{\text{row}} \neq \emptyset$ and $B_k^{\text{row}} \neq \emptyset$, and finally let h_3 be the number of rows such that $A_k^{\text{row}} \neq \emptyset$ and $B_k^{\text{row}} = \emptyset$. Similarly to previous classes, the energy may be expressed as

$$E(A, B) = -2(N_A + N_B) + (l_1 + l_2 + l_3) + (h_1 + h_2 + h_3) + (1 - \beta)(l_2 + h_2). \quad (6.4)$$

The situation is presented in Figure 16.

6.4. Class \mathcal{IV}

We say that an admissible configuration (A, B) belongs to Class \mathcal{IV} if there exist $l_1, l_2, h_1, h_2 > 0$ such that $N_{\text{row}} + N_{\text{col}} - (l_1 + l_2 + h_1 + h_2) > 0$ and the following conditions hold: for each $k = 1, \dots, l_1$, we have $n_k^{\text{col}} > 0$ and $m_k^{\text{col}} = 0$. For each $k = l_1 + 1, \dots, l_1 + l_2$, we have $n_k^{\text{col}} > 0$ and $m_k^{\text{col}} > 0$. Finally, for all $k = l_1 + l_2 + 1, \dots, N_{\text{row}}$ (this may possibly be empty), we have $n_k^{\text{col}} = 0$ and $m_k^{\text{col}} > 0$. Similarly, for each $l = 1, \dots, h_1$, we have $n_l^{\text{row}} > 0$ and $m_l^{\text{row}} = 0$. For each $l = h_1 + 1, \dots, h_1 + h_2$, we have $n_l^{\text{row}} > 0$ and $m_l^{\text{row}} > 0$. Finally, for all $l = h_1 + h_2 + 1, \dots, N_{\text{col}}$ (this may possibly be empty) we have $n_l^{\text{row}} = 0$ and $m_l^{\text{row}} > 0$. Setting $l_3 = N_{\text{col}} - l_1 - l_2$ and $h_3 = N_{\text{row}} - h_1 - h_2$ we observe

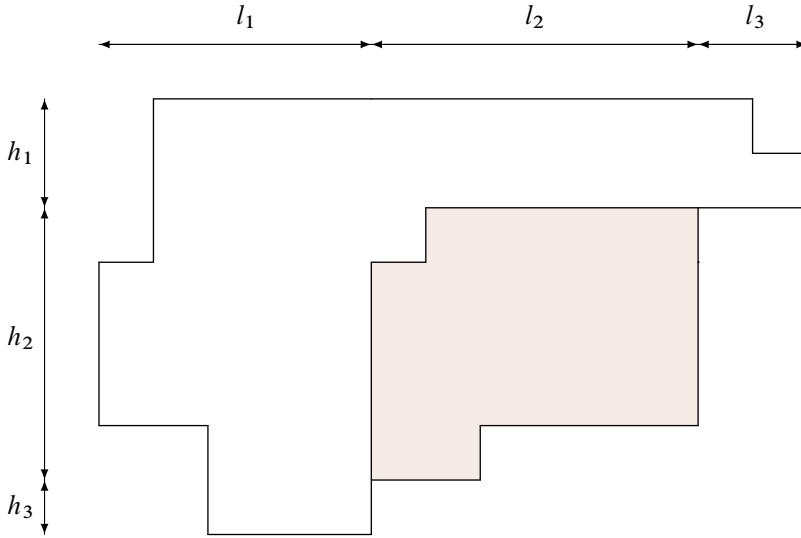


Figure 16. Class III .

$l_3 > 0$ or $h_3 > 0$; i.e., the configuration does not lie in Class III . The energy may be expressed as

$$E(A, B) = -2(N_A + N_B) + (l_1 + l_2 + l_3) + (h_1 + h_2 + h_3) + (1 - \beta)(l_2 + h_2). \quad (6.5)$$

The situation is presented in Figure 17. Examples of optimal configurations in this class can be found in Figure 10 (on the right) and in Figure 11 (both in the middle).

6.5. Class \mathcal{V}

We say that an admissible configuration (A, B) belongs to Class \mathcal{V} if there exist $l_1, l_2, l_3, h_1, h_2, h_3 > 0$ such that $l_1 + l_2 + l_3 = N_{\text{col}}$, $h_1 + h_2 + h_3 = N_{\text{row}}$ and the following conditions hold: for each $k = 1, \dots, l_1$, we have $n_k^{\text{col}} > 0$ and $m_k^{\text{col}} = 0$. For each $k = l_1 + 1, \dots, l_1 + l_2$, we have $n_k^{\text{col}} > 0$ and $m_k^{\text{col}} > 0$. Finally, for all $k = l_1 + l_2 + 1, \dots, N_{\text{row}}$, we have $n_k^{\text{col}} > 0$ and $m_k^{\text{col}} = 0$. On the other hand, for each $l = 1, \dots, h_1$ we have $n_l^{\text{row}} > 0$ and $m_l^{\text{row}} = 0$. For each $l = h_1 + 1, \dots, h_1 + h_2$ we have $n_l^{\text{row}} > 0$ and $m_l^{\text{row}} > 0$. Finally, for all $l = h_1 + h_2 + 1, \dots, N_{\text{col}}$ we have $n_l^{\text{row}} = 0$ and $m_l^{\text{row}} > 0$. The energy may be expressed as

$$E(A, B) = -2(N_A + N_B) + (l_1 + l_2 + l_3) + (h_1 + h_2 + h_3) + (1 - \beta)(l_2 + h_2).$$

The situation is presented in Figure 18.

We close this section with the observation that the five classes cover all possible cases up to isometries, reflections, and changing roles of the types.

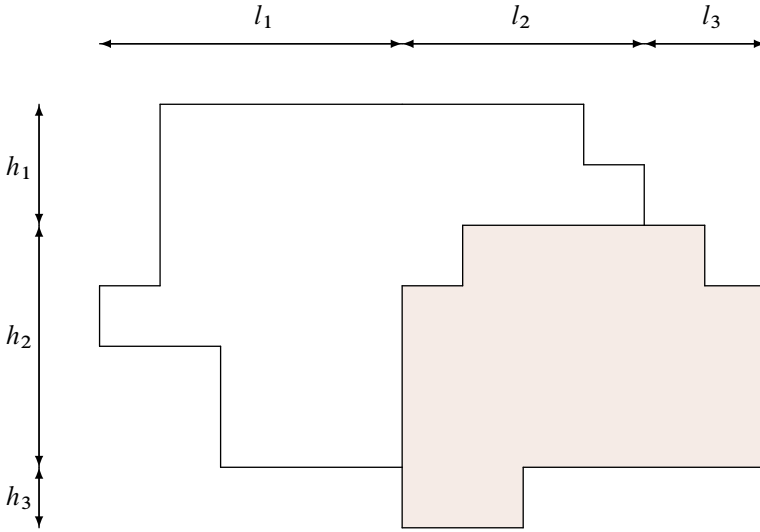


Figure 17. Class \mathcal{IV} .

7. Analysis of Class \mathcal{I}

7.1. Regularisation inside Class \mathcal{I}

The goal of this section is to make the configuration in Class \mathcal{I} more regular without increasing the energy. This regularisation will facilitate the computation of the minimal energy. We keep the notation as in the previous section and begin with the following observation.

Proposition 7.1. *Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{I}$ is an optimal configuration. Then, we either have $l_2 = 0$ or $l_2 = 1$.*

Both cases can happen, take $N_A = N_B = 3$ and $\beta \in (0, 1)$. Then, there are two optimal configurations, one with $l_2 = 0$ and the other one with $l_2 = 1$, see Figure 8.

Proof. The idea of the proof is the following: we suppose by contradiction that $l_2 \geq 2$. We add more points to the configuration (A, B) , so that it becomes a full rectangle, keeping track of the change of the energy in the process. Then, we exchange a number of points, making the interface shorter and causing a drop in the energy. Finally, we remove the added points, again keeping track of the energy. This yields strictly smaller total energy, a contradiction. The argument is presented in Figure 19.

To be exact, let us modify the configuration (A, B) as follows. We add N'_A A -points on the left and N'_B B -points on the right such that (A, B) becomes a full rectangle with sides $l_1 + l_2 + l_3$ and h . Notice that in this way we do not alter the surface energy. Meanwhile, the bulk energy changes by $-2(N'_A + N'_B)$. Now, look at the rectangle in the

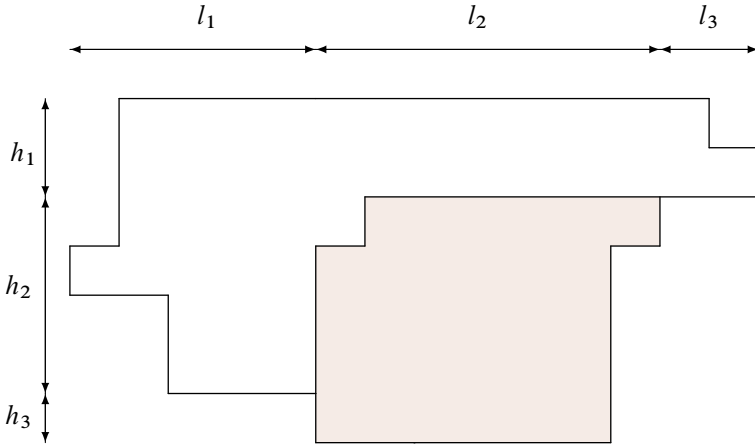


Figure 18. Class \mathcal{V} .

middle with sides l_2 and h . If we exchange A -points from its rightmost column and B -points from its leftmost column (as many as we can), we will make one column (or two) full of points of one type. Hence, in the formula for the energy, see (6.2), we replace l_2 by $l_2 - 1$ (respectively, $l_2 - 2$), and $l_1 + l_3$ by $l_1 + l_3 + 1$ (respectively, $l_1 + l_3 + 2$). This causes a drop in the surface energy by $(1 - \beta)$ or $2(1 - \beta)$.

Finally, we take care of the added points. We remove N'_A A -points, starting from the leftmost column, going from top to bottom. In the process, the surface energy decreases or remains the same (since l_1 may decrease or remain the same). Similarly, we remove N'_B B -points, starting from the rightmost column and going from top to bottom.

In this way, we have obtained a configuration (\hat{A}, \hat{B}) with the same number of A - and B -points as (A, B) , but with energy lower at least by $(1 - \beta)$. After this operation, we possibly end up with a shape of the interface different from the one in Class \mathcal{I} , but this does not matter since we only wanted to show that (A, B) was not optimal. Hence, if (A, B) is an optimal configuration, then $l_2 = 0$ or $l_2 = 1$. ■

By performing the modification described in the proof, we get that we may assume that the configuration is as compact as possible: given h , the values of l_1 and l_3 are as small as possible, and all the columns except for the leftmost and rightmost ones are full (i.e., have h points). This is a property that we will use several times in the sequel.

We provide an exact formula for the minimal energy in Theorem 7.4. This requires fixing $N_A = N_B$, which will be assumed throughout. Note however that some of the intermediate lemmas below may be adapted for the case $N_A \neq N_B$, as well. Let us first prove that we may assume that $l_2 = 0$. To this end, let us first state the following technical lemma.

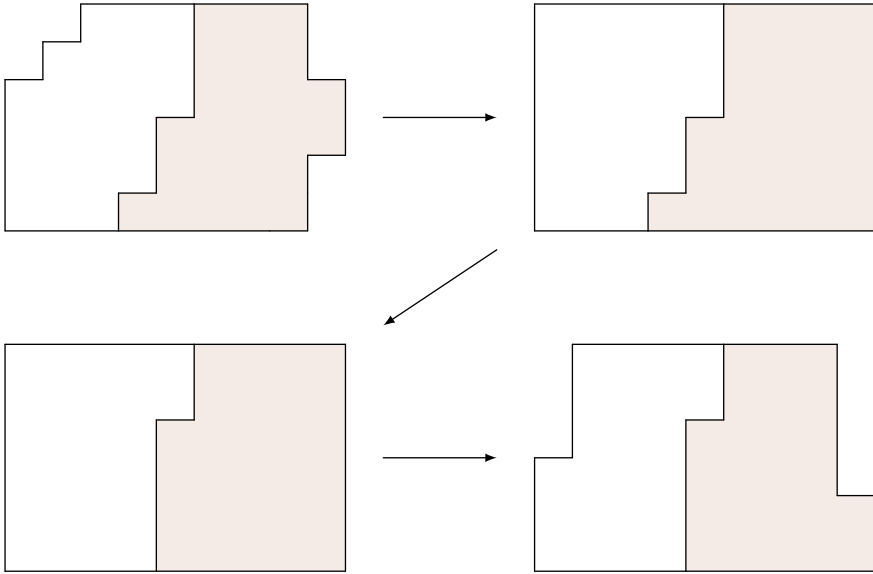


Figure 19. Regularisation of Class \mathcal{I} .

Lemma 7.2. Fix $N := N_A = N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{I}$ is an optimal configuration such that $l_1 = l_3$ and $l_2 = 1$. Then, we have $l_1 = l_3 \geq h/2$.

Proof. Without restriction, we assume that (A, B) has the form described before the statement of the lemma, see also the last picture in Figure 19. Let $k = \lceil h/2 \rceil$. Suppose by contradiction that the statement does not hold, i.e., $l_1 = l_3 < k$ (in particular, $k \geq 2$).

Consider two cases: first, assume that h is even, so that $h = 2k$. Then, the whole configuration fits into a rectangle with height $2k$ and width $2l_1 + 1$, where $l_1 \leq k - 1$. Let us rearrange all the points so that the resulting configuration lies in a rectangle with height $2k - 1$ and width $2l_1 + 2$. We place the points by filling the columns from left to right, first with A -points and then with B -points so that the resulting configuration lies in Class \mathcal{I} and has $l_2 \leq 1$. In fact, all points may be placed in this rectangle since the assumption $l_1 \leq k - 1$ implies that

$$(2k - 1)(2l_1 + 2) \geq 2k(2l_1 + 1).$$

But then the new configuration has strictly smaller energy since h decreased by 1, $l_2 \leq 1$, and $l_1 + l_3$ grew by at most 1. Hence, the original configuration was not optimal, a contradiction.

In the second case, h is odd so that $h = 2k - 1$. Then, the whole configuration fits into a rectangle with height $2k - 1$ and width $2l_1 + 1$, where $l_1 \leq k - 1$. Let us again

rearrange all the points using the procedure from the previous paragraph so that the resulting configuration lies in a rectangle with height $2k - 2$ and width $2l_1 + 2$ and satisfies $l_2 \leq 1$. Indeed, if $l_1 \leq k - 2$, all points may be placed in this rectangle since in this case we have

$$(2k - 2)(2l_1 + 2) \geq (2k - 1)(2l_1 + 1). \quad (7.1)$$

On the other hand, if $l_1 = k - 1$, we have

$$(2k - 2)(2l_1 + 2) = (2k - 1)(2l_1 + 1) - 1,$$

so the inequality (7.1) is not satisfied. In this case, however, $(2k - 1)(2l_1 + 1)$ is odd. Thus, since the total number of points $2N$ is even, it is not possible that the entire rectangle with height $2k$ and width $2l_1 + 1$ was full in the original configuration. Therefore, we can still place all the points in the rectangle with height $2k - 2$ and width $2l_1 + 2$. As before, the new configuration has strictly smaller energy since h decreased by 1, $l_2 \leq 1$, and $l_1 + l_3$ grew by at most 1, a contradiction. ■

Now, we proceed to prove the main result for Class \mathcal{I} ; namely, that for the purpose of the computation of the minimal energy, we may assume that $l_2 = 0$.

Proposition 7.3. *Fix $N := N_A = N_B > 0$ and $\beta \in (0, 1)$. Then, if $(A, B) \in \mathcal{I}$ is an optimal configuration, then there exists an optimal configuration $(\hat{A}, \hat{B}) \in \mathcal{I}$ with $l_2 = 0$.*

Proof. If $(A, B) \in \mathcal{I}$ such that $l_2 = 0$, there is nothing to prove. Suppose to the contrary that $l_2 > 0$. Then, by Proposition 7.1, we have that $l_2 = 1$. We introduce the following notation: again, l_1 is the number of columns with only A -points and l_3 is the number of columns with only B -points. We can assume that all columns except for the leftmost and rightmost ones are full, cf. last picture in Figure 19. By $r_1 \in \{1, \dots, h\}$ we denote the number of A -points in the leftmost column, and $r_4 \in \{1, \dots, h\}$ is the number of B -points in the rightmost column. By $r_2, r_3 \in \{1, \dots, h - 1\}$ we denote the numbers of A - and B -points, respectively, in the single column which contains points of both types.

Since $N_A = N_B$, we compute the number of points of each type, and we get that

$$(l_1 - 1)h + r_1 + r_2 = (l_3 - 1)h + r_3 + r_4,$$

so

$$(l_1 - l_3)h = r_3 + r_4 - r_1 - r_2. \quad (7.2)$$

Due to the range of r_1, \dots, r_4 , the left-hand side can take only values between $-2h + 3$ and $2h - 3$, so it needs to take values in the set $\{-h, 0, h\}$. Hence, up to exchanging the roles of the two types, we either have $l_1 = l_3$ or $l_1 = l_3 + 1$.

First, suppose that $l_1 = l_3 + 1$. Then, by (7.2), we have $r_1 + r_2 + h = r_3 + r_4$. In particular, $r_1 + r_2 < h$ as $r_3 + r_4 \leq 2h - 1$. Hence, we may move the r_2 A -points from the single column with both types to the leftmost column and replace them by r_2 B -points from the rightmost column. In this way, the double-type column disappeared altogether.

This process strictly decreases the energy (6.2) since l_1 stays the same, l_2 decreases by 1, and l_3 increases by 1 or stays the same. This is a contradiction.

Now, suppose that $l_1 = l_3$. Then, by (7.2), we have $r_1 + r_2 = r_3 + r_4$. If $r_1 + r_2 \leq h$, we proceed as in the previous paragraph. Suppose otherwise; i.e., $r_1 + r_2 = r_3 + r_4 > h$. Without restriction, we can suppose that $r_3 \geq r_2$. Let $k \in \mathbb{N}$ such that $k = \lceil h/2 \rceil$. Notice that we may modify the configuration so that $r_2 = \lfloor h/2 \rfloor$ and $r_3 = k$. Indeed, otherwise, we move $\lfloor h/2 \rfloor - r_2 (= r_3 - k)$ B -points from the double-type column to the rightmost column and move $\lfloor h/2 \rfloor - r_2$ A -points from the leftmost column to the double-type column so that both types have $\lfloor h/2 \rfloor$ and k points, respectively, in the double-type column. In this way, since

$$r_4 + \lfloor h/2 \rfloor - r_2 = (r_1 + r_2 - r_3) + \lfloor h/2 \rfloor - r_2 = r_1 + \lfloor h/2 \rfloor - r_3 \leq h,$$

where we used $r_1 \leq h$ and $r_3 \geq \lfloor h/2 \rfloor$, we did not add any additional column on the right. Thus, the total energy did not increase.

As $l_1 = l_3$ and $l_2 = 1$, by Lemma 7.2, we have that $l_1 = l_3 \geq k$. Now, remove all the points in the double-type column and place them directly above the first row, $\lfloor h/2 \rfloor$ A -points directly above the l_1 A -points (starting from the right) and k B -points directly above the l_3 B -points (starting from the left). Finally, we merge the two connected components of the resulting configuration by moving the connected component on the left by $(1, 0)$. In this way, h increased by 1, l_2 decreased by 1, and l_1 and l_3 remain unchanged so that the energy remains the same, see (6.2). Hence, the resulting configuration (\hat{A}, \hat{B}) is minimal, lies in Class \mathcal{I} , and satisfies $l_2 = 0$. This concludes the proof. ■

7.2. Exact calculation for Class \mathcal{I}

The regularisation procedure presented in the previous section enables us to compute directly the minimal energy for configurations in Class \mathcal{I} for any $\beta \in (0, 1)$. In this section, we suppose that $N_A = N_B$ and denote the common value by N . Later, in Section 8, we will show that there exists always a minimiser in Class \mathcal{I} which induces that the energy computed below coincides with the minimal energy.

Theorem 7.4. *Fix $N := N_A = N_B > 0$ and $\beta \in (0, 1)$. Suppose that a minimal configuration (A, B) is in Class \mathcal{I} . Then, its energy is equal to*

$$-4N + \min_{h \in \mathbb{N}} (2\lceil N/h \rceil + h(2 - \beta)),$$

where all minimisers h satisfy $|h - \sqrt{2N/(2 - \beta)}| \leq C_\beta N^{1/4}$ for some constant C_β only depending on β . For $\beta \in \mathbb{R} \setminus \mathbb{Q}$, there exists a unique minimiser.

Proof. By Proposition 7.3, for the purpose of the computation of the minimal energy, we may assume that $l_2 = 0$. Hence, we also have $l_1 = l_3$, and denote the common value by ℓ . Notice that we may minimise the energy under the constraint

$$h, \ell \in \mathbb{N}, \quad N = h\ell + r \quad \text{with } r \in \mathbb{N}, \quad 0 \leq r \leq h - 1.$$

This constraint is natural since for fixed h , the length ℓ is minimal whenever all the columns except for the leftmost and rightmost ones are full (i.e., have h points). We also refer to the configuration given in Theorem 1.1 (v). Under these assumptions, we may rewrite the energy (6.2) as

$$E(A, B) = -4N + 2(\ell + \min\{r, 1\}) + h(2 - \beta).$$

In particular, one can express the energy solely in terms of $h \in \mathbb{N}$ as

$$E(h) := -4N + 2 \left\lceil \frac{N}{h} \right\rceil + h(2 - \beta).$$

It is clear that the minimum of E over \mathbb{N} is unique in case that $\beta \in \mathbb{R} \setminus \mathbb{Q}$ as $E(h_1) - E(h_2) \notin \mathbb{Q}$ for all $h_1, h_2 \in \mathbb{N}$ with $h_1 \neq h_2$.

It remains to check that minimisers h satisfy $|h - \sqrt{2N/(2 - \beta)}| \leq C_\beta N^{1/4}$ for some constant C_β . The function

$$\bar{E}(h) = -4N + 2N/h + h(2 - \beta)$$

is strictly convex and attains its minimum at

$$\bar{h} := \sqrt{2N/(2 - \beta)} \quad \text{with} \quad \bar{E}(\bar{h}) = -4N + 2\sqrt{2N(2 - \beta)}.$$

For $h_* = \lceil \bar{h} \rceil$, we get for $\beta \in (0, 1)$

$$\begin{aligned} E(h_*) &= -4N + 2 \left\lceil \frac{N}{h_*} \right\rceil + h_*(2 - \beta) \leq -4N + 2\frac{N}{h_*} + 2 + h_*(2 - \beta) \\ &\leq -4N + 2\frac{N}{\bar{h}} + \bar{h}(2 - \beta) + 4 = \bar{E}(\bar{h}) + 4. \end{aligned} \quad (7.3)$$

Let us now determine those $h \in \mathbb{N}$ such that the inequality $\bar{E}(h) \leq \bar{E}(\bar{h}) + 4$ holds. By determining the roots of the quadratic equation $h\bar{E}(h) = h(\bar{E}(\bar{h}) + 4)$, one can check that $\bar{E}(h) \leq \bar{E}(\bar{h}) + 4$ is equivalent to

$$\begin{aligned} h &\in I_{N,\beta} \\ &:= \frac{2}{2 - \beta} + \sqrt{2N/(2 - \beta)} + \frac{2}{2 - \beta} \left[-\sqrt{1 + \sqrt{2N(2 - \beta)}}, \sqrt{1 + \sqrt{2N(2 - \beta)}} \right]. \end{aligned}$$

Note that $h \notin I_{N,\beta}$ cannot be a minimiser of E since then by (7.3) we have $E(h) \geq \bar{E}(h) > \bar{E}(\bar{h}) + 4 \geq E(h_*)$. Clearly, the definition of $I_{N,\beta}$ implies $|h - \sqrt{2N/(2 - \beta)}| \leq C_\beta N^{1/4}$ for all $h \in I_{N,\beta}$ for some C_β sufficiently large. This concludes the proof. \blacksquare

We close this section with the observation that, once we have guaranteed the existence of a minimiser in Class \mathcal{I} (see Theorem 8.15 below), Theorem 1.1 (iv) follows from Theorem 7.4 and (2.2). The construction of the configuration in the previous proof also yields the explicit solution in Theorem 1.1 (v).

8. Analysis and regularisation of other classes

In this section, we show how to regularise configurations related to classes $\mathcal{II}-\mathcal{V}$. Our main goal is to show that for $N_A = N_B$, it is not possible that a minimiser lies in Class \mathcal{II} or Class \mathcal{III} . While it is possible that a minimiser lies in Class \mathcal{IV} , see Proposition 8.16 below, we will show that under the constraint $\beta \leq 1/2$ we can modify an optimal configuration so that it lies in Class \mathcal{I} .

8.1. Class \mathcal{II}

Since the definition of Class \mathcal{II} already involved a very regular interface, namely, a straight line, the situation here is much simpler with respect to Class \mathcal{I} . In fact, the whole analysis of the problem boils down to the following simple result.

Proposition 8.1. *Fix $N := N_A = N_B > 0$ and $\beta \in (0, 1)$. If (A, B) is an optimal configuration, then $(A, B) \notin \mathcal{II}$.*

Proof. Suppose otherwise. Then, recalling (6.3), notice that we may rewrite the energy as

$$E(A, B) = -4N + E_A + E_B - \beta h_2,$$

where

$$E_A = l_1 + h_1 + h_2 \quad \text{and} \quad E_B = l_3 + h_2$$

are the energy between the void and A and B , respectively, and the last term corresponds to the interface energy.

Suppose first that $E_A > E_B$. Then, we modify the configuration as follows: set $\hat{B} = B$ and let \hat{A} be the symmetric image of B under the reflection along the interface. In this way, we obtain

$$E(\hat{A}, \hat{B}) = -4N + 2E_B - \beta h_2 < -4N + E_A + E_B - \beta h_2 = E(A, B),$$

a contradiction to minimality of (A, B) . Now, we suppose $E_A \leq E_B$ instead. We modify the configuration as follows: set $\hat{A} = A$ and let \hat{B} be the symmetric image of A under the reflection along the interface. In this way, the part of the energy corresponding to the shape of A stays the same, the part corresponding to B drops or stays the same, and the length h_2 of the interface increases at least by 1. Hence, the total energy decreases, so (A, B) was not a minimal configuration.

Let us remark that Proposition 8.1 does not hold if $N_A \neq N_B$, a counterexample being provided by Figure 10. ■

8.2. Class \mathcal{III}

Using again the notation introduced in the previous section, our first goal is to show that we can modify an admissible configuration in Class \mathcal{III} such that we remain in Class \mathcal{III} and $l_3 = h_3 = 0$ without increasing the energy. Then, we will prove that such a configuration cannot be optimal if $N_A = N_B$.

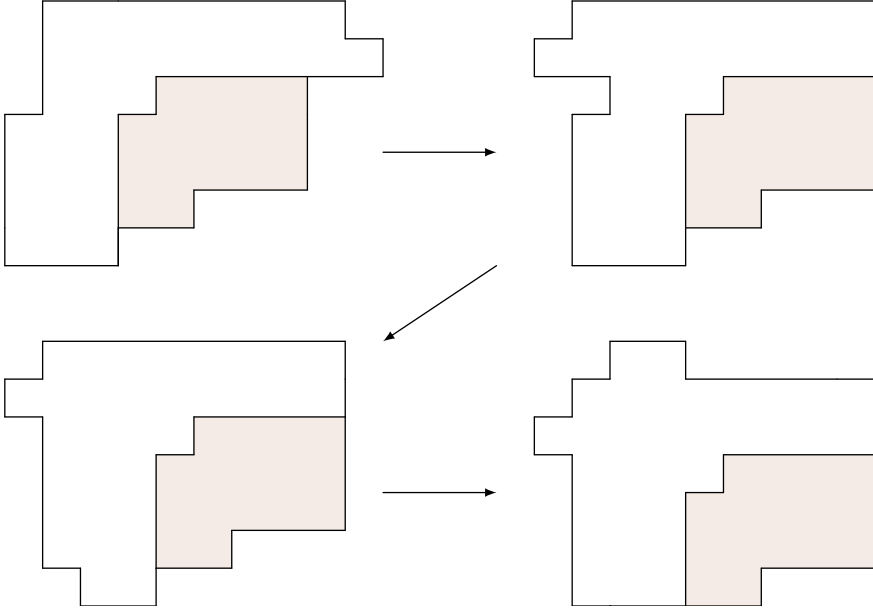


Figure 20. Regularisation of Class III : part one.

Proposition 8.2. Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in III$ is a minimal configuration and $l_3 > 0$ (respectively, $h_3 > 0$). Then, there exists a minimal configuration $(\hat{A}, \hat{B}) \in III$ with $l_3 = 0$ (respectively, $h_3 = 0$).

Proof. Assume that $l_3 > 0$ (the proof in the case $h_3 > 0$ is analogous). Our construction is presented in Figure 20. We will modify the top h_1 rows of the configuration (A, B) in the following way, for every $1 \leq k \leq N_{\text{row}}$, denote by x_k the first coordinate in the rightmost point of $(A \cup B)_k^{\text{row}}$. Then, for $k \leq h_1$, we set

$$\hat{A}_k := A_k^{\text{row}} + (\min\{x_{h_1+1} - x_k, 0\}, 0);$$

i.e., each row which has points further to the right than the rightmost point of B_{h_1+1} is translated to the left, in such a way that its rightmost point aligns with the rightmost point of B_{h_1+1} . As we made no modifications inside rows,

$$E_k^{\text{row}}(\hat{A}, \hat{B}) = E_k^{\text{row}}(A, B)$$

for all $k = 1, \dots, N_{\text{row}}$, see (4.1). Regarding E_k^{inter} , observe that for $k \geq h_1 + 1$ nothing changed in the configuration, so

$$E_k^{\text{inter}}(\hat{A}, \hat{B}) = E_k^{\text{inter}}(A, B).$$

On the other hand, for $k < h_1$, we either left two adjacent rows intact (so the number of connections between them stayed the same); moved both of them to the left so that their

rightmost points align (so the number of connections between them stayed the same or increased); or moved only one of them to the left, but because the rightmost point of the other one has first coordinate smaller than or equal to the first coordinate of B_{h_1+1} , this shift did not destroy any bonds and possibly created new ones. In every case, all these connections are of type A - A , so we have

$$E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B).$$

Finally, for $k = h_1$, we did not change the number of A - B connections and possibly added some A - A connections. Thus,

$$E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B).$$

Note that after this procedure all columns A_l^{col} for $l \leq l_1$ are still connected, as otherwise this would contradict Theorem 4.5 and the minimality of the original configuration. Hence, the resulting configuration lies in Class III . ■

In order to facilitate the proof that configurations in Class III cannot be optimal, we further modify the configuration without increasing the energy.

Lemma 8.3. *Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in III$ is a minimal configuration. Then, there exists a minimal configuration $(\hat{A}, \hat{B}) \in III$ such that for every $k = 1, \dots, N_{\text{row}}$ the rightmost point of $(\hat{A} \cup \hat{B})_k^{\text{row}}$ has the same first coordinate and for every $k = 1, \dots, N_{\text{col}}$ the lowest point of $(\hat{A} \cup \hat{B})_k^{\text{col}}$ has the same second coordinate.*

Proof. By Proposition 8.2, we may assume that $l_3 = h_3 = 0$. We will use a version of the technique used for Class I , and refer to Figure 21 for an illustration of the construction. Note that if we add N'_A A -points on the top and on the left and N'_B B -points on in the bottom right corner so that the configuration (A, B) becomes a full rectangle with sides $l_1 + l_2$ and $h_1 + h_2$, we do not alter the surface energy, but the bulk energy changes by $-2(N'_A + N'_B)$.

Having fixed $N'_B > 0$, let us remove the topmost A -point in the leftmost column and change the type of the topmost B -point in the leftmost column to A . In this way, we removed a B -point, without increasing the energy (6.4). We repeat this procedure until we remove N'_B B -points. Then, we remove N'_A A -points, starting from the top of the leftmost column. Again, this cannot increase the energy. Moreover, the resulting configuration lies in Class III because if in this last step we removed a whole column or a point which lies next to the interface, we would decrease the energy. Hence, the resulting configuration is also minimal and satisfies the desired property. ■

These regularisation results imply that in the case when the numbers of points in the two types are equal, then the minimising configuration cannot lie in Class III .

Proposition 8.4. *Fix $N_A = N_B > 0$ and $\beta \in (0, 1)$. Then, if (A, B) is a minimal configuration, $(A, B) \notin III$.*

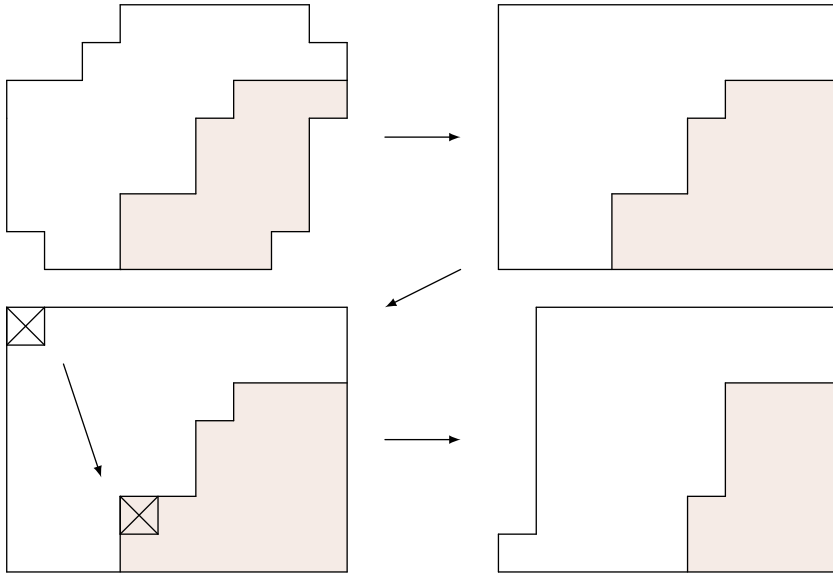


Figure 21. Regularisation of Class III: part two.

Proof. Suppose otherwise and let $(A, B) \in III$ be a minimal configuration. Apply the regularisation procedure described in Proposition 8.2 and Lemma 8.3. After these operations, (A, B) lies in a rectangle R with sides $h_1 + h_2$ and $l_1 + l_2$. Then, the length of the interface equals $l_2 + h_2$. Without loss of generality, $h_1 + h_2 \leq l_1 + l_2$ (otherwise, this is true after applying a symmetry with respect to the line $\mathbb{R}(-1, 1)$). Then, we compare (A, B) with a configuration $(\hat{A}, \hat{B}) \in I$ which fits into the rectangle R , with A -points on the left and B -points on the right such that the length of the interface is either $h_1 + h_2$ or $h_1 + h_2 + 1$, depending on whether $l_2 = 0$ or $l_2 = 1$. Hence, by minimality of (A, B) , we have $l_2 + h_2 \leq h_1 + h_2 + 1$; i.e.,

$$l_2 \leq h_1 + 1. \tag{8.1}$$

This gives a contradiction to the assumption $N_A = N_B$. To see this, first recall that the configuration is *full*, in the sense that the construction in Lemma 8.3 ensures that all the columns except for the leftmost one have the same number of points. Therefore, we may first estimate from above the number of B -points by

$$N_B \leq l_2 h_2 \leq h_1 h_2 + h_2$$

and the number of A -points from below by

$$\begin{aligned} N_A &\geq h_1 l_2 + h_1(l_1 - 1) + h_2(l_1 - 1) = h_1(l_1 + l_2) - h_1 + h_2(l_1 - 1) \\ &\geq h_1(h_1 + h_2) - h_1 + h_2(l_1 - 1) = h_1 h_2 + h_1(h_1 - 1) + h_2(l_1 - 1), \end{aligned}$$

where we used the assumption that $h_1 + h_2 \leq l_1 + l_2$. Hence, whenever $h_1, l_1 \geq 2$ or $l_1 \geq 3$, we have $N_A > N_B$, which would contradict the assumption $N_A = N_B$. Moreover, we get that necessarily $h_1 \leq h_2$.

Finally, we have to take into consideration the case when $l_1 = 1$ (with h_1 arbitrary) or when $h_1 = 1$ and $l_1 = 2$. In the first case, by (8.1), we have $h_1 + h_2 \leq l_2 + 1 \leq h_1 + 2$, so $h_2 \leq 2$. But then, $h_1 \leq h_2 \leq 2$, and thus, $l_2 \leq h_1 + 1 \leq 3$. This leaves us with a finite (and small) number of configurations to consider separately, and it may be checked that none of them is optimal. In the second case, again by (8.1), we have $l_2 \leq h_1 + 1 = 2$. Furthermore, $l_1 + l_2 \geq h_1 + h_2$, so $h_1 + h_2 \leq 4$, and hence $h_2 \leq 3$. Again, we end up with a small number of configurations. A direct exhaustive analysis guarantees that none of them is optimal. ■

8.3. Class \mathcal{IV} , part one

The situation in Class \mathcal{IV} is not as clear-cut as in Classes \mathcal{II} and \mathcal{III} : whereas configurations in Classes \mathcal{II} and \mathcal{III} are never optimal, the problem is that, even for $N_A = N_B$ and $\beta = 1/2$, an optimal configuration may actually lie in Class \mathcal{IV} , see Figure 11. Hence, the goal in this section is a bit different: we will prove that even though minimal configurations in Class \mathcal{IV} may exist, there also exists an optimal configuration in Class \mathcal{I} . Moreover, the reasoning will also provide some further properties of optimal configurations in Class \mathcal{IV} . In particular, a careful inspection of the forthcoming constructions will show a fluctuation estimate for minimisers in Class \mathcal{IV} , see Section 9 below.

This goal is achieved as follows: in the first part, we regularise our configuration such that $h_3 = 0$ and $h_1 \leq l_1$. This is achieved in Proposition 8.7, with the key part of the reasoning proved in Proposition 8.6. These arguments are valid for any $\beta \in (0, 1)$. Then, in the second part, under the restriction $\beta \leq 1/2$, we regularise a configuration with $h_3 = 0$ and $h_1 \leq l_1$ to obtain a configuration in Class \mathcal{I} . This is achieved in Propositions 8.10–8.13. We break the reasoning into smaller pieces in order to highlight different techniques and different assumptions required at each point.

Lemma 8.5. *Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{IV}$ is a minimal configuration. Then, there exists a minimal configuration $(\hat{A}, \hat{B}) \in \mathcal{I} \cup \mathcal{IV}$ such that $l_2 \leq h_2$,*

$$\min\{h_1, h_1 + h_2 - l_1 - l_2\} \leq 0 \quad \text{and} \quad \min\{h_3, h_2 + h_3 - l_2 - l_3\} \leq 0.$$

Proof. Choose a minimal configuration (A, B) in Class \mathcal{IV} . Without loss of generality, we may assume that $l_2 \leq h_2$. Otherwise, consider a reflection of the original configuration with respect to the line $\mathbb{R}(-1, 1)$. Then, we end up with a configuration of the same type with the roles of h_i and l_i reversed. We suppose that $h_1 \geq 1$ as otherwise the second condition in the statement of the lemma is satisfied. We modify the configuration without increasing the energy such that $h_1 = 0$ or $l_1 + l_2 \geq h_1 + h_2$. To see this, suppose that $l_1 + l_2 < h_1 + h_2$. Then, we remove all the points in the first row, and place them on the left-hand side starting from the second row, one in each row, possibly forming one

additional column. The assumption guarantees that there was enough space to place all the points. In this way, h_1 decreases by 1 and l_1 increases possibly by 1, so the total energy decreases (in which case (A, B) was not a minimal configuration) or stays the same, cf. (6.5). We repeat this procedure until $h_1 = 0$ or $l_1 + l_2 \geq h_1 + h_2$.

In a similar fashion, we modify the configuration to obtain $\min\{h_3, h_2 + h_3 - l_2 - l_3\} \leq 0$. Finally, if $h_1 = h_3 = 0$, the configuration is in Class \mathcal{I} . Otherwise, if $h_1 \geq 1$, the configuration is in Class \mathcal{IV} , and if $h_1 = 0, h_3 \geq 1$, after a rotation by π and interchanging the roles of the two types, we obtain a configuration in Class \mathcal{IV} . ■

We continue the regularisation in the following proposition.

Proposition 8.6. *Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{IV}$ is a minimal configuration. Then, there exists a minimal configuration $(\hat{A}, \hat{B}) \in \mathcal{I} \cup \mathcal{IV}$ which satisfies $l_2 \leq h_2$, $\min\{h_1, h_1 + h_2 - l_1 - l_2\} \leq 0$, $\min\{h_3, h_2 + h_3 - l_2 - l_3\} \leq 0$, and at least one of the following two properties:*

- (1) $l_2 = 1$,
- (2) $h_3 = 0$.

For the proof, we introduce the following notation specific for Class \mathcal{IV} . With the notation of Figure 17, we will refer to the nine rectangles with sides l_i and h_j as $l_i : h_j$. For instance, the rectangle in the middle with sides l_2 and h_2 will be referred to as rectangle $l_2 : h_2$. A priori, some of these rectangles may be not full or even empty, for instance, the rectangle $l_3 : h_1$.

Proof. Let $(A, B) \in \mathcal{IV}$ be a minimal configuration from Lemma 8.5 which does not satisfy the desired properties, i.e., $l_2 > 1$ and $h_1, h_3 > 0$ ($l_2 = 0$ is not possible as it would imply $(A, B) \in \mathcal{II}$). Then, we first make a similar regularisation as we did for Class \mathcal{I} . We add N'_A A -points to the configuration (A, B) so that the interface between A and the void consists of four line segments (of lengths $l_1, h_1 + h_2, l_1 + l_2$, and h_1). This does not increase the surface energy. Then, we remove N'_A A -points, column by column, starting from the leftmost column in (A, B) . If we removed a whole column, or if we removed a point which lies at the interface, the energy drops, so the original configuration (A, B) was not minimal. Hence, the resulting configuration lies in Class \mathcal{IV} . We proceed in a similar fashion for the B -points. In particular, the rectangle $l_2 : h_2$ (in the middle) is full.

Now, let us look at the (full) rectangle $l_2 : h_2$. It contains exactly $l_2 h_2$ points, N''_A of them of type A and N''_B of them of type B . We rearrange them (i.e., remove all the points in $l_2 : h_2$ and place them back in $l_2 : h_2$) in the following way: we start with the leftmost column and we fill the columns one by one with A -points until we end up with less than h_2 points to place. Then, we place the remaining points in the next column, starting from the top. Similarly, we place the B -points starting from the rightmost column and we fill the columns one by one until we end up with less than h_2 points. We place the remaining points on the bottom of the next column. In this way, the resulting configuration has an

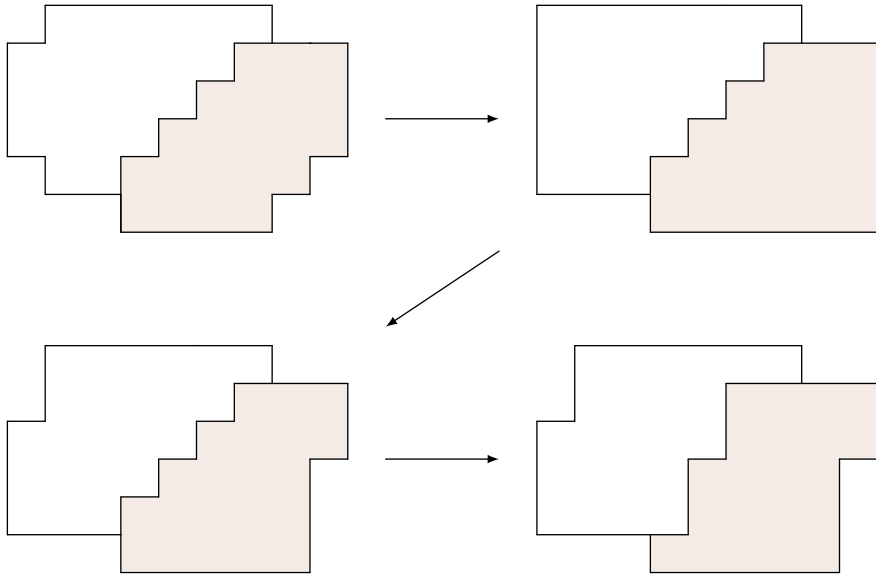


Figure 22. Regularisation of Class $\mathcal{I}\mathcal{V}$: part one.

interface with at most one step in $l_2 : h_2$, and we did not change the energy. By Lemma 8.5, we also have

- (i) $l_2 \leq h_2$,
- (ii) $l_1 \geq h_1$,
- (iii) $l_3 \geq h_3$.

Indeed, (i) is clear. If $h_1 = 0$, (ii) is obvious. Otherwise, we have $h_1 + h_2 - l_1 - l_2 \leq 0$ which along with (i) shows (ii). The proof of (iii) is similar. The procedure described above is presented in Figure 22.

As $l_2 \geq 2$ and the interface has at most one step, we observe that at least one of the following cases holds true: (a) the rightmost column of $l_2 : h_2$ consists only of points of type B . (b) The leftmost column of $l_2 : h_2$ consists only of points of type A . Then, we apply one of the two following procedures:

(a) We move the A -points from the rightmost column of the rectangle $l_2 : h_1$ (in the upper right corner) to the rectangle $l_1 : h_3$ (in the bottom left corner) and place them in its highest row (starting from the right). Here, we use (ii) and $h_3 \geq 1$. In this way, we do not increase the surface energy, see (6.5), since we have $h_2 \rightarrow h_2 + 1, l_2 \rightarrow l_2 - 1, h_3 \rightarrow h_3 - 1, l_3 \rightarrow l_3 + 1$, and h_1 and l_1 remain unchanged. Finally, we perform a rearrangement in the new rectangle $l_2 : h_2$ as above. An example of such construction is given by the top arrow in Figure 23.

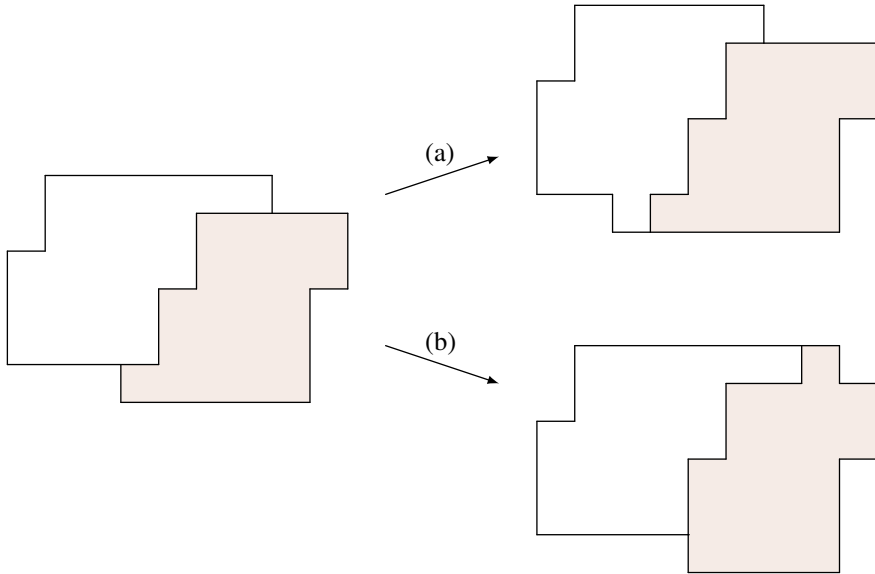


Figure 23. Regularisation of Class $\mathcal{I}\mathcal{V}$: part two.

(b) We move the B -points from the leftmost column of the rectangle $l_2 : h_3$ (in the bottom left corner) to the rectangle $l_3 : h_1$ (in the upper right corner) and place them in its lowest row (starting from the left). Here, we use (iii) and $h_1 \geq 1$. In this way, we do not increase the surface energy since we have $h_2 \rightarrow h_2 + 1$, $l_2 \rightarrow l_2 - 1$, $h_1 \rightarrow h_1 - 1$, $l_1 \rightarrow l_1 + 1$, and h_3 and l_3 remain unchanged. Finally, we perform a rearrangement in the new rectangle $l_2 : h_2$ as above. An example of such construction is given by the bottom arrow in Figure 23.

In both cases, after applying the procedure, the conditions (i), (ii), and (iii) are still satisfied, so we may repeat it. We repeat it until $l_2 = 1$, $h_1 = 0$, or $h_3 = 0$. Indeed, this follows after a finite number of steps since in each step l_2 decreases. If $l_2 = 1$ or $h_3 = 0$ holds, the proof is concluded. Otherwise, $h_3 = 0$ holds after a rotation by π and interchanging the roles of the two types. ■

We now come to the main result of this section.

Proposition 8.7. Fix $N_A = N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{I}\mathcal{V}$ is a minimal configuration. Then, there exists a minimal configuration $(A, B) \in \mathcal{I} \cup \mathcal{I}\mathcal{V}$ such that $l_2 \leq h_2$, $h_1 \leq l_1$, and $h_3 = 0$.

Proof. Let (A, B) be a configuration from Proposition 8.6. Suppose by contradiction that (A, B) (up to a rotation by π and interchanging the roles of the two types) does not have

the desired properties. Since (i), (ii), and (iii) hold, we thus get that $l_2 = 1$ and $h_1, h_3 > 0$. By Proposition 8.6 and $h_1, h_3 > 0$, we also have

$$l_1 + 1 \geq h_1 + h_2 \quad \text{and} \quad l_3 + 1 \geq h_2 + h_3.$$

As $h_2 \geq 1$, this particularly implies that $h_1 \leq l_1$. We can thus move the single column $l_2 : h_1$ to the empty rectangle $l_1 : h_3$ without increasing the energy. Note that $l_1 \geq h_1$ guarantees that there was enough space to place all the points. The resulting configuration has a straight interface with $h_1 > 0$; i.e., lies in Class \mathcal{II} . In view of Proposition 8.1, however, this contradicts the optimality of the original configuration. ■

Hence, for $N_A = N_B$ and any $\beta \in (0, 1)$, we may require that $h_3 = 0$ and $h_1 \leq l_1$. We continue the analysis in the next section, with an additional requirement on β .

8.4. Class \mathcal{IV} , part two

From now on, we will work with configurations which satisfy the statement of Proposition 8.7, i.e., $h_1 \leq l_1$ and $h_3 = 0$. Our goal is to perform a further modification such that configurations lie in Class \mathcal{I} . To this end, we assume without restriction that configurations from Proposition 8.7 lie in Class \mathcal{IV} and that $N := N_A = N_B$. In due course, we will introduce an additional assumption on $\beta \in (0, 1)$.

As a first step of the regularisation procedure, we again straighten the interface such that it has at most one step.

Lemma 8.8. *Fix $N_A = N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{IV}$ is an optimal configuration with $h_3 = 0$. Then, there exists a minimal configuration with the same properties and at most one step in the interface.*

Proof. We proceed similarly to our reasoning in Class \mathcal{I} ; i.e., as in the proof of Proposition 7.1. We add points to the configuration such that the rectangles $l_i : h_j$ for $i = 1, 2, 3$ and $j = 1, 2$, except for $l_3 : h_1$ are full. In this way, the surface part of the energy did not change. Then, we remove the same number of A - and B -points that we added, starting with the leftmost and rightmost column. If we removed a full column, then the energy would drop and the original configuration would not be minimal. Hence, the rectangle $l_2 : h_2$ is necessarily full. Let us now reorganise it in the following way: we put all the A -points to the left and all the B -points to the right so that the interface between them (inside $l_2 : h_2$) is vertical except for a single possible step to the right. Its length did not change, so the resulting configuration is optimal. ■

Lemma 8.9. *Fix $N_A = N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{IV}$ is an optimal configuration such that $h_1 \leq l_1$ and $h_3 = 0$. Then, $h_1 \leq h_2$.*

Proof. Suppose otherwise, i.e., $h_1 > h_2$. First, we can assume that $l_3 \leq h_2$. Indeed, if not, we can remove the whole rectangle $l_3 : h_2$, rotate it by $\pi/2$ and reattach it to the configuration, adding at least one additional bond, a contradiction to minimality of (A, B) .

Moreover, we can assume that $l_1 \geq 2$ as $l_1 = 1$ implies also $h_1 = 1$, and the inequality $h_1 \leq h_2$ is automatically satisfied. Finally, we can suppose that the interface has at most one step, see Lemma 8.8. The main step of the proof is to show that $l_1 < l_3$. Indeed, then, we obtain the contradiction

$$h_2 \leq h_1 \leq l_1 < l_3 \leq h_2.$$

Let us now prove $l_1 < l_3$. To this end, we will calculate the total number of points in two ways. Denote by r_1 the number of A -points in the leftmost column, by $h_1 + r_2$ the number of A -points in the leftmost double-type column, by r_3 the number of B -points in the leftmost double-type column, and by r_4 the number of B -points in the rightmost column. Then, we have

$$N_A = (l_1 - 1)(h_1 + h_2) + l_2 h_1 + r_1 + r_2$$

and

$$N_B = (l_2 + l_3 - 2)h_2 + r_3 + r_4.$$

Now, we subtract one of these equations from the other. Since $r_1 > 0$, $r_2 \geq 0$, and $r_3, r_4 \leq h_2$, we get

$$\begin{aligned} 0 &= N_A - N_B = l_1 h_1 + l_1 h_2 + l_2 h_1 - h_1 - h_2 + r_1 + r_2 \\ &\quad - l_2 h_2 - l_3 h_2 + 2h_2 - r_3 - r_4 \\ &> (l_1 - 1)h_1 - h_2 + (l_1 - l_3)h_2 + l_2(h_1 - h_2) \geq (l_1 - l_3)h_2, \end{aligned}$$

where, in the last step, we used $l_1 \geq 2$ and the assumption (by contradiction) that $h_1 \geq h_2$. This shows that $l_1 < l_3$ and concludes the proof. ■

Proposition 8.10. *Fix $N_A = N_B > 0$ and $\beta \leq 1/2$. Suppose that $(A, B) \in \mathcal{IV}$ is an optimal configuration such that $h_1 \leq l_1$ and $h_3 = 0$. Then, there exists an optimal configuration (\hat{A}, \hat{B}) such that $(\hat{A}, \hat{B}) \in \mathcal{IV}$ with $h_3 = 0$ and $l_2 \in \{1, 2\}$.*

Proof. Suppose that (A, B) satisfies $l_2 \geq 3$. By Lemma 8.9, we have $h_1 \leq h_2$. Then, let us remove the rightmost two layers in $l_2 : h_1$ and place the (at most $2h_1$) A -points on the left of the configuration, at most one point in every row. Since $h_1 \leq h_2$, there is enough space to place all the points. In this way, since the configuration can be assumed to have only one step in the interface (see Lemma 8.8), l_1 increases by at most 1, l_2 decreases by 2, l_3 increases by 2, and all h_i stay the same. Hence, by formula (6.5), we see that the energy stays the same (for $\beta = 1/2$), so the resulting configuration is optimal or decreases (for $\beta < 1/2$), so the original configuration was not optimal. We repeat this procedure until $l_2 \in \{1, 2\}$. ■

Hence, in order to prove the existence of an optimal configuration in Class \mathcal{I} , we have two special cases to consider, depending on the value of l_2 . We start with the case $l_2 = 1$.

Proposition 8.11. Fix $N_A = N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{IV}$ is an optimal configuration such that $h_3 = 0$ and $l_2 = 1$. Then, $h_1 = 1$. Furthermore, there exists an optimal configuration $(\hat{A}, \hat{B}) \in \mathcal{I}$.

Proof. As in (4.2), let us write the energy as

$$E(A, B) = E_A + E_B - (h_2 + 1)\beta,$$

where E_A is minus the number of bonds between points in A and E_B is minus the number of bonds between points in B .

We consider two cases. First, suppose that $E_B < E_A$. We do the following rearrangement of points: we separate A and B and suppose without restriction that the leftmost column of B is full as otherwise we can move the points in this column to the right-hand side of B , without changing the E_B . We replace A by \hat{A} , a reflection of B along the vertical axis. Then, we reconnect \hat{A} and B along the vertical line segment of length h_2 . In this way, the resulting configuration has energy

$$E(\hat{A}, B) = E_B + E_B - h_2\beta.$$

Hence, as $E_B \leq E_A - 1$, the energy drops by at least $1 - \beta$, so the original configuration was not optimal, a contradiction.

Now, suppose that $E_A \leq E_B$. We do the following: we keep A fixed (or, as above, we make A flat on one side without changing E_A) and replace B by \hat{B} , a reflection of A along the vertical axis. Then, we join A and \hat{B} along the vertical line segment of length $h_1 + h_2$. In this way, the resulting configuration lies in Class \mathcal{I} , has a flat interface, and the energy is given by

$$E(A, \hat{B}) = E_A + E_A - (h_1 + h_2)\beta.$$

Therefore, the only way in which the energy does not decrease is that $E_A = E_B$ and $h_1 = 1$. ■

We will employ another variant of the reflection argument to deal with the case $l_2 = 2$. This is formalised in the next proposition.

Proposition 8.12. Fix $N_A = N_B > 0$ and $\beta \leq 1/2$. Suppose that $(A, B) \in \mathcal{IV}$ is an optimal configuration such that $h_3 = 0$ and $l_2 = 2$. Then, $h_1 \leq 2 + 1/\beta$ and there exists an optimal configuration $(\hat{A}, \hat{B}) \in \mathcal{I}$.

Proof. Again, as in (4.2), we write the energy as

$$E(A, B) = E_A + E_B - (h_2 + 2)\beta.$$

We consider three cases: first, suppose that either $E_B \leq E_A - 2$ or $E_B = E_A - 1$ and $h_1 \leq 2 + 1/\beta$. We do the following rearrangement of points: we keep B fixed (up to making one side flat, as in the previous proof) and replace A by \hat{A} , a reflection of B along

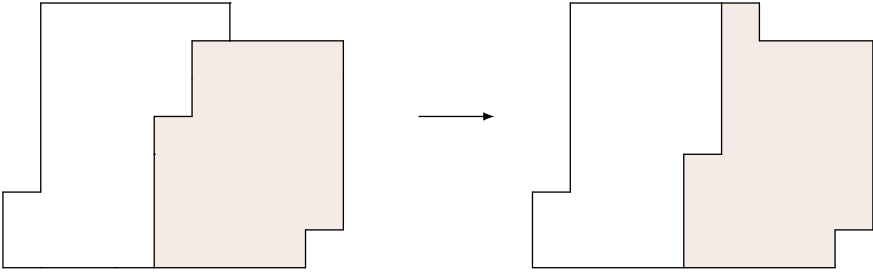


Figure 24. Final step of modification into Class \mathcal{I} .

the vertical axis. Then, we join \hat{A} and B along the vertical line segment of length h_2 . The resulting configuration lies in Class \mathcal{I} and satisfies

$$E(\hat{A}, B) = E_B + E_B - h_2\beta.$$

Hence, the energy drops by $k - 2\beta$, where $k = E_A - E_B \geq 1$. Thus, either the original configuration was not optimal (for $k \geq 2$ or $k = 1$ and $\beta < 1/2$) or the resulting configuration is optimal (for $k = 1$ and $\beta = 1/2$). Moreover, the resulting configuration lies in Class \mathcal{I} .

Now, suppose that either $E_B = E_A - 1$ and $h_1 > 2 + 1/\beta$ or $E_B = E_A$ and $h_1 \geq 2$ or $E_A < E_B$. This time, we keep A fixed (up to making one side flat) and replace B by \hat{B} , a reflection of A along the vertical axis. Then, we join A and \hat{B} along the vertical line segment of length $h_1 + h_2$. In this way, the resulting configuration lies in Class \mathcal{I} , has a flat interface, and the energy is given by

$$E(A, \hat{B}) = E_A + E_A - (h_1 + h_2)\beta.$$

Thus, the energy decreases by $k + (h_1 - 2)\beta$, where $k = E_B - E_A$. In particular, for $k = -1$ and $h_1 > 2 + 1/\beta$ or $k = 0$ and $h_1 \geq 3$ or $k > 0$, the energy drops. For $k = 0$ and $h_1 = 2$, it stays the same, so the resulting configuration is optimal and lies in Class \mathcal{I} .

The only case left to consider is when $E_A = E_B$ and $h_1 = 1$. We proceed as follows: we exchange the rightmost A -point (i.e., the rightmost point of the rectangle $l_2 : h_1$) with the top B -point from column C_{l_1+1} , i.e., the point with two connections to points of type A and two connections to points of type B . If C_{l_1+1} contains only one B -point, then the interface becomes shorter (without changing the overall shape of the configuration) and the energy actually drops. If it contains more than one B -point, this procedure does not change the energy. Moreover, the resulting configuration is in Class \mathcal{I} . The construction is presented in Figure 24.

Summarising, we have shown that $h_1 \leq 2 + 1/\beta$ and that there exists an optimal configuration in Class \mathcal{I} . ■

We summarise the reasoning from this section in the following result.

Proposition 8.13. *Fix $N_A = N_B > 0$ and $\beta \leq 1/2$. Suppose that $(A, B) \in \mathcal{IV}$ is an optimal configuration. Then, there exists an optimal configuration $(\hat{A}, \hat{B}) \in \mathcal{I}$.*

Proof. By Proposition 8.7, there exists an optimal configuration with $h_1 \leq l_1$ and $h_3 = 0$. Since $\beta \leq 1/2$, by Proposition 8.10, one may require additionally that $l_2 = 1$ or $l_2 = 2$. In both cases, the existence of an optimal configuration in Class \mathcal{I} is guaranteed by Proposition 8.11 and by Proposition 8.12, respectively. ■

8.5. Class \mathcal{V}

Finally, we show that we can modify optimal configurations in Class \mathcal{V} to optimal configuration in Class \mathcal{IV} . Along with Proposition 8.13, this shows that there always exists a minimiser in Class \mathcal{I} . This is done in the following proposition which employs a similar technique to the one used for Class \mathcal{III} .

Proposition 8.14. *Fix $N_A, N_B > 0$ and $\beta \in (0, 1)$. Suppose that $(A, B) \in \mathcal{V}$. Then, there exists $(\hat{A}, \hat{B}) \in \mathcal{IV}$ with $E(\hat{A}, \hat{B}) \leq E(A, B)$.*

Proof. We will modify the top h_1 rows of the configuration (A, B) in a similar fashion to the proof of Proposition 8.2. For every $k \leq h_1$, we set $\hat{A}_k := A_k^{\text{row}} + (-1, 0)$. This translation implies that

$$E_k^{\text{row}}(\hat{A}, \hat{B}) = E_k^{\text{row}}(A, B)$$

for all $k = 1, \dots, N_{\text{row}}$. Regarding E_k^{inter} , a change is possible at most for $k = h_1$, where we did not change the number of A - B connections and added zero or one A - A connections, so $E_k^{\text{inter}}(\hat{A}, \hat{B}) \leq E_k^{\text{inter}}(A, B)$. Hence, the total energy did not increase. We repeat this procedure for all rows with index $k \leq h_1$ until the rightmost point of all A_k^{row} with $k \leq h_1$ does not lie right to the rightmost point of $B_{h_1+1}^{\text{row}}$. We thus get a configuration which lies in Class \mathcal{IV} . ■

8.6. Conclusion

Finally, we are in the position to state another of the main results, which, together with Theorem 7.4, gives the exact formula for the minimal energy see Theorem 1.1 (iv).

Theorem 8.15. *Fix $N_A = N_B > 0$ and $\beta \leq 1/2$. Then, there exists an optimal configuration (A, B) which lies in Class \mathcal{I} and has a straight interface.*

Proof. Since the number of points is finite, there exists an optimal configuration. By Theorem 4.5 and the discussion below it, it lies in one of the five classes. However, it cannot lie in Class \mathcal{II} by Proposition 8.1. It also cannot lie in Class \mathcal{III} by Proposition 8.4. If it lies in Class \mathcal{V} , then there exists a minimal configuration in Class \mathcal{IV} by virtue of Proposition 8.14. If it lies in Class \mathcal{IV} , then by Proposition 8.13 there exists a minimal

configuration in Class \mathcal{I} . Finally, since there is an optimal configuration in Class \mathcal{I} , by Proposition 7.3, we may suppose that it has a flat interface. ■

Let us note that in the above theorem we only state that a solution in Class \mathcal{I} exists and that we cannot fully exclude the existence of solutions in other classes. In particular, the following result shows that there exist arbitrarily large optimal configurations in Class \mathcal{IV} .

Proposition 8.16. *Let $\beta \in (0, 1/2] \cap \mathbb{Q}$, $r, s \in \mathbb{N}$ with $r/s = 1 - \beta/2$, and $k \in \mathbb{N}$. Then, the Class- \mathcal{IV} configuration (A, B) with*

$$\begin{aligned} A &= \{(x, y) \in \mathbb{Z}^2 : x \in [-kr + 1, 0], y \in [1, ks]\} \cup (1, ks), \\ B &= \{(x, y) \in \mathbb{Z}^2 : x \in [1, kr], y \in [0, ks - 1]\} \cup (0, 0) \end{aligned}$$

is optimal.

Proof. Using (2.2) and formula (6.5), one can directly compute

$$P(A, B) = 4kr + 2(ks + 1) + 2(1 - \beta)(ks + 1). \tag{8.2}$$

To prove optimality, it hence suffices to check that $P(A, B) = \min\{P_*, P^*\}$, where P_* and P^* are defined in Theorem 1.1 (iv) for $N := N_A = N_B = k^2rs + 1$. From $\beta \in (0, 1/2]$, we get that $s/r = 2/(2 - \beta) \in (1, 4/3]$. This in particular entails that $s > r \geq 2$, which in turn allows to prove that

$$\sqrt{\frac{2N}{2 - \beta}} = \sqrt{\frac{k^2rs + 1}{r/s}} = \sqrt{k^2s^2 + s/r} \in (ks, ks + 1).$$

In particular, we have checked that

$$\left\lfloor \sqrt{\frac{2N}{2 - \beta}} \right\rfloor = ks \quad \text{and} \quad \left\lceil \sqrt{\frac{2N}{2 - \beta}} \right\rceil = ks + 1.$$

One can hence compute

$$\begin{aligned} P_* &= 4 \left\lceil \frac{N}{\lfloor \sqrt{\frac{2N}{2 - \beta}} \rfloor} \right\rceil + 2 \left\lfloor \sqrt{\frac{2N}{2 - \beta}} \right\rfloor (2 - \beta) \\ &= 4 \left\lceil \frac{k^2rs + 1}{ks} \right\rceil + 2ks(2 - \beta) = 4[kr + 1/ks] + 2ks(2 - \beta) \\ &= 4kr + 4 + 2ks(2 - \beta). \end{aligned}$$

On the other hand, using again the fact that for $s > r \geq 2$, we get that

$$\frac{k^2rs + 1}{ks + 1} \in (kr - 1, kr],$$

and we can compute

$$\begin{aligned} P^* &= 4 \left\lceil \frac{N}{\lceil \sqrt{\frac{2N}{2-\beta}} \rceil} \right\rceil + 2 \left\lceil \sqrt{\frac{2N}{2-\beta}} \right\rceil (2-\beta) \\ &= 4 \left\lceil \frac{k^2rs + 1}{ks + 1} \right\rceil + 2(ks + 1)(2-\beta) = 4kr + 2(ks + 1)(2-\beta). \end{aligned}$$

We conclude that

$$\min\{P_*, P^*\} = P^* \stackrel{(8.2)}{=} P(A, B),$$

which proves that (A, B) is optimal. ■

9. $N^{1/2}$ -law and $N^{3/4}$ -law for minimisers

In this section, we give a quantitative upper bound on the difference of two optimal configurations, see Theorem 1.1 (vi). The goal is to prove that, even though in general there is no uniqueness of the optimal configurations and some of them may even not be in Class \mathcal{I} they all have the same approximate shape. In the following, an isometry $T: \mathbb{Z}^2 \rightarrow \mathbb{Z}^2$ indicates a composition of the translations $x \mapsto x + \tau$ for $\tau \in \mathbb{Z}^2$, the rotation $(x_1, x_2) \mapsto (-x_2, x_1)$ by the angle $\pi/2$, and the reflections $(x_1, x_2) \mapsto (x_1, -x_2)$, $(x_1, x_2) \mapsto (-x_1, x_2)$.

Theorem 9.1 ($N^{1/2}$ - and $N^{3/4}$ -law). *Fix $N := N_A = N_B > 0$ and $\beta \leq \frac{1}{2}$. Then, there exists a constant C_β only depending on β such that for each two optimal configurations (A, B) and (A', B') it holds that*

$$\min\{\#(A \Delta T(A')) + \#(B \Delta T(B')) : T : \mathbb{Z}^2 \rightarrow \mathbb{Z}^2 \text{ is an isometry}\} \leq C_\beta N^\gamma(\beta), \quad (9.1)$$

where $\gamma(\beta) = 1/2$ if $\beta \in \mathbb{R} \setminus \mathbb{Q}$ and $\gamma(\beta) = 3/4$ if $\beta \in \mathbb{Q}$.

Proof. Throughout the proof, C_β is a constant which depends only on β whose value may vary from line to line. We start the proof by mentioning that it suffices to check the assertion only for $N \geq N_0$ for some $N_0 \in \mathbb{N}$ depending only on β . As observed in the proof of Theorem 8.15, every optimal configuration lies in the Classes \mathcal{I} , $\mathcal{I}\mathcal{V}$, \mathcal{V} . In Step 1, we show (9.1) for two optimal configurations in Class \mathcal{I} . Afterwards, in Step 2, we show that for each optimal configuration (A, B) in Class $\mathcal{I}\mathcal{V}$ there exists (A', B') in Class \mathcal{I} such that (9.1) holds. Eventually, in Step 3, we check that for each optimal configuration (A, B) in Class \mathcal{V} there exists (A', B') in Class $\mathcal{I}\mathcal{V}$ such that (9.1) holds. The combination of these three steps yields the statement.

Step 1: Class \mathcal{I} . Let first (A, B) be an optimal configuration in Class \mathcal{I} such that $l_2 = 0$. Then, by Theorem 1.1 (iv), we find $\bar{h} \in \mathbb{N}$ with $|\bar{h} - \sqrt{2N/(2-\beta)}| \leq C_\beta N^{1/4}$ such that

$$h \sim \bar{h}, \quad l_1 = l_3 \sim \sqrt{N/\bar{h}}, \quad (9.2)$$

where here and in the following \sim indicates that the equality holds up to a constant $C_\beta N^{\nu(\beta)-1/2}$. Indeed, for $\beta \in \mathbb{R} \setminus \mathbb{Q}$, the value \bar{h} is unique, whereas for $\beta \in \mathbb{Q}$ it lies in an interval whose diameter is at most of order $N^{1/4}$. Consequently, two optimal configurations in Class \mathcal{I} with $l_2 = 0$ clearly satisfy (9.1). Also, notice that since the interface is straight, reflection along the interface exchanges the roles of the sets A and B . Now, consider an optimal configuration (A, B) in Class \mathcal{I} with $l_2 > 0$. Then, we get $l_2 = 1$ by Proposition 7.1. The regularisation of Proposition 7.3 shows that (A, B) can be modified to a configuration (A', B') in Class \mathcal{I} with $l_2 = 0$ such that (9.1) holds. Indeed, in this regularisation, we only alter the configurations involving the single column containing points of both types and possibly merge two connected components by moving one connected component by $(1, 0)$. This concludes Step 1 of the proof.

Step 2: Class \mathcal{IV} . We now consider an optimal configuration in Class \mathcal{IV} and show that it can be modified to a configuration in Class \mathcal{I} such that (9.1) holds. We will work through the proofs in Sections 8.3 and 8.4 in reverse order. Our strategy is as follows: we use the knowledge of the structure of the final step of the regularisation procedure, obtain some a posteriori bounds on the size of l_i and h_i , and go back to see how these can change at every step of the regularisation procedure. Eventually, this will allow us to show that already after the first modification described in Lemma 8.5 we obtain an optimal configuration in Class \mathcal{I} , by moving at most $C_\beta N^{1/2}$ many points. This will conclude Step 2 of the proof.

Step 2.1. Our starting points are Propositions 8.11 and 8.12: recall that applying all the intermediate steps, in the end, we have $h_3 = 0$ and we land with an alternative $l_1 = 1$ (which is covered in Proposition 8.11) or $l_2 = 2$ (which is covered by Proposition 8.12). In both cases, before applying these propositions, we have

$$l_2 \leq 2, \quad h_1 \leq 2 + \frac{1}{\beta}, \quad h_3 = 0, \quad h_2 \sim \bar{h}, \quad l_1, l_3 \sim \sqrt{N/\bar{h}}. \quad (9.3)$$

In fact, the last conditions follow from (9.2) (for $h = h_2$) and the reflection procedure described in the propositions.

Step 2.2. Now, we go a step back in the regularisation procedure. In Proposition 8.10, for $\beta < 1/2$ nothing changes and the same bounds hold. For $\beta = 1/2$, (9.3) yields that $\frac{h_1}{h_2} \rightarrow 0$ as $N \rightarrow \infty$. This implies that in Proposition 8.10, for sufficiently large N , we move at most two layers. In fact, if we moved at least three layers, the energy would strictly decrease since all of them fit into a single column. Hence, for sufficiently big N (depending only on β), we have the following bounds:

$$l_2 \leq 4, \quad h_1 \leq 2 + \frac{1}{\beta}, \quad h_3 = 0, \quad h_2 \sim \bar{h}, \quad l_1, l_3 \sim \sqrt{N/\bar{h}}. \quad (9.4)$$

Finally, let us take one more step back in the regularisation procedure. In Lemma 8.8, we actually modify the configuration only slightly inside the rectangle $l_2 : h_2$. In this way, h_i and l_i are not altered, so the bounds (9.4) still hold.

Step 2.3. Now we come to the main part of the regularisation procedure, i.e., Proposition 8.6. In its proof, we apply an iterative procedure, and at every step one of the following changes happens:

- (a) $h_2 \rightarrow h_2 + 1, l_2 \rightarrow l_2 - 1, h_3 \rightarrow h_3 - 1, l_3 \rightarrow l_3 + 1, h_1 \rightarrow h_1, l_1 \rightarrow l_1$ or
- (b) $h_2 \rightarrow h_2 + 1, l_2 \rightarrow l_2 - 1, h_1 \rightarrow h_1 - 1, l_1 \rightarrow l_1 + 1, h_3 \rightarrow h_3, l_3 \rightarrow l_3$.

Notice that in both cases l_1 and l_3 cannot decrease during this procedure, and exactly one of them increases at every step. The procedure can end in two ways: $h_3 = 0$ (or equivalently $h_1 = 0$) or $l_2 = 1$. In the latter case, however, the proof of Proposition 8.7 implies that the original configuration was not optimal, so we only need to examine the former case.

Consider the last step of the regularisation procedure in the proof of Proposition 8.6, i.e., the one before we reach $h_3 = 0$. Denote by \hat{h}_1 the value of h_1 at the end of the regularisation procedure, and note that $\hat{h}_1 \leq 2 + \frac{1}{\beta}$ by (9.4). There are two possible situations: either

$$\hat{l}_1 \leq 2\hat{h}_1 \quad \text{or} \quad \hat{l}_1 > 2\hat{h}_1.$$

In the second case, notice that we cannot have applied the construction from case (a) twice as otherwise a slightly modified procedure would give the following: we move the A -points from the rightmost two columns of the rectangle $l_2 : h_1$ to the rectangle $l_1 : h_3$, but we place them in a single row. In this way, we have

$$h_2 \rightarrow h_2 + 1, \quad l_2 \rightarrow l_2 - 2, \quad h_3 \rightarrow h_3 - 1, \quad l_3 \rightarrow l_3 + 2, \quad h_1 \rightarrow h_1, \quad l_1 \rightarrow l_1.$$

This shows that the energy (6.5) strictly decreases as the length of the interface is decreased. Hence, the original configuration was not optimal, so either $\hat{l}_1 \leq 2\hat{h}_1$ or we have applied a step of type (a) at most once.

Similarly, since \hat{h}_3 at the end of the procedure equals zero, we consider the alternative

$$\hat{l}_3 \leq 2 \quad \text{or} \quad \hat{l}_3 > 2.$$

We apply a similar argument to conclude that either $\hat{l}_3 \leq 2$ or that we have applied a step of type (b) at most once.

In view of (9.4), and because l_1 and l_3 can only increase during the regularisation procedure, we see that $l_1 \leq 2\hat{h}_1$ and $l_3 \leq 2$ lead to contradictions for N sufficiently large depending only on β . This implies that there can be at most one step of types (a) and (b), respectively. Therefore, using again (9.4), we see that before the application of Proposition 8.6 it holds that

$$l_2 \leq 6, \quad h_1 \leq 4 + \frac{1}{\beta}, \quad h_3 \leq 2, \quad h_2 \sim \bar{h}, \quad l_1, l_3 \sim \sqrt{N/\bar{h}}. \quad (9.5)$$

Step 2.4. Finally, we consider the modification in Lemma 8.5. For simplicity, we only address the modification leading to $\min\{h_1, h_1 + h_2 - l_1 - l_2\} \leq 0$. Note that each step of the procedure consists in $h_1 \rightarrow h_1 - 1$ and $l_1 \rightarrow l_1 + 1$. As after the application of

Lemma 8.5, we have $\hat{h}_2/\hat{l}_1 \geq 2/(2 - \beta) + O(1/\sqrt{N})$, see (9.5), and during its application h_2 does not change and l_1 can only increase, at each step of the procedure, it holds that $h_2/l_1 \geq 2/(2 - \beta) + O(1/\sqrt{N})$. In view of (9.5), in particular the fact that $l_2 \leq 6$, for N sufficiently large depending only on β , we have

$$(h_1 + h_2)/(l_1 + l_2) \geq h_2/(l_1 + l_2) \geq c_\beta \tag{9.6}$$

at each step of the procedure, for some constant $c_\beta > 1$ only depending on β . This ensures that at the beginning we have $h_1 \leq M$ for $M \in \mathbb{N}$ such that $(M + 1)/M < c_\beta$ since otherwise $M + 1$ rows could be moved to M columns leading to a strictly smaller energy. This along with (9.5) shows that at most $C_\beta N^{1/2}$ are moved. Moreover, the modifications stop once $h_1 = 0$ or $h_1 + h_2 \leq l_1 + l_2$ has been obtained. By (9.6), we see that it necessarily holds $h_1 = 0$. In a similar fashion, one gets $h_3 = 0$. This shows that, directly after the application of Lemma 8.5, we obtain a configuration in Class \mathcal{I} . This concludes the proof as we have seen that in the modification of Lemma 8.5 only $C_\beta N^{1/2}$ points are moved.

Step 3: Class \mathcal{V} . We now consider an optimal configuration in Class \mathcal{V} and show that it can be modified to a configuration in Class $\mathcal{I}\mathcal{V}$ such that (9.1) holds. The modification in Proposition 8.14 consists in moving at most h_1 rows to the left. By Step 2, we know that $h_1 \leq C_\beta$ which implies that we have moved at most $C_\beta N^{1/2}$ many points. This concludes the proof of Step 3. ■

Let us highlight that in the proof of Theorem 9.1 we have not only shown the $N^{1/2}$ -law and $N^{3/4}$ -law for minimisers, but we also get explicit estimates on the shape of the configuration, written as a separate statement here below. The following corollary is a consequence of equations (9.5), (9.6), and the procedure from Step 3 of the proof of Theorem 9.1.

Corollary 9.2. *Suppose that $(A, B) \in \mathcal{I}\mathcal{V} \cup \mathcal{V}$ is an optimal configuration. Then,*

$$l_2, h_1, h_3 \leq C_\beta, \quad h_2 \sim \bar{h}, \quad l_1, l_3 \sim \sqrt{N/\bar{h}},$$

where \bar{h} is a minimiser of (1.3).

Recall that for $\beta \in \mathbb{R} \setminus \mathbb{Q}$ the minimiser \bar{h} is unique. Thus, in this case, the quantitative bound given in Theorem 9.1 is sharp, the optimal configuration in Class $\mathcal{I}\mathcal{V}$ given by Proposition 8.16 differs from the one given in Theorem 1.1 (v) by a number of points of exactly this order. In the case $\beta \in \mathbb{Q}$, the $N^{3/4}$ -law can again be checked to be sharp. This will be addressed in a forthcoming paper.

10. Proofs in the continuum setting

We conclude by providing the proofs of Corollaries 1.2 and 1.3 from the Introduction.

Proof of Corollary 1.2. For the explicit solution (A'_N, B'_N) in Theorem 1.1 (v) with $N_A = N_B =: N$, one can directly verify that $\mu_{A'_N} \xrightarrow{*} \mathcal{L} \llcorner \mathcal{A}$ and $\mu_{B'_N} \xrightarrow{*} \mathcal{L} \llcorner \mathcal{B}$, where \mathcal{A} and \mathcal{B} are given in (1.5). For a general sequence of solutions (A_N, B_N) of (1.1), the statement follows from the fluctuation estimate in Theorem 1.1 (vi). ■

Proof of Corollary 1.3. We start by relating point configurations with sets of finite perimeter: given (A_N, B_N) with $N_A = N_B =: N$, we define the sets

$$\begin{aligned} A^N &:= \frac{1}{\sqrt{N}} \operatorname{int} \left(\bigcup_{p \in A_N} p + \left[-\frac{1}{2}, \frac{1}{2} \right]^2 \right), \\ B^N &:= \frac{1}{\sqrt{N}} \operatorname{int} \left(\bigcup_{p \in B_N} p + \left[-\frac{1}{2}, \frac{1}{2} \right]^2 \right). \end{aligned} \quad (10.1)$$

Clearly, A^N and B^N satisfy

$$A^N \cap B^N = \emptyset \quad \text{and} \quad \mathcal{L}(A^N) = \mathcal{L}(B^N) = 1.$$

It is an elementary matter to check that (1.1) and (1.6) coincide in this case up to normalisation, i.e.,

$$\begin{aligned} N^{-1/2} P(A_N, B_N) &= P_{\operatorname{cont}}(A^N, B^N) \\ &:= \operatorname{Per}(A^N) + \operatorname{Per}(B^N) - 2\beta \mathcal{L}(\partial^* A^N \cap \partial^* B^N). \end{aligned} \quad (10.2)$$

Now, consider any pair of sets of finite perimeter with

$$A \cap B = \emptyset \quad \text{and} \quad \mathcal{L}(A) = \mathcal{L}(B) = 1.$$

Given $\varepsilon > 0$, by the density result [10, Theorem 2.1 and Corollary 2.4] (for \mathcal{Z} consisting of three values representing A , B , and the empty set) we can find A' and B' with polygonal boundary such that

$$A' \cap B' = \emptyset, \quad \mathcal{L}(A') = \mathcal{L}(B') = 1$$

and

$$P_{\operatorname{cont}}(A', B') \leq P_{\operatorname{cont}}(A, B) + \varepsilon.$$

(Strictly speaking, the constraint $\mathcal{L}(A') = \mathcal{L}(B') = 1$ has not been addressed there. However, possibly after scaling, one can assume that $\mathcal{L}(A') \leq 1$, $\mathcal{L}(B') \leq 1$, and then it suffices to add a disjoint squares of small volume and surface to satisfy the constraint.) We define a point configuration related to A' and B' by setting

$$\begin{aligned} A_N &= \{p \in \mathbb{Z}^2: p/\sqrt{N} \in A'\}, \\ B_N &= \{p \in \mathbb{Z}^2: p/\sqrt{N} \in B'\}. \end{aligned}$$

By A^N and B^N we denote the corresponding sets of finite perimeter defined in (10.1). Note that the sets A^N and B^N may have different cardinalities, although $\mathcal{L}(A') = \mathcal{L}(B') = 1$. Still, equal cardinalities can be restored by adding points to one of the two sets. This can be achieved at the price of making a small error in the perimeter, which goes to 0 with N after rescaling. The fact that (A', B') have polygonal boundary along with the properties of $\|\cdot\|_1$ implies that

$$\lim_{N \rightarrow \infty} P_{\text{cont}}(A^N, B^N) = P_{\text{cont}}(A', B').$$

In fact, each segment of the polygonal boundary of (A', B') is approximated by a path consisting of horizontal and vertical segments which is contained in the boundary of the squares forming (A^N, B^N) , see (10.1). The l^1 -norm of the segment and of the path coincide, up to an error of order $\frac{1}{\sqrt{N}}$. This along with (10.2) and Theorem 1.1 (iv) yields

$$\begin{aligned} P_{\text{cont}}(A, B) &\geq \liminf_{N \rightarrow \infty} P_{\text{cont}}(A^N, B^N) - \varepsilon \\ &\geq \liminf_{N \rightarrow \infty} N^{-1/2} \min_{h \in \mathbb{N}} (4\lceil N/h \rceil + 2h(2 - \beta)) - \varepsilon \\ &= \liminf_{N \rightarrow \infty} \min_{h \in \mathbb{N}} \left(4\sqrt{N}/h + 2\frac{h}{\sqrt{N}}(2 - \beta) \right) - \varepsilon. \end{aligned}$$

Optimisation with respect to h yields

$$P_{\text{cont}}(A, B) \geq 4\frac{1}{\sqrt{\frac{2}{2-\beta}}} + 2\sqrt{\frac{2}{2-\beta}}(2 - \beta) - \varepsilon = 4\sqrt{2}\sqrt{2-\beta} - \varepsilon.$$

We directly compute $P_{\text{cont}}(\mathcal{A}, \mathcal{B}) = 4\sqrt{2}\sqrt{2-\beta}$. As $\varepsilon > 0$ is arbitrary, we conclude that the pair $(\mathcal{A}, \mathcal{B})$ is a solution of (1.6). ■

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Manuel Friedrich

Department of Mathematics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Cauerstraße 1, 91058 Erlangen, Germany; manuel.friedrich@uni-muenster.de

Wojciech Górny

Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Banacha 2, 02-097 Warsaw, Poland; Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria; wojciech.gorny@univie.ac.at

Ulisse Stefanelli

Faculty of Mathematics, University of Vienna, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria; Vienna Research Platform on Accelerating Photoreaction Discovery, University of Vienna, Währingerstraße 17, 1090 Vienna, Austria; Istituto di Matematica Applicata e Tecnologie Informatiche *E. Magenes*, via Ferrata 1, 27100 Pavia, Italy; ulisse.stefanelli@univie.ac.at