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Ph.D. Thesis

Some asymptotic results on the global shape of planar clusters

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Abstract

In this thesis we analyze the problem of the global shape of perimeter-minimizing planar N-clusters, which represent a model for soap bubbles. A planar N-cluster is a collection $\mathscr{E}_N = (\mathscr{E}_N(1), \ldots, \mathscr{E}_N(N))$ of disjoint finite perimeter sets in $\mathbb{R}^2$ with unit area, called *bubbles* or *chambers* (to which we add for convenience the *exterior chamber* $\mathscr{E}(0) = \mathbb{R}^2 \setminus \bigcup_{i=1}^N \mathscr{E}(i)$), and its perimeter is given by

$$P(\mathscr{E}_N) = \frac{1}{2}\sum_{i=0}^{N} P(\mathscr{E}(i)).$$

The problem of understanding the asymptotic global (or outer) shape of minimizing N-clusters as $N \to \infty$ has been considered by various authors [CG03], [HM05], [CMG13].

We prove under some assumptions that the asymptotic global shape of the rescaled minimal clusters

$$E_\infty := \lim_{N\to\infty} \frac{1}{\sqrt{N}}\mathscr{E}(0)^c$$

exists as a finite perimeter set, and we prove the mild regularity result that the set of zero Lebesgue density $E_\infty^{(0)}$ is an open set. Moreover the asymptotic perimeter density is that of a hexagonal lattice, up to lower order terms.

We then consider some variants of this problem:

- *Anisotropic perimeter.* If we consider an anisotropic perimeter with cubic Wulff shape then the asymptotic global shape is itself a cube in any dimension, with a precise rate of convergence that is given by the quantitative anisotropic isoperimetric inequality [FMP10].

- *Fixed shape of chambers.* If we require all chambers to be squares (respectively hexagons) then again the global shape is a square (respectively hexagon). In both cases the rate of convergence to the global shape coincides with the $N^{3/4}$ law already proven for crystallized configurations of particles in either the square or the triangular lattice [Sch13], [DPS17]. This is proved again thanks to the quantitative isoperimetric inequality, which gives also an alternative way of proving the above cited $N^{3/4}$ law for crystallized particles .

- *Weighted clusters.* We put different weights at different interfaces and prove that in a suitable "repulsive" asymptotic regime minimizers converge to configurations of disjoint disks that maximize the number of tangencies among them. In other words, the weighted perimeter functionals Γ-converge to the sticky-disk problem. This suggests that for certain choices of weights the global shape of minimizing clusters should be close to a hexagon.

We then estimate the perimeter of the hexagonal honeycomb $\mathscr{H}$ contained in a disk of radius r proving the remainder estimate $P(\mathscr{H}, B_r) - \sqrt[4]{12}\pi r^2 = \mathscr{O}(r^{2/3})$ (observe that the remainder term is smaller than the trivial "surface" term $\mathscr{O}(r)$) and proving an analogue result for any periodic measure in $\mathbb{R}^n$.

Finally we consider the *interface problem* where we ask what is the optimal way to fill the region contained between two honeycombs whose orientations differ by an angle θ, proving that some defects must appear and proving that, as the size of the chambers goes to zero, we can extract a "limit *BV* orientation" that describes the asymptotic orientation of the hexagonal chambers.

Contents

Introduction

Many physical systems at rest exhibit a regular structure of some kind when there is a large number of elements involved. Among these systems we can cite: particles interacting via some kind of repulsive-attractive potential; soap bubbles forming foams; crystalline structures in materials.

The aim of this thesis is to study some of these pattern occurrences with a particular focus on the case of perimeter-minimizing planar clusters (which represent a model for soap bubbles) but also to highlight the interplay of this model with the other aforementioned physical systems.

One of the most famous results on this topic is the proof of the *honeycomb conjecture* by T.C. Hales [Hal01]: the optimal partition of the plane in equal-area cells (bubbles) that minimizes perimeter is given by the hexagonal honeycomb. Of course we have to specify what we mean by perimeter-minimizing since the perimeter of an equal-area partition of the plane is infinite. For instance given any partition $\mathscr{E} = (\mathscr{E}(1), \mathscr{E}(2), \dots)$ of $\mathbb{R}^2$ we can define its asymptotic perimeter density as

$$\rho(\mathscr{E}) := \limsup_{r \to \infty} \frac{P(\mathscr{E}, B_r)}{\pi r^2}$$

where

$$P(\mathscr{E}, B_r) := \frac{1}{2} \sum_i \mathrm{length}(\partial \mathscr{E}(i) \cap B_r)$$

is the perimeter of $\mathscr{E}$ contained in a disk of radius r. Then the honeycomb conjecture amounts to say that for any partition $\mathscr{E}$ with $Area(\mathscr{E}(i)) = 1$ we have

$$\rho(\mathscr{E}) \geq \rho(\mathscr{H}) = \sqrt[4]{12}$$

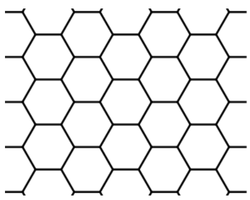


Figure 1: A portion of the honeycomb $\mathscr{H}$.

where $\mathscr{H}$ is the hexagonal honeycomb with unit areas (see Figure 1).

Hales proved that even if we consider a finite number N of bubbles we still can not beat the average perimeter-to-area ratio of $\sqrt[4]{12}$: for any given *N-cluster* $\mathscr{E}_N = (\mathscr{E}_N(1), \dots, \mathscr{E}_N(N))$ (also called *N-bubble*) of sets with pairwise disjoint interiors with $Area(\mathscr{E}_N(i)) = 1$ we have

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}N \tag{1}$$

where

$$P(\mathscr{E}_N) := \frac{1}{2}\sum_{i=0}^{N} \text{length}(\partial \mathscr{E}_N(i))$$

and where we have introduced for convenience the exterior chamber

$$\mathscr{E}_N(0) := \mathbb{R}^2 \setminus \bigcup_{i=1}^{N} \mathscr{E}_N(i).$$

The case of a finite number of bubbles presents however a non trivial effect of the outer boundary on the shape of minimizing configurations: while a hexagonal interior structure is expected by the honeycomb conjecture, the outer layer of bubbles tends to be rounder to minimize the outer unshared perimeter (see Figure 2) and therefore there is a competition between the six-fold symmetry of the honeycomb and the isoperimetric inequality which would yield a round outer shape. The understanding of what is the optimal outer shape when $N \to \infty$ was considered by various authors [CG03], [HM05], [CMG13] and is the main question that initiated the various topics discussed in the present thesis. We highlight it here:

Question 1. *What is the asymptotic outer shape of equal-area perimeter-minimizing planar N-clusters when $N \to \infty$?*

In order to have a meaningful result we have to rescale the clusters so that their total area remains fixed, and in particular given an N-cluster with unit areas we define its *global shape* as

$$E_N := \frac{1}{\sqrt{N}} \bigcup_{i=1}^{N} \mathscr{E}_N(i)$$

and then we ask if the limit

$$E_\infty = \lim_{N \to \infty} E_N$$

exists in a suitable sense (up to subsequence and rigid motions) when $\mathscr{E}_N$ are minimizing N-clusters for the given unit-area constraint.

Another related problem is considering optimal *partitions* of a given open set $\Omega \subset \mathbb{R}^2$: minimize $P(\mathscr{E}_N)$ among all N-clusters with areas $\frac{|\Omega|}{N}$ such that

$$\Omega = \bigcup_{i=1}^{N} \mathscr{E}(i).$$

In this case the outer shape is fixed and the focus is on the creation of hexagonal patterns in the interior of the configuration.

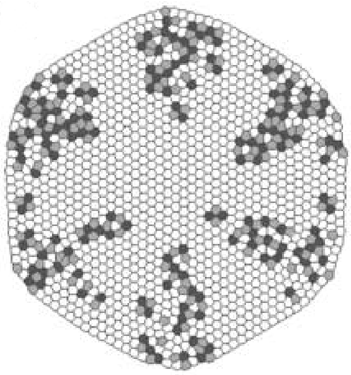


Figure 2: An example of N-bubble with $N = 1261$, taken from [CG03]. A regularity result [Mor94] assures that in a minimizing cluster the boundary of the bubbles is made of a finite number of segments and circular arcs. The different grey scale indicates the number of sides of the bubble, and more precisely the discrepancy between the expected number of sides (6 for interior bubbles, 5 for boundary bubbles) and the actual one. As the number of bubbles goes to infinity we want to understand what is the asymptotic outer shape of equal-areas minimizing clusters.

Question 2. *Both in the case of N-clusters and N-partitions can we define a notion of "orientation" of the underlying hexagonal pattern? Can we prove a compactness result about these orientations for minimizing configurations when $N \to \infty$?*

The basic existence and regularity result for perimeter-minimizing planar clusters is the following [Mor94]: for any given choice of positive numbers $m_1, \dots, m_N$ the area-constrained minimization problem

$$\min\{P(\mathscr{E}_N) : \mathscr{E}_N \text{ is an } N\text{-cluster with } Area(\mathscr{E}_N(i)) = m_i\}$$

admits a solution. Moreover each chamber of a minimizer is equivalent to a (possibly disconnected) open set whose boundary is composed by a finite number of circular arcs or straight segments; these arcs meet in triple points forming equal angles of 120 degrees.

We now briefly summarize the content of the thesis, referring to each individual chapter for a detailed explanation.

Existence of the global shape (Chapter 3)

The first step to confront Question 1 is proving the existence in a suitable sense of a limit global shape. This will be the goal of Chapter 3. We will see that, under some assumptions, the limit shape exists as a finite perimeter set. In particular we apply a standard compactness result for finite perimeter sets (see Theorem 1.2) which is based on proving the following equiboundedness property for unit-areas perimeter-minimizing N-clusters $\bar{\mathscr{E}}_N$:

$$\sup_{N\in\mathbb{N}} P(\bar{E}_N) < +\infty$$

where $\bar{E}_N$ is the global shape defined above. This estimate, in terms of the original non-rescaled clusters $\bar{\mathscr{E}}_N$, is equivalent to

$$P(\bar{\mathscr{E}}_N(0)) \leq C\sqrt{N}$$

for a constant C. We underline that this task is non-trivial due to the bulk scaling of the total perimeter: while for unit-areas minimal N-clusters the total perimeter $P(\bar{\mathscr{E}}_N)$ (the quantity to be minimized) goes like N as $N \to \infty$, the estimate that we want to obtain concerns a quantity (the *outer* perimeter) which is of a lower order, $\sqrt{N}$.

The above estimate is an immediate consequence of the following two results:

- an upper bound (Lemma 3.7) for minimizing configurations

  $$P(\bar{\mathscr{E}}_N) \leq \sqrt[4]{12}N + C\sqrt{N}$$

  obtained by constructing a simple competitor with unit-area hexagons placed in a spiral configuration (but any reasonable "not too squeezed" configuration would suffice);

- a lower bound (Lemma 3.6) that holds for any unit-areas N-cluster:

  $$P(\mathscr{E}_N) \geq \sqrt[4]{12}N + cP(\mathscr{E}_N(0))$$

  for a constant $c > 0$. Observe that this is a refinement of the honeycomb inequality (1) which takes into accout also the outer perimeter.

The proof of the lower bound estimate relies on an isoperimetric inequality for curvilinear polygons, which we call *Hales inequality*, and which is the key tool employed in [Hal01] to prove the honeycomb conjecture. To obtain the final result however we have to require that the area of each component of each chamber in a minimizing N-cluster satisfies a lower bound that depends on the number of curvilinear sides which compose its boundary, see (3.5). This assumption is satisfied if for instance we know that each chamber is connected (which however is not known in general and is an open problem) or if we consider a different setting where, roughly speaking, if a chamber has many connected components we still count an infinitesimally thin interface that connects them (that is we view each chamber not as a finite perimeter set but as the area enclosed by a closed rectifiable curve, whose length gives the perimeter). We could avoid this additional assumption if we knew that a slightly better Hales inequality holds. We refer to Section 3.3 for a discussion on this topic.

After having established existence of the limit global shape E_∞ we prove a weak regularity result: the measure-theoretic exterior $E_\infty^{(0)}$, that is the set of points of Lebesgue density zero, is an open set (Theorem 3.15).

Finally we prove the equipartition of the asymptotic energy density (Theorem 3.17): consider minimal N-clusters $\bar{\mathscr{E}}_N$ whose global shape converge to E_∞, and define the measures $\nu_N := \frac{1}{\sqrt{N}}\mathscr{H}^1 \llcorner \partial\bar{\mathscr{E}}_N$, that is the 1-dimensional Hausdorff measures restricted to the interfaces between bubbles, suitably rescaled to have bounded mass. Then ν_N weakly converge to the uniform Lebesgue measure on E_∞ with density $\sqrt[4]{12}$:

$$\nu_N \overset{*}{\rightharpoonup} \sqrt[4]{12}\mathscr{L}^2 \llcorner E_\infty \quad \text{as } N \to \infty.$$

This result tells us that the interior structure of minimal N-clusters when N is big is close, at least energetically speaking, to a regular honeycomb.

We actually prove these last results in a slighlty different setting where we impose a relaxed constraint on the chambers: given a parameter $\varepsilon > 0$ we fix the total area of the cluster $\mathscr{E}$ to be 1 and we require $Area(\mathscr{E}(i)) \leq \varepsilon^2$ for every i, then send $\varepsilon \to 0$.

Weighted clusters (Chapter 2)

A variant of the problem of perimeter-minimizing N-clusters is given by computing the perimeter with different weigths at different interfaces. This problem is often referred to as the *immiscible fluids* problem. In particular given a cluster $\mathscr{E} = (\mathscr{E}(1), \dots, \mathscr{E}(N))$ and given some non-negative weights c_{ij} we consider the following weighted perimeter

$$P(\mathscr{E}) := \sum_{i=0}^{N} c_{ij} \, \text{length}(\partial\mathscr{E}(i) \cap \partial\mathscr{E}(j))$$

which counts the interface between bubbles $\mathscr{E}(i)$ and $\mathscr{E}(j)$ with weight c_{ij} and represents different surface tensions between different fluids.

In Chapter 2 we analyze a special case where the weights depend on a small parameter $\varepsilon > 0$, which is then sent to zero. Specifically we consider

$$P_\varepsilon(\mathscr{E}) := \sum_{i=0}^{N} c_{ij}(\varepsilon) \, \text{length}(\partial\mathscr{E}(i) \cap \partial\mathscr{E}(j)) \qquad c_{ij}(\varepsilon) = \begin{cases} 2 - \varepsilon & \text{if } i, j \neq 0 \\ 1 & \text{if } i = 0 \text{ or } j = 0 \end{cases}$$

which amounts to say that interfaces between different bubbles are given almost twice the weight given to the interfaces between a bubble and the exterior. We explain this choice: if we put weight 2 instead of $2 - \varepsilon$ then the problem splits into N separate isoperimetric problems, since it amounts to minimize

$$\sum_{i=1}^{N} P(\mathscr{E}(i))$$

which is minimized by any configuration of disjoint disks. If instead we put the slightly lower weight $2 - \varepsilon$ the effect is that the bubbles tend to “repel” each other but have still interest in sharing tiny portions of their boundary (see Figure 3).

We are then interested in the following asymptotic behaviour: instead of sending the number of bubbles to infinity we fix their number N and fix an area constraint and we ask what happens to P_ε-minimizing N-bubbles $\overline{\mathscr{E}_\varepsilon} = (\overline{\mathscr{E}_\varepsilon}(1), \dots \overline{\mathscr{E}_\varepsilon}(N))$ when $\varepsilon \to 0$. A first simple consequence of the isoperimetric inequality is that each bubble converges to a disk, and in the limit we only see configurations of disks with pairwise disjoint interiors. We expect however to see in the limit $\varepsilon \to 0$ only certain configurations of disks, and indeed the following is the main result of the chapter (see Theorem 2.2):

Theorem (Sticky-disk limit). *As $\varepsilon \to 0$ minimizers $\overline{\mathscr{E}_\varepsilon}$ of P_ε converge up to subsequence and rigid motions to a cluster of disks that maximizes the number of contact points among the disks, each contact point counted with factor $\frac{r_i r_j}{r_i + r_j}$, where r_i, r_j are the radii of the touching disks.*

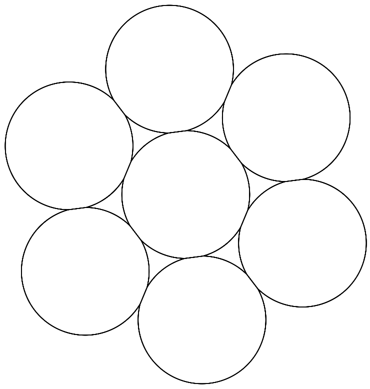


Figure 3: A numerical candidate for being a minimizer of the weighted perimeter P_ε when $\varepsilon = 0.02$, for $N = 7$ bubbles with equal area. This competitor was obtained by means of the Surface Evolver developed by Ken Brakke [Bra92].

The proof of the above theorem relies on a quantitative-type isoperimetric inequality involving the curvature of the boundary (Theorem 2.14), which can be seen as a sort of Taylor expansion of the perimeter functional with base point the disk. In the same way Hales inequality (3.6) can be seen as a Taylor expansion of the perimeter with base point the hexagon, and it would be interesting to understand more deeply the relation between the two and whether they are an instance of a more general Taylor-type expansion of the perimeter.

The name "sticky-disk" comes from the following fact: if the radii of the disks are equal (say $\frac{1}{2}$) then maximizing the number of their contact points is equivalent to minimizing the energy

$$E(X_N) = \sum_{1\le i<j\le N} V(|x_i - x_j|)$$

among configurations $X_N = \{x_1, \dots, x_N\}$ of N points in $\mathbb{R}^2$, where

$$V(r) = \begin{cases} +\infty & \text{if } 0 \le r < 1 \\ -1 & \text{if } r = 1 \\ 0 & \text{if } r > 1 \end{cases}$$

is the so-called *sticky-disk* or *Heitmann-Radin* potential. We know that minimizers of the sticky-disk are *crystallized* [HR80], that is they form a subset of the triangular lattice, and as $N \to \infty$ the global shape of minimal configurations converges to a hexagon [AYFS12], [Sch13], [DPS16], see also Section 4.1. This is a hint that, for a fixed but small ε, minimizers of P_ε could have an almost-hexagonal limit global shape as $N \to \infty$ (see Section 3.6).

In proving the theorem above we also obtain some information on the structure of P_ε-minimizing clusters for small ε (Theorem 2.7). We then discuss the extension of the above theorem to higher dimensions.

Variants on the global shape problem (Chapter 4)

We consider some variants on the asymptotic global shape problem, where we impose some constraint on the chambers or consider special perimeters.

In the first we consider N-clusters whose chambers are *regular* hexagons of unit area. We prove that minimizers are crystallized, that is they can be realized as a subset of the honeycomb $\mathscr{H}$, and as a consequence of [AYFS12], [DPS16] we obtain a hexagonal asymptotic global shape.

Then we consider anisotropic clusters, in particular with a cubic anisotropy, where to compute the perimeter of each chamber we take into consideration the direction of its unit normals. Using the quantitative anisotropic isoperimetric inequality [FMP10] we prove that in this case the global shape is a cube, with a precise rate of convergence. In particular in $\mathbb{R}^n$ the global shape of minimizers with N chambers of unit volume differs from a big cube of side $N^{1/n}$ by at most a volume $\approx N^{1-\frac{1}{2n}}$. The same estimate holds for discrete configurations of N points in $\mathbb{Z}^n$ that minimize the edge-perimeter. In particular in dimension 2 we recover the $N^{3/4}$ law [Sch13]. In three dimensions this estimate is not sharp, since the optimal rate is again $N^{3/4}$ [Mai+18], and in higher dimension it is an open question.

Then we look at N-clusters whose chambers are squares of area $\frac{1}{N}$ in the plane, but this time we are interested not only in the asymptotic global shape of minimizers (which is a square) but also on the formation of an interior crystalline structure in low energy configurations: we prove a Γ-convergence result that implies that if we take into account also the orientations of the square chambers then sequences $\mathscr{E}_N$ with low energy, i.e.

$$P(\mathscr{E}_N) \leq 4\sqrt{N} + C$$

converge in a suitable sense, up to subsequence and rigid motions (and up to a confinement assumption), to a *polycrystal* with square Wulff shape.

More precisely, the first step is defining in a suitable way what we can call an *orientation* for any minimizing N-cluster. In the case where all chambers are squares it is natural to define an orientation as a vectorfield $\theta_N : E_N \to \mathbb{S}^1$ which is constant on every square and is parallel to one of the sides (see Figure 4 for the equally natural case of hexagonal bubbles). To factor out the rotational invariance modulo $\frac{\pi}{2}$ we can decide that the angle that the vectorfield makes with the x axis belongs to $[0, \frac{\pi}{2})$ (counterclockwise). In particular this vectorfield is a piecewise constant *SBV* (*special bounded variation*) function. Then by standard compactness results about *SBV* functions we ensure that there exists a limit vectorfield $\theta_\infty = \lim_{N\to\infty} \theta_N$ which is still an *SBV* vectorfield, with values in $\mathbb{S}^1$, which is constant on each set of a (countable) partition of $\mathbb{R}^2$ in sets of finite perimeter. This limit vectorfield describes what is the asymptotic infinitesimal orientation of the underlying square lattice.

The second step is to obtain a variational problem for the limit vectorfields obtained in the first step, that is to compute the Γ-limit. This is in general a more delicate issue, but in the case of square chambers we can exactly compute it: we obtain a model for polycrystals with square anisotropy. If we write the

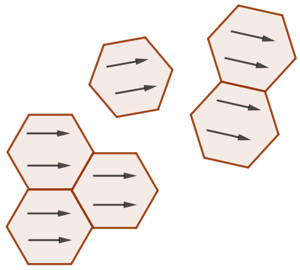


Figure 4: An example of the orientation vectorfield ϕ in the case of hexagonal bubbles: constant on each hexagon and parlallel to one side.

limit vectorfield as

$$\theta_\infty = \sum_{i=1}^{\infty} \theta_\infty^i \mathbb{1}_{C_i}$$

then the limit functional is

$$\sum_{i=1}^{\infty} P_{\theta_\infty^i}(C_i)$$

where $P_{\theta_\infty^i}(C_i)$ is the anisotropic square perimeter of C_i rotated in direction θ_∞^i.

A similar compactness result (i.e. in the limit we obtain a countable collection of sets and orientations) holds also for hexagonal chambers.

Finally we consider the sticky-disk model, where we expect again a triangular pattern to appear in low energy configurations. We define a notion of orientation that describes the underlying triangular pattern and exploting the above cited compactness result for hexagonal chambers we prove an analogous compactness result for low energy configurations of the sticky-disk as $N \to \infty$. Again in the limit we obtain a polycrystal, but again we can not compute the exact Γ-limit. In [DLNP18] the authors prove an analogous compactness result and give some estimates on the Γ-limit.

Mass distribution of periodic measures (Chapter 5)

A natural question regarding the honeycomb partition $\mathscr{H}$ of the plane is the following: can we estimate the perimeter contained in a disk of radius r when $r \to \infty$? The leading term is easily obtainable and more precisely we have

$$P(\mathscr{H}, B_r) = \sqrt[4]{12}\pi r^2 + o(r^2).$$

The goal is to find estimates for the remainder term

$$\Delta(r) := P(\mathscr{H}, B_r) - \sqrt[4]{12}\pi r^2.$$

More generally we can consider a lattice $\Lambda = A\mathbb{Z}^n$ for some invertible linear transformation A and a Λ-periodic measure μ: we start from a measure μ_0 on the fundamental cell $Q = A([0,1)^n)$, consider the

Λ-periodized measure

$$\mu := \sum_{k \in \Lambda} (\tau_k)_{\#}\mu_0$$

obtained by summing the pushforward through all the translations by a vector in the lattice Λ and estimate the remainder term

$$\Delta_\mu(r) := \mu(B_r) - \|\mu_0\||B_r|$$

where $\|\mu_0\| := \mu_0(Q)/|Q|$ and $|\cdot|$ denotes the Lebesgue measure. We will show that

$$\Delta_\mu(r) = \|\mu_0\|\mathscr{O}(r^{(n-1)\frac{n}{n+1}})$$

by adapting the proof by C.S. Herz [Her62b] for the Gauss Circle Problem (counting the number of lattice points of $\mathbb{Z}^n$ contained in B_r) which can be seen as a particular case of the above setting with $\mu_0 = \delta_0$. In particular the estimate is smaller than a "surface" term $\mathscr{O}(r^{n-1})$ that one could naively expect, and in the planar case coincides with $\mathscr{O}(r^{2/3})$.

Interface problem (Chapter 6)

In order to describe the asymptotic behaviour of both N-clusters and N-partitions we would like to prove a Γ-convergence result, of which we now give a rough outline. This outline actually works in the simplified case considered in Chapter 4 (square chambers) but the general Γ-convergence for clusters is out of reach for now, and that's why we will focus on an intermediate problem. We consider for simplicity the case of polygonal partitions, that is when all chambers are polygons.

The ideal Γ-convergence result follows these steps:

- *Defining an orientation.* The first step is to define a suitable notion of orientation that describes the direction of the hexagonal chambers, which by the honeycomb inequality constitute the majority. We can imagine for instance a vectorfield $\phi_N : E_N \to \mathbb{S}^1$ defined on

$$E_N = \frac{1}{\sqrt{N}} \bigcup_{i=1}^{N} \mathscr{E}_N(i)$$

  which is ideally parallel to the sides of the hexagons.

- *Compactness of orientations.* The second step is obtaining a compactness result for the orientations ϕ_N of minimizing clusters. A likely situation (that occurs in the case of square chambers) is compactness in SBV: we thus obtain a limit vectorfield $\phi_\infty = \lim_{N\to\infty} \phi_N$ which describes locally the asymptotic direction of the underlying honeycomb.

- Γ*-convergence.* The final step is obtaining a limit functional defined on the limit vectorfields obtained in the previous step. Such a limit functional would have to take into account the energy

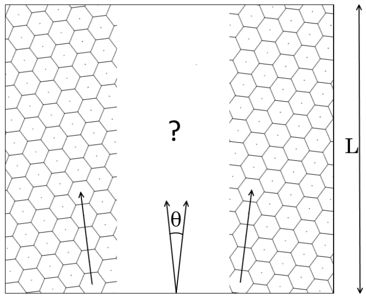


Figure 5: The *interface problem*: what is the optimal way of filling the middle region with chambers of area $\frac{|\Omega|}{N}$ in order to minimize the total perimeter? Do we have to insert non-hexagonal chambers? What is the energy excess with respect to the honeycomb?

of passing from one orientation to another and the effect of the boundary, and could roughly have the following simplified form:

$$F(\phi) = \int_{\Omega} \psi(D\phi(x))dx + \int_{\partial\Omega} b(\phi(x), \nu_{\Omega}(x))d\mathscr{H}^1(x)$$

where $D\phi$ is the distributional gradient of ϕ. $b(\cdot,\cdot)$ measures the effect on the energy of having a specific orientation near the boundary $\partial\Omega$, while ψ measures the effect of changing orientation.

An intermediate problem in the series of steps above is what we can call a *cell problem*: localize the problem in a square and study minimal configurations with some fixed "boundary conditions". A particular case that we consider in this chapter is the following:

- *Interface problem* (also *grain boundary problem*). We fix a square Ω of side L, fix an angle θ and consider all N-partitions of Ω that on two lateral zones of the square coincide with two honeycombs whose orientations differ by an angle θ (see Figure 5) and ask what is the optimal way of filling the middle region to minimize the total perimeter.

Hales inequality (1) tells us that optimal configurations should be hexagonal, but the impossibility of filling the middle region with a honeycomb matching both sides makes the problem non-trivial. Also, the possibility of using deformed hexagons or even non-hexagonal chambers, which we generically call *defects*, introduces a competition between elastic and plastic effects and makes the problem much more difficult than the rigid situations considered in Chapter 4 where we use chambers with a fixed shape (square or hexagonal). We therefore have the following questions, with a particular focus on the limit $N \to \infty$:

Question 3. *Do defects (non-hexagonal chambers) necessarily appear at an interface of a minimizing (or low energy) partition? If so, what is their total number in terms of the parameters L, θ and N?*

Question 4. *Can we estimate in terms of L, θ, N the energy excess created at an interface with respect to the ideal hexagonal ground state?*

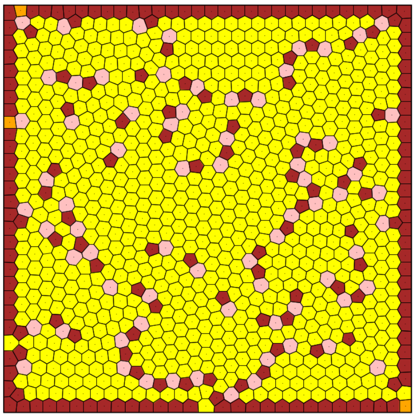


Figure 6: A numerical candidate for a local minimizer of an energy modeling block copolymers considered in [BPT14] and given by a perimeter term of the cells plus a Wasserstein transport term. Zones with hexagonal cells having almost constant orientation are separated by "lines" of defects (pentagonal and heptagonal cells). Observe also that isolated pentagonal or heptagonal defects are rare and are close to some other defect.

An answer to the last question above would give an indication also on which vectorfields ϕ_∞ we have to expect in the limit. Indicating by $\mathscr{E}_N(\theta)$ the energy excess with respect to a honeycomb, a superlinear behaviour in θ

$$\lim_{\theta \to 0} \frac{\mathscr{E}_N(\theta)}{\theta} = \infty$$

would suggest that vectorfields are piecewise constant (that is their gradient $D\phi$ has only a jump part) because a gradual change in the orientation is penalized. This is precisely what we expect, and in particular we expect the following Read-Shockley type law:

$$\mathscr{E}_N(\theta) \geq C\theta|\log\theta|.$$

The reason behind this expectation is twofold: from an experimental viewpoint, a similar behaviour is observed in nature for the energy of grain boundaries, that is the interface between two regular crystalline configurations with mismatching orientations; from a theoretical viewpoint, a similar law has been proved in [LL16] for the energy of a grain boundary in a semidiscrete model for dislocations. Also, as observed above the consequence of a superlinear behaviour in θ is the creation of big regular zones separated by lines of defects, and this can be witnessed in some numerical simulations for energies similar to the perimeter (see Figure 6).

More specifically we expect defects to appear, that is non-hexagonal chambers, because putting a stretched honeycomb (*elastic* competitor) would increase the perimeter by a big amount, much bigger than the amount due to a competitor built extending the two honeycombs on both sides until they almost touch, and filling the middle region with equispaced deformed chambers (*plastic* competitor; see Figure 7).

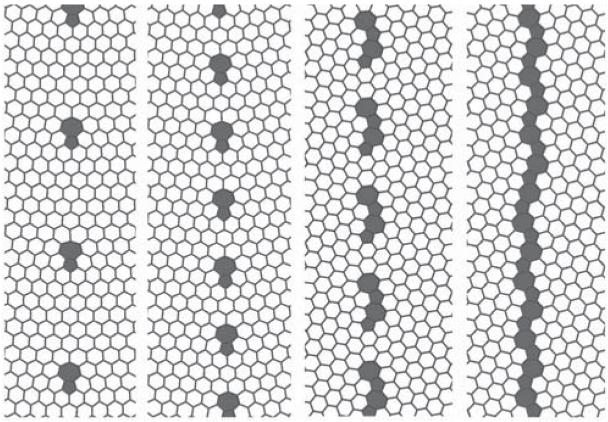


Figure 7: It is expected that between two honeycombs with different orientations some defects (non-hexagonal cells, here greyed out) will appear. Their number (or rather, their number per unit length of the interface) depends on the misorientation angle θ. Figure taken from [Ge+16]

Since the emergence of defects seems to be a common feature of many different mathematical models we decide to remain in a quite abstract framework, which can then be adapted to the specific model under consideration. We therefore start from a graph with triangular faces, that ideally represents our model in a simplified way. For instance:

- for perimeter-minimizing partitions we can consider the dual graph of the given partition, where each chamber represent a vertex and two vertices are connected by an edge if the corresponding chambers share some boundary.

- for particles interacting via a Lennard-Jones type potential with a minimum at 1 (for instance the sticky disk) we can consider the *bond graph* given by all pairs of particles x, x' such that $\big||x-x'|-1\big| < \alpha$ for a certain $\alpha > 0$, and then triangulate it;

In both cases the expected pattern is a triangular lattice. Starting from a graph G we will therefore give a notion of topological defect, that is a face/vertex that constitutes a non-removable type of singularity (i.e. it has degree different from 6), and then gradually we will start introducing more metric notions that take into account the elastic energy given by the deformation of the regular faces.

We stress again that one of the first goals is to attach a notion of orientation, and more precisely this will be a matrix-field $\beta : \Omega(G) \to \mathbb{R}^{2\times 2}$ that locally represents the deformation which each face is subject to, with respect to the ideal situation when the faces are equilateral triangles.

In order to do this we first introduce a parameter $\varepsilon > 0$ that represents the microscopic lengthscale of the system. Then for each triangular face we consider an affine map u that sends the vertices into the vertices of an equilateral triangle of side ε, and define the orientation as $\beta := \nabla u$. Doing this for each face we obtain a global matrix-field β defined on the faces of the graph. Of course β is defined on each face up to rotations, because there is some freedom in the choice of the map u.

We then define an energy $\mathscr{E}_\varepsilon$ on graphs that depends on the parameter $\varepsilon > 0$ and which has the following form:

$$\mathscr{E}_\varepsilon = \frac{1}{\varepsilon}\int_{\Omega(G)} \operatorname{dist}(\beta, SO(2))^2 + \varepsilon \# V_{def}(G) \tag{2}$$

where $\Omega(G)$ is the domain of the graph G (the union of its faces) and $V_{def}(G)$ is the number of defects, that is vertices with degree different from 6. The first term represent an elastic energy that takes into account the deformations of the faces and vanishes if and only if the face is an equilateral triangle of side ε. Notice that the freedom in the definition of β has no influence on the energy. The second term takes into account defects, each of which contributes with a fixed amount ε to the energy. The two different scalings in ε are deduced considering the case of perimeter-minimizing N-partitions where $\varepsilon \approx \frac{1}{\sqrt{N}}$ and where non-hexagonal chambers are considered as defects, and also considering the case of particles interacting through an attractive-repulsive potential (see the subsection *Motivating examples* in Section 6.6).

The essential tool that we use at this point is the Rigidity Theorem by Friesecke, James and Müller [FJM02] and especially the subsequent generalization by Müller, Scardia and Zeppieri [MSZ14]:

Theorem (**Generalized Rigidity Estimate** [MSZ14, Theorem 3.3]). *Let $\Omega \subset \mathbb{R}^2$ be open, bounded, simply connected and Lipschitz. There exists a constant $C = C(\Omega) > 0$ (scaling-invariant) with the following property: for every $\beta \in L^2(\Omega;\mathbb{R}^{2\times 2})$ with $\mu := \operatorname{curl}\beta \in \mathscr{M}_b(\Omega;\mathbb{R}^2)$ there is an associated rotation $R \in SO(2)$ such that*

$$\|\beta - R\|_{L^2(\Omega;\mathbb{R}^{2\times 2})} \le C(\|\operatorname{dist}(\beta, SO(2))\|_{L^2(\Omega)} + \|\operatorname{curl}\beta\|).$$

In order to fruitfully apply the Rigidity Theorem we now have to care about the specific choce of β, because of the presence of the term $\|\operatorname{curl}\beta\|$. We will see that in the absence of “essential defects” in the graph (basically, isolated vertices with degree different from 6, corresponding e.g. to isolated pentagons or heptagons) we are able to construct a matrix-field β whose curl is concentrated around defects and is therefore directly related to the second term of the energy $\mathscr{E}_\varepsilon$ in (2). In this case without essential defects we can then prove the following things:

- Some defects have to appear in the interface problem, and in particular their number is at least of order $\frac{L\theta}{\varepsilon}$.
- The orientations converge strongly in L^2 to a BV limit matrix field, with values in $SO(2)$.
- The energy excess at an interface with mismatch angle θ is at least of order $L\theta$.

The presence of essential defects introduces some difficulties that are currently under study. Moreover we expect a stronger lower bound for the energy: instead of $L\theta$ we expect $L\theta|\log\theta|$. In the last part of the chapter we explain why, and describe the difficulties we encounter in proving such a result.

Chapter 1

Preliminaries

We recall without proof some basic definitions and results about finite perimeter sets, BV functions, N-clusters and Γ-convergence. The main references are Maggi's book [Mag12], the book by Ambrosio, Fusco and Pallara [AFP00] and the book by Braides [Bra02].

Contents

1.1 Measures

Let $\mathscr{F}$ be a σ-algebra on X. $(X,\mathscr{F})$ will be called a measure space. A **measure** μ on $(X,\mathscr{F})$ is a σ-additive map $\mu : \mathscr{F} \to [0,+\infty]$ such that $\mu(\emptyset) = 0$. Given a set $A \in \mathscr{F}$ we denote by $\mu \llcorner A$ the **restriction** of μ to A, that is the measure defined by $\mu \llcorner A(S) := \mu(A \cap S)$. Given a measurable map $f : (X,\mathscr{F}) \to (Y,\mathscr{G})$ between two measure spaces and a measure on $(X,\mathscr{F})$ we denote by $f_\#\mu$ the **pushforward** measure given by $f_\#\mu(A) := \mu(f^{-1}(A))$.

We will consider **Radon measures** on $\mathbb{R}^n$, that is measures μ on the Borel σ-algebra such that $\mu(K) < \infty$ for any compact set K and the regularity properties

$$\mu(A) = \inf\{\mu(U) : U \supset A,\, U \text{ open}\}$$
$$\mu(A) = \sup\{\mu(K) : K \subset A,\, K \text{ compact}\}$$

hold for every Borel set A. The Lebesgue measure on $\mathbb{R}^n$ will be denoted by $\mathscr{L}^n$.

We denote by $\mathscr{M}_b(\Omega)$ the space of bounded signed Radon measures on the Borel σ-algebra of a given open set Ω. This space arises as the dual of the space $C_c(\Omega)$ of continuous functions with compact support in Ω. Given $\mu \in \mathscr{M}_b(\Omega)$ and $\varphi \in C_c(\Omega)$ we will write

$$\langle \mu, \varphi \rangle := \int \varphi \, d\mu.$$

On the space of measures we consider the **weak* convergence**: $\mu_k \overset{*}{\rightharpoonup} \mu$ if and only if $\langle \mu_k, \varphi \rangle \to \langle \mu, \varphi \rangle$ for every $\varphi \in C_c(\Omega)$. Similar definitions hold for vector-valued measures. Given a (vector-valued) measure μ we define its **total variation** measure $|\mu|$ as

$$|\mu|(A) := \sup \left\{ \sum_{i \in \mathbb{N}} |\mu(A_i)| : A_i \text{ is a partition of } A \right\}.$$

If μ is defined on $\mathbb{R}^n$ then we denote by $\|\mu\|$ the total mass of μ, that is $|\mu|(\mathbb{R}^n)$. We define the **flat norm** of μ as

$$\|\mu\|_F := \sup \left\{ \int_{\mathbb{R}^n} \phi \, d\mu : \phi \text{ is 1-Lipschitz and } \|\phi\|_{W^{1,\infty}} \leq 1. \right\} \tag{1.1}$$

Given an $\mathbb{R}^m$-valued measure μ on Ω there exists a unique function $f \in L^1(\Omega, |\mu|)^m$ with values in $\mathbb{S}^{m-1}$ such that $\mu = f|\mu|$. This is called **polar decomposition**.

1.2 Functions of bounded variation

Given an open set $\Omega \subset \mathbb{R}^n$, a function $u \in L^1(\Omega)$ is said to be of **bounded variation in** Ω, and we write $u \in BV(\Omega)$, if its distributional gradient $Du = (D_1 u, \ldots, D_n u)$ is a vector-valued Radon measure in Ω, that is if

$$\int_\Omega \operatorname{div} \phi \, dx = -\int_\Omega \phi \cdot dDu(x)$$

for every $\phi \in C_c^1(\Omega, \mathbb{R}^n)$. We say that u is of **bounded variation** if $u \in BV(\mathbb{R}^n)$. If u is vector valued, that is $u \in L^1(\Omega, \mathbb{R}^m)$, we say that u is of bounded variation, and write $u \in BV(\Omega, \mathbb{R}^m)$, if each component of u is in $BV(\Omega)$. In this case Du is a $m \times n$ matrix of Radon measures. We also abbreviate "bounded variation" by "BV". The notion of function of local bounded variation is obtained when the above property holds for any open set compactly supported in Ω. The main kinds of convergence we consider on $BV(\Omega)$ are the L^1 (or L^1_{loc}) and the **weak* convergence**: a sequence $(u_k) \subset BV(\Omega)$ is said to weak* converge to $u \in BV(\Omega)$, and we write $u_k \overset{*}{\rightharpoonup} u$, if

$$u_k \to u \text{ in } L^1 \qquad \text{and} \qquad Du_k \overset{*}{\rightharpoonup} Du \text{ as Radon measures.}$$

By the Riesz representation theorem, $u \in BV(\Omega)$ if and only if $u \in L^1(\Omega)$ and

$$\sup \left\{ \int_\Omega u \operatorname{div} \phi : \phi \in C_c^1(\mathbb{R}^n, \mathbb{R}^n), |\phi| \leq 1 \right\} < \infty,$$

and the value of the supremum coincides with the total mass of the total variation measure $|Du|$, that is with $\|Du\| := |Du|(\Omega)$. Moreover, $u \mapsto |Du|(\Omega)$ is lower semicontinuous in $BV(\Omega)$ with respect to the $L^1_{loc}(\Omega)$ topology.

A third equivalent approach to define BV functions is by approximation with smooth functions: $u \in L^1(\Omega, \mathbb{R}^m)$ is in $BV(\Omega, \mathbb{R}^m)$ if and only if there exists an approximating sequence $(u_k) \subset C^\infty(\Omega, \mathbb{R}^m)$ such that

$$\begin{aligned} u_k \to u \quad &\text{in } L^1(\Omega) \\ L := \lim_{k\to\infty} \int_\Omega &|\nabla u_k| dx < \infty. \end{aligned}$$

Moreover, the least constant L coincides with $|Du|(\Omega)$.

For any BV function u the **coarea formula** holds: for any open set A

$$|Du|(A) = \int_{\mathbb{R}} P(\{u > t\}) dt. \tag{1.2}$$

Decomposition of *BV* functions, *SBV*

Given $u \in L^1_{loc}(\Omega, \mathbb{R}^m)$, we say that u has **approximate limit** at x if there exists $z \in \mathbb{R}^m$ such that

$$\lim_{r\to 0} \fint_{B_r(x)} |u(y) - z| dy = 0,$$

and the set S_u where this property does not hold is called **approximate discontinuity set**. We say that $x \in \Omega$ is an **approximate jump point** of $u \in BV(\Omega, \mathbb{R}^m)$ if there exist $a, b \in \mathbb{R}^m$ and $\nu \in \mathbb{S}^{n-1}$ such that $a \neq b$ and

$$\lim_{r\to 0} \fint_{B_r^+(x,\nu)} |u(y) - a| dy = 0 \qquad \lim_{r\to 0} \fint_{B_r^-(x,\nu)} |u(y) - b| dy = 0$$

where

$$\begin{aligned} B_r^+(x,\nu) &:= \{y \in B_r(x) : \langle y - x, \nu \rangle > 0\} \\ B_r^-(x,\nu) &:= \{y \in B_r(x) : \langle y - x, \nu \rangle < 0\}. \end{aligned}$$

The triplet (a, b, ν) is determined unniquely up to a permutation of (a, b) ad a change of sign of ν, and is denoted by $(u^+(x), u^-(x), \nu_u(x))$. The set of approximate jump points of u is denoted by J_u. By [AFP00, Theorem 3.78] the set S_u is countably $\mathscr{H}^{n-1}$-rectifiable and $\mathscr{H}^{n-1}(S_u \setminus J_u) = 0$.

Given any function $u \in BV(\Omega)$ we can decompose its derivative Du in an **absolutely continuous part** w.r.t. the Lebesgue measure $D^a u$ and a singular part $D^s u$. We can further decompose $D^s u$ in a **jump part** $D^j u := D^s u \llcorner J_u$ and a **Cantor part** $D^c u := D^s u \llcorner (\Omega \setminus S_u)$. The jump part can be written as

$$D^j u = (u^+ - u^-) \otimes \nu_u \mathscr{H}^{n-1} \llcorner J_u.$$

We define the space of functions of **special bounded variation** in Ω, denoted by $SBV(\Omega)$, as the set of BV functions with zero Cantor part

$$SBV(\Omega) := \{u \in BV(\Omega) : D^c u = 0\}.$$

1.3 Finite perimeter sets

A **finite perimeter set** (also *set of finite perimeter*) is a Lebesgue measurable set E in $\mathbb{R}^n$ such that $\mathbb{1}_E \in BV(\mathbb{R}^n)$, or equivalently if

$$\sup\left\{\int_E \operatorname{div}\phi : \phi \in C_c^1(\mathbb{R}^n,\mathbb{R}^n), |\phi| \leq 1\right\} < \infty \tag{1.3}$$

and the value of the supremum is called **perimeter** of E and denoted by $P(E)$. We say that E is of **locally finite perimeter** if for every bounded open set Ω (1.3) holds with $C_c^1(\mathbb{R}^n,\mathbb{R}^n)$ replaced by $C_c^1(\Omega,\mathbb{R}^n)$. Equivalently, by the Riesz representation theorem, E is of (locally) finite perimeter if and only if the distributional gradient of the characteristic function $\mathbb{1}_E$ is a (locally) finite vector valued Radon measure (usually denoted by μ_E or $D\mathbb{1}_E$), that is

$$\int_E \operatorname{div}\phi(x)dx = \int_{\mathbb{R}^n} \phi \cdot d\mu_E \quad \text{for every } \phi \in C_c^\infty(\mathbb{R}^n,\mathbb{R}^n).$$

The total variation of μ_E is also called the **perimeter measure**. Given a Borel subset A of $\mathbb{R}^n$ we define the perimeter of E inside A as $P(E,A) := |D\mathbb{1}_E|(A)$. It is easy to see that if $|E\Delta E'| = 0$ then $P(E,A) = P(E',A)$ for every Borel set A. We thus consider on the measurable sets of $\mathbb{R}^n$ the equivalence relation given by $E \sim E' \iff |E\Delta E'| = 0$, and we usually think of a set of finite perimeter as an equivalence class (although we can at time consider a precise representative). We introduce the distance $d(E,E') := |E\Delta E'|$ among (equivalence classes of) measurable sets with finite measure. In particular we say that E_k **converge** to E, and write $E_k \to E$, if $d(E_k,E) \to 0$ and that E_k **locally converge** to $\mathscr{E}$, and write $E_k \overset{loc}{\to} E$, if for every compact set K in $\mathbb{R}^n$ $E_k \cap K \to E \cap K$.

A consequence of the coarea formula (1.2) is the following property which we will use in Section 2.5:

$$|E \cap B(x,r)| = \int_0^r \mathscr{H}^{n-1}(E \cap \partial B(x,t))dt \tag{1.4}$$

for any finite perimeter set E. We also cite the following result, which is a consequence of [Mag12, Theorem 16.3] and which we will use in Chapter 2, Section 2.5: for any finite perimeter set E and a.e. $r > 0$

$$P(E \cap B_r) = P(E,B_r) + \mathscr{H}^{n-1}(E \cap \partial B_r). \tag{1.5}$$

When working on minimum problems in calculus of variations two essential tools are lower semicontinuity and compactness.

Theorem 1.1 (**Lower semicontinuity of perimeter** [Mag12, Proposition 12.15])**.** *If $\{E_k\}_{h\in\mathbb{N}}$ is a sequence of finite perimeter sets in $\mathbb{R}^n$ such that*

$$E_k \overset{loc}{\to} E, \qquad \limsup_{k\to\infty} P(E_k,K) < \infty$$

for every compact set K in $\mathbb{R}^n$, then E is of locally finite perimeter in $\mathbb{R}^n$, $D\mathbb{1}_{E_k} \overset{*}{\rightharpoonup} D\mathbb{1}_E$ and for every open set A in $\mathbb{R}^n$ we have

$$P(E,A) \leq \liminf_{k\to\infty} P(E_k,A).$$

Theorem 1.2 (**Compactness of finite perimeter sets** [Mag12, Theorem 12.26])**.** *If $R > 0$ and $\{E_k\}_{k\in\mathbb{N}}$ are finite perimeter sets in $\mathbb{R}^n$ such that*

$$(i) \quad \sup_k P(E_k) < \infty$$
$$(ii) \quad E_k \subset B_R \quad \textit{for all } k \in \mathbb{N}$$

then there exists E of finite perimeter in $\mathbb{R}^n$ and a subsequence $k(h) \to \infty$ with

$$E_{k(h)} \to E, \qquad D\mathbb{1}_{E_{k(h)}} \overset{*}{\rightharpoonup} D\mathbb{1}_E, \qquad E \subset B_R.$$

Reduced and essential boundary, De Giorgi and Federer's theorems

We define the **reduced boundary** $\mathscr{F}E$ as the set of points $x \in \mathbb{R}^n$ where the limit

$$\nu_E(x) := \lim_{r\to 0} \frac{D\mathbb{1}_E(B(x,r))}{|D\mathbb{1}_E|(B(x,r))}$$

exists and is a unit vector, called the **inner normal** of E at x. The following fundamental structure theorem of finite perimeter sets is due to De Giorgi:

Theorem 1.3 (**De Giorgi's structure theorem**)**.** *If E is a finite perimeter set in $\mathbb{R}^n$ then*

$$D\mathbb{1}_E = \nu_E \mathscr{H}^{n-1} \llcorner \mathscr{F}E \qquad |D\mathbb{1}_E| = \mathscr{H}^{n-1} \llcorner \mathscr{F}E$$

and therefore

$$\int_E \operatorname{div}\phi = \int_{\mathscr{F}E} \phi \cdot \nu_E \, d\mathscr{H}^{n-1} \quad \textit{for every } \phi \in C^1_c(\mathbb{R}^n, \mathbb{R}^n). \tag{1.6}$$

Moreover $\mathscr{F}E$ is countably $\mathscr{H}^{n-1}$-rectifiable, that is there exist countably many C^1 hypersurfaces M_h in $\mathbb{R}^n$, compact sets $K_h \subset M_h$ and a measurable set F with $\mathscr{H}^{n-1}(F) = 0$ such that

$$\mathscr{F}E = F \cup \bigcup_h K_h$$

and moreover, for every $x \in K_h$, $\nu_E^\perp(x) = T_x M_h$, the tangent space to M_h at x.

Given $\theta \in [0,1]$ define the set of points of **density** θ of a set E in $\mathbb{R}^n$ by

$$E^{(\theta)} := \left\{ x \in \mathbb{R}^n : \lim_{r\to 0} \frac{|E \cap B(x,r)|}{|B(x,r)|} = \theta \right\}. \tag{1.7}$$

Then by the Lebesgue differentiation theorem, $\mathscr{L}^n$-a.e. point of E belongs to $E^{(1)}$. Given a finite perimeter set E, we define the **essential boundary** $\partial^* E$ by

$$\partial^* E = \mathbb{R}^2 \setminus (E^{(0)} \cup E^{(1)}).$$

The following theorem, due to Federer, implies that when working with finite perimeter sets we can use interchangeably either $\mathscr{F}E$ or $\partial^* E$ or $E^{(1/2)}$.

Theorem 1.4 (Federer's theorem). *Given a finite perimeter set E, the reduced boundary $\mathscr{F}E$, the essential boundary ∂^*E and $E^{(1/2)}$ all coincide up to $\mathscr{H}^{n-1}$-negligible sets. More precisely, $\mathscr{F}E \subseteq E^{(1/2)} \subseteq \partial^*E$, and $\mathscr{H}^{n-1}(\partial^*E \setminus \mathscr{F}E) = 0$.*

In particular, the divergence theorem (1.6) holds with $\mathscr{F}E$ replaced by ∂^*E.

Isoperimetric inequality

For any set $E \subset \mathbb{R}^n$ of finite perimeter and finite volume the **isoperimetric inequality** holds:

$$\mathscr{H}^{n-1}(\partial^*E) = P(E) \geq n\omega_n^{\frac{1}{n}}|E|^{\frac{n-1}{n}}$$

where $\omega_n := |B_1|$ is the volume of the unit ball in $\mathbb{R}^n$. The **relative isoperimetric inequality** in a (sufficiently regular) open set Ω states that for every set of finite perimeter $E \subset \Omega$

$$P(E,\Omega) \geq c(\Omega)\min\{|E|,|\Omega \setminus E|\}^{\frac{n-1}{n}}.$$

A particular case is when $\Omega \subset \mathbb{R}^2$ is a half-plane, which we call **Dido's inequality**:

$$P(E,\{y>0\}) \geq \sqrt{2\pi|E|} \tag{1.8}$$

for every set $E \subset \{y > 0\}$ with finite area.

Consider now an open, bounded convex set K symmetric with respect to the origin in $\mathbb{R}^n$. We define its Minkowski functional $\|\cdot\|_K : \mathbb{R}^n \to [0,\infty)$ as

$$\|x\|_K = \inf\left\{\rho > 0 : \frac{x}{\rho} \in K\right\}.$$

This functional defines a norm on $\mathbb{R}^n$ whose unit ball centered at the origin is exactly K. Then $X = (\mathbb{R}^n, \|\cdot\|_K)$ is a Banach space, and since it is finite dimensional we can identify its dual X^* with $\mathbb{R}^n$ itself through the standard scalar product. In this way the dual norm as a Banach space becomes

$$\|\xi\|_* := \sup_{\|x\|<1}\{\langle\xi,x\rangle\} = \sup_{x\in K}\{\xi \cdot x\}$$

whose unit ball is by definition K^*, the dual of K. We have $\|x\|_* = \|x\|_{K^*}$.
Given a finite perimeter set E we define the **anisotropic perimeter** related to K as

$$P_K(E) := \int_{\partial^*E} \|\nu_E(x)\|_{K^*} d\mathscr{H}^{n-1}(x). \tag{1.9}$$

The **anisotropic isoperimetric inequality** says that, among all sets E with fixed volume in $\mathbb{R}^n$, up to translations the unique minimizer of $P_K(E)$ (also called **Wulff shape**) is given by a rescaled copy of K, that is by

$$K_E := \left(\frac{|E|}{|K|}\right)^{1/n} K.$$

and in particular

$$P_K(E) \geq P_K(K_E) = n|K|^{\frac{1}{n}}|E|^{\frac{n-1}{n}} \tag{1.10}$$

A quantitative version of this inequality was proved in [FMP10] (and earlier in [FMP08] for the isotropic perimeter; see also [CL12]). In order to state it, let us introduce the **isoperimetric deficit**

$$\delta_K(E) := \frac{P_K(E)}{n|K|^{\frac{1}{n}}|E|^{\frac{n-1}{n}}} - 1$$

and the **asymmetry index**

$$A_K(E) := \inf\left\{ \frac{|E\Delta(\tau + K_E)|}{|E|} : \tau \in \mathbb{R}^n \right\}. \tag{1.11}$$

The **quantitative anisotropic isoperimetric inequality** states the following.

Theorem 1.5 ([FMP10])**.** *There is a constant $C(n)$, depending only on the dimension, such that*

$$A_K(E) \leq C(n)\sqrt{\delta_K(E)}.$$

1.4 N-Clusters

An N**-cluster** (or simply cluster) is a family $\mathscr{E} = (\mathscr{E}(1), \dots, \mathscr{E}(N))$ of finite perimeter sets, called **chambers** or also **bubbles**, such that $0 < |\mathscr{E}(i)| < \infty$ for $i = 1, \dots, N$ and $|\mathscr{E}(i) \cap \mathscr{E}(j)| = 0$ for $i \neq j$, $i, j = 1, \dots, N$. By convention $\mathscr{E}(0) := \mathbb{R}^n \setminus \bigcup_{i=1}^N \mathscr{E}(i)$ denotes the **exterior chamber** of $\mathscr{E}$, while the others are called **interior chambers**. We denote by $\mathscr{E}(i,j) := \partial^*\mathscr{E}(i) \cap \partial^*\mathscr{E}(j)$ the common **interface** between chambers i and j. The standard perimeter of a cluster is

$$P(E) := \sum_{0 \leq i < j \leq N} \mathscr{H}^{n-1}(\mathscr{E}(i,j)) = \frac{1}{2}\sum_{i=0}^{N} P(\mathscr{E}(i)).$$

The last equality is a consequence of Federer's theorem. The distance in $F \subset \mathbb{R}^n$ of two clusters is defined as

$$d_F(\mathscr{E}, \mathscr{E}') := \sum_{i=1}^{n} |F \cap \big(\mathscr{E}(i)\Delta\mathscr{E}'(i)\big)|$$

and we set $d(\mathscr{E}, \mathscr{E}') := d_{\mathbb{R}^n}(\mathscr{E}, \mathscr{E}')$. We say that $\mathscr{E}_k$ **converges** to $\mathscr{E}$ if $d(\mathscr{E}_k, \mathscr{E}) \to 0$ as $k \to \infty$, and that **locally converges** to $\mathscr{E}$ if for every compact set K in $\mathbb{R}^n$ we have $d_K(\mathscr{E}_k, \mathscr{E}') \to 0$ as $k \to \infty$.

We also consider the case of countably many chambers: a **Caccioppoli partition** is a partition $\mathscr{E} = (\mathscr{E}(i))_{i \in \mathbb{N}}$ of $\mathbb{R}^n$ such that $\sum_{i \in \mathbb{N}} P(\mathscr{E}(i)) < \infty$. We say that it is **ordered** if $|\mathscr{E}(i)| \geq |\mathscr{E}(j)|$ whenever $i \leq j$. We define the perimeter of a Caccioppoli partition as

$$P(\mathscr{E}) := \frac{1}{2}\sum_{i \in \mathbb{N}} P(\mathscr{E}(i)).$$

The following compactness result holds.

Theorem 1.6 (**Compactness of Caccioppoli partitions**, [AFP00, Theorem 4.19]). *Let* $(\mathscr{E}^h(i))_{i\in\mathbb{N}}$, $h\in\mathbb{N}$ *be Caccioppoli partitions of* $\mathbb{R}^n$ *satisfying*

$$\sup_{h\in\mathbb{N}}\{P(\mathscr{E}^h)\}<\infty.$$

Then if the partitions are ordered there exists a Caccioppoli partition $(\mathscr{E}(i))_{i\in\mathbb{N}}$ and a subsequence $h(k)$ such that $\mathscr{E}^{h(k)}$ locally converges in measure in $\mathbb{R}^n$ to E_i for any $i\in\mathbb{N}$.

1.5 Surface energies for partitions

In the following we will also consider more general variants of perimeter, also called surface energies, because we will introduce a *weight* on different interfaces and an *anisotropy* depending on the direction of the unit normal. We refer to [AFP00] for a more detailed discussion. Set $I:=\{0,\dots,N\}$ and consider a function $\phi: I\times I\times\mathbb{S}^{n-1}\to\mathbb{R}$. Then the perimeter associated to ϕ is given by

$$P_\phi(\mathscr{E}):=\frac{1}{2}\sum_{i\neq j}\int_{\mathscr{E}(i,j)}\phi(i,j,\nu_{\mathscr{E}(i)}(x))d\mathscr{H}^{n-1}(x). \tag{1.12}$$

The two particular cases we will consider are:

(i) **Weighted perimeter**, where ϕ does not depend on the unit normal but just on i and j. In this case we can always rewrite the perimeter as

$$\sum_{0\le i<j\le N} c_{ij}\mathscr{H}^{n-1}(\mathscr{E}(i,j)) \tag{1.13}$$

and we suppose for simplicity that $c_{ij}=c_{ji}$. See Chapter 2.

(i) **Anisotropic perimeter**, where ϕ does not depend on i and j but just on the unit normal. In particular, the relevant functionals will be of the form

$$\sum_{0\le i<j\le N}\int_{\mathscr{E}(i,j)}\|\nu_{\mathscr{E}(i)}\|d\mathscr{H}^{n-1} \tag{1.14}$$

where $\|\cdot\|$ is a norm on $\mathbb{R}^n$. See Section 4.2.

As for the case of finite perimeter sets, we are interested in compactness and lower semiconinuity results. For the standard perimeter, they are an easy consequence of the corresponding theorems for finite perimeter sets (Theorem 1.1 and Theorem 1.2). For the more general surface energy (1.12), we need to introduce the notion of BV-ellipticity, originally introduced by Ambrosio and Braides [AB90]. We denote by $Q_\rho(\nu)$ any open cube with centre in the origin, side length ρ and faces either parallel or orthogonal to $\nu\in\mathbb{S}^{n-1}$. We denote by $u_{i,j,\nu}$ the function jumping between values i and j across the hyperplane $\{x: x\cdot\nu=0\}$.

Let $I \subset \mathbb{R}^m$ and $\phi : I \times I \times \mathbb{S}^{n-1} \to [0,\infty]$. We say that ϕ is **BV-elliptic** if

$$\int_{J_u} \phi(u^+, u^-, \nu_u) d\mathscr{H}^{n-1} \geq \phi(i, j, \nu)$$

for any bounded piecewise constant function $u : Q_1(\nu) \to I$ such that $\{u \neq u_{i,j,\nu_u}\} \Subset Q_1(\nu)$ and any triplet (i, j, ν) in the domain of ϕ.

We denote by $BV^*(\Omega, I)$ the space of I-valued BV functions u such that Du is concentrated on J_u and $\mathscr{H}^{n-1}(J_u) < \infty$. In particular $BV^*(\Omega, I) \subset SBV(\Omega)^m$.

We have the following result:

Theorem 1.7 ([AFP00, Theorem 5.14])**.** *Let $\phi : I \times I \times \mathbb{S}^{n-1} \to [0,\infty)$ be a bounded continuous function. Then the functional*

$$\mathscr{F}(u) := \int_{J_u} \phi(u^+, u^-, \nu_u) d\mathscr{H}^{n-1}$$

is lower semicontinuous in the space $BV^*(\Omega, I)$ (with respect to the L^1 convergence) if and only if ϕ is BV-elliptic.

In particular the surface energy P_ϕ defined by (1.12) is lower semicontinuous in the space of N-clusters if and only if ϕ is BV-elliptic. BV-ellipticity can be seen as an analogue of Morrey's quasiconvexity in the setting of BV functions. As for quasiconvexity, the condition is not so easily checked in practical examples. It is useful to have some simpler sufficient conditions that ensure lower semicontinuity. With reference to the two examples (1.13) and (1.14), we have the following results.

Theorem 1.8 (**Lower semicontinuity of weighted perimeter**, [AFP00, Example 5.23(a)])**.** *The weighted perimeter given by* (1.13) *is lower semicontinuous in the space of N-clusters if and only if $c_{ij} = c_{ji}$ are non-negative weights satisfying*

$$c_{ik} \leq c_{ij} + c_{ik} \text{ for every } i, j, k.$$

We state the following result as a theorem even though it is a simple consequence of the lower semicontinuity of the anisotropic perimeter on each chamber.

Theorem 1.9 (**Lower semicontinuity of anisotropic perimeter**)**.** *The anisotropic perimeter given by* (1.14) *is lower semicontinuous on the space of N-clusters.*

A more general notion which is still sufficient to ensure lower semicontinuity is joint convexity: given $K \subset \mathbb{R}^m$ compact we say that $\phi : K \times K \times \mathbb{R}^n \to [0,\infty]$ is **jointly convex** if

$$\phi(i, j, p) = \sup_{h \in \mathbb{N}} \langle g_h(i) - g_h(j), p \rangle \quad \forall (i, j, p) \in K \times K \times \mathbb{R}^n$$

for some sequence $(g_h) \subset C(K)^n$.

As a special case we mention the following example [AFP00, Example 5.23(b)]: let $K \subset \mathbb{R}^m$ be compact and $\psi : K \times \mathbb{R}^n \to [0, \infty]$ a lower semicontinuous function, positively 1-homogeneous and convex in the second variable. Then the function

$$\phi(i, j, p) = \begin{cases} \psi(i, p) + \psi(j, -p) & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases} \tag{1.15}$$

is jointly convex.

1.6 Γ-convergence

Given a sequence of functionals $F_h : X \to \mathbb{R} \cup \{+\infty\}$ defined on a metric space (X, d), a functional $F : X \to \mathbb{R} \cup \{\infty\}$ is said to be the **Γ-limit** of F_h for the distance d if the following two conditions hold:

- $\liminf$ inequality: for every $x \in X$ and every sequence $x_h \to x$ we have

$$F(x) \leq \liminf_{h \to \infty} F_h(x_h);$$

- $\limsup$ inequality: for every $x \in X$ there exists a sequence $x_h \to x$ (called **recovery sequence**) such that

$$F(x) \geq \limsup_{h \to \infty} F_h(x_h).$$

We also say that F_h **Γ-converge** to F with respect to the distance d.

The basic property of Γ-convergence is convergence of minimizers of F_h to a minimizer of F:

Theorem 1.10 (Fundamental property of Γ-convergence). *If the functionals F_h Γ-converge to F, $\bar{x}_h$ are minimizers of F_h and $\bar{x}_h \to \bar{x}$ then $\bar{x}$ is a minimizer of F.*

In particular under a coercivity assumption on F_h we can ensure that every sequence of minimizers $\bar{x}_h$ admits a convergent subsequence: assume that F_h are equicoercive, meaning that for every real t $\{F_h \leq t\}$ is compact; then any sequence of minimizers $\bar{x}_h$ admits a subsequence converging to a minimizer $\bar{x}$ of F.

Chapter 2

Sticky-disk limit of weighted N-clusters

We study planar N-clusters that minimize, under an area constraint, a weighted perimeter P_ε depending on a small parameter $\varepsilon > 0$. Specifically we weight $2-\varepsilon$ the boundary between the interior chambers and 1 the boundary between an interior chamber and the exterior one. We prove that as $\varepsilon \to 0$ minimizers of P_ε converge to configurations of disjoint disks that maximize the number of tangencies, each weighted by the harmonic mean of the radii of the two tangent disks. We also obtain some information on the structure of minimizers for small ε. Lastly, we partially extend the results to higher dimension. The content of this chapter, except for the last Section *Higher dimension*, is basically part of [DN18], with a few modifications.

Contents

In this chapter we are interested in studying the optimal way to enclose and separate N volumes in order to minimize a specific weighted perimeter. We restrict for the first part of the chapter to the planar case, and in the last section prove some partial results about the higher dimensional case.

We recall that an N-bubble, or N-cluster, is a family $\mathscr{E} = (\mathscr{E}(1), \dots \mathscr{E}(N))$ of finite perimeter sets in the plane, called *bubbles* or *chambers*, that are of finite positive volume and are essentially disjoint:

$$0 < |\mathscr{E}(i)| < \infty \qquad |\mathscr{E}(i) \cap \mathscr{E}(j)| = 0 \text{ for every } i \neq j$$

The weighted perimeter of an N-bubble is given by the weighted sum of the Hausdorff measures of all the interfaces, that is

$$P(\mathscr{E}) = \frac{1}{2} \sum_{\substack{0 \le i,j \le N \\ i \neq j}} c_{ij} \mathscr{H}^1 \big(\partial^* \mathscr{E}(i) \cap \partial^* \mathscr{E}(j)\big) \tag{2.1}$$

for some fixed positive weights $c_{ji} = c_{ij} > 0$. In the following we will fix the areas $m_1, \dots, m_N$ of the bubbles and seek the configurations that minimize the perimeter $P(\mathscr{E})$ under this constraint.

The exact characterization of perimeter minimizing N-bubbles is currently known only in very few situations. The case $N = 1$ is the classical isoperimetric problem, whose well-known solution is a disk. If $N = 2$ the solution is the *standard weighted double bubble* made of three circular arcs meeting in two triple points forming angles which depend on the specific weights (see [Foi+93] in the case of unit weights, [Law14] in general). If $N = 3$ the solution is known only for equal weights ($c_{ij} = 1$), and it is the *standard triple bubble* made of six circular arcs meeting in four points [Wic04]. When $N = 4$ and the weights are equal the minimal configuration has a determined topology and is conjectured to be the *symmetric sandwich* [PT18].

For general N only existence and regularity of minimizers is known: under the strict triangle inequalities $c_{ij} < c_{ik} + c_{kj}$ for any distinct i, j, k, minimizers exist and their boundary is made of a finite number of circular arcs, meeting at a finite number of singular points where they satisfy a condition on the incidence angles [Mor98, Proposition 4.3].

The exact characterization of minimizers seems an intractable problem already for small values of N. For this reason, in this work we consider a special asymptotic regime. Indeed for $\varepsilon \geq 0$ we define

$$\begin{aligned} P_\varepsilon(\mathscr{E}) &= \frac{1}{2} \sum_{\substack{0 \le i,j \le N \\ i \neq j}} c_{ij}(\varepsilon) \mathscr{H}^1 (\partial \mathscr{E}(i) \cap \partial \mathscr{E}(j)), \\ c_{ij}(\varepsilon) &= \begin{cases} 1 & \text{if } i = 0 \text{ or } j = 0 \\ 2 - \varepsilon & \text{if } i, j \neq 0 \end{cases}. \end{aligned} \tag{2.2}$$

Problem We want to study the asymptotic behaviour as $\varepsilon \to 0$ of N-bubbles which minimize the energy P_ε with an area constraint $|\mathscr{E}(i)| = m_i$ for $i = 1, \dots, N$.

We denote by $\overline{\mathscr{E}}_\varepsilon$ minimizers of P_ε. We call a *cluster of disks* any cluster made of disks with pairwise disjoint interiors.

Proposition 2.1 (First-order behaviour). *As $\varepsilon \to 0$ minimizers of P_ε converge to a cluster of disks.*

At this level however we have no information on the disposition of the limit disks, since any collection of disks with pairwise disjoint interiors is a possible candidate. On the other hand we expect to see only

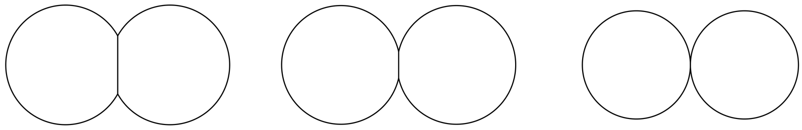


Figure 2.1: When $N = 2$ we know the explicit shape of the (unique) minimizers of P_ε, and as $\varepsilon \to 0$ (from left o right) they converge to two tangent disks. Depicted here is the case of equal areas.

certain configurations of disks: if we look for instance at the case $N = 2$ with equal areas the limit disks must be tangent (see Figure 2.1). To obtain more information we then perform a second-order expansion of the perimeter functional, that is we subtract the limit energy $P_0(\mathscr{B}) = \sum_{i=1}^{N} P(B_i)$, rescale by the right power of ε and analyze these rescaled functionals. To find the right scaling we look again at the completely solved case of two bubbles with equal areas $|\mathscr{E}(1)| = |\mathscr{E}(2)| = \pi$: an explicit computation shows that

$$P_\varepsilon(\overline{\mathscr{E}_\varepsilon}) = 4\pi - \frac{4}{3}\varepsilon^{3/2} + O(\varepsilon^{5/2}) \tag{2.3}$$

hence the relevant next order is $\varepsilon^{3/2}$ and we are led to consider the rescaled functionals

$$P_\varepsilon^{(1)}(\mathscr{E}) := \frac{P_\varepsilon(\mathscr{E}) - P_0(\mathscr{B})}{\frac{4}{3}\varepsilon^{3/2}}. \tag{2.4}$$

Of course they have the same minimizers as P_ε but allow us to analyze the finer behaviour at scale $\varepsilon^{3/2}$. We expect that, as in the case of the double bubble, these functionals "see" the tangency points in the limit cluster $\mathscr{B}$. Indeed, this is precisely what happens. The following is the main result of this chapter:

Theorem 2.2 (Sticky-disk limit). *As $\varepsilon \to 0$ minimizers $\overline{\mathscr{E}_\varepsilon}$ of P_ε converge up to subsequence and rigid motions to a cluster of disks that maximizes the number of contact points among the disks, each contact point counted with factor $\frac{r_i r_j}{r_i + r_j}$, where r_i, r_j are the radii of the touching disks.*

Remark 2.3. Theorem 2.2 selects, among all possible clusters of disks with the right area constraint, those which maximize the number of (weighted) tangencies; equivalently, those which minimize the following *tangency functional*

$$\mathscr{T}(\mathscr{E}) = \begin{cases} -\sum\limits_{1 \le i < j \le N} \sigma_{ij} \dfrac{2 r_i r_j}{r_i + r_j} & \text{if } \mathscr{E} = (B_1, \ldots, B_N) \text{ is a cluster of disks} \\ +\infty & \text{otherwise} \end{cases} \tag{2.5}$$

where r_i is the radius of the disk B_i and

$$\sigma_{ij} = \begin{cases} 1 & \text{if } B_i \text{ and } B_j \text{ touch} \\ 0 & \text{otherwise} \end{cases}.$$

In the case of equal radii, the tangency functional $\mathscr{T}$ coincides, up to a suitable rescaling, with the energy of N particles associated to the centers of B_i and interacting by means of the *sticky disk* (or *Heitmann-Radin*) potential

$$V(r) = \begin{cases} +\infty & \text{if } r < 1 \\ -1 & \text{if } r = 1 \\ 0 & \text{if } r > 1 \end{cases},$$

hence the name of the Theorem above. Heitmann and Radin proved in [HR80] that minimizers for the sticky disk with a fixed number of particles N are crystallized, that is they form a subset of the triangular lattice. Moreover as $N \to \infty$ the global shape of minimizers converges to a hexagon [AYFS12], [Sch13], [DPS17]. In view of Theorem 2.2 this translates in the context of N-clusters minimizing P_ε in the following information: if we first send $\varepsilon \to 0$ and then $N \to \infty$ we obtain as an asymtptotic global shape a hexagon. If it were possible to exchange the order of the limits we would obtain that, for sufficiently small ε, the global shape of N-clusters minimizing P_ε is almost hexagonal in the limit $N \to \infty$. This would give a partial answer in the case of weighted clusters to a question considered by Cox, Morgan and Graner [CMG13] about the global shape of minimal N-clusters for large N, and it was actually the initial motivation for this work. See also Chapter 3 for the global shape problem.

The main ingredient in the proof of Theorem 2.2 is the lower-bound inequality given by Theorem 2.14, which can be seen as an asymptotic quantitative isoperimetric inequality involving the "curvature deficit" of the boundary.

Finally, as a byproduct of the proof of Theorem 2.2, we also obtain information on the structure of minimizers $\overline{\mathscr{E}_\varepsilon}$ for small ε:

Theorem 2.4 (**Structure of minimizers**). *Minimizing clusters $\overline{\mathscr{E}_\varepsilon}$ have the following properties: let $\mathscr{B} = (B_1, \dots, B_N)$ be a cluster of disks with radii $r_1, \dots, r_N$ to which $\overline{\mathscr{E}_\varepsilon}$ converge; then for small $\varepsilon > 0$, in addition to the standard regularity given by Theorem 2.7, the following hold:*

- *each chamber is connected;*
- *different arcs can meet only in a finite number of triple points, and when this happens exactly one of the chambers meeting there is the exterior one. In particular, the angles formed at a triple point are $2\theta_\varepsilon, \pi - \theta_\varepsilon, \pi - \theta_\varepsilon$, where $\theta_\varepsilon = \arccos\left(1 - \frac{\varepsilon}{2}\right)$.*
- *between each pair of chambers $\overline{\mathscr{E}_\varepsilon}(i)$ and $\overline{\mathscr{E}_\varepsilon}(j)$ such that B_i and B_j are tangent, there is a single arc of constant curvature κ_{ij}^ε and length of respective chord ℓ_{ij}^ε where*

$$\kappa_{ij}^\varepsilon = \frac{1}{2}\left(\frac{1}{r_j} - \frac{1}{r_i}\right) + o(1) \qquad \textit{and} \qquad \ell_{ij}^\varepsilon = \frac{4r_ir_j}{r_i + r_j}\varepsilon^{1/2} + o(\varepsilon^{1/2})$$

  while in the remaining portion of the boundaries, that is between any chamber $\overline{\mathscr{E}_\varepsilon}(i)$, $i \geq 1$, and the exterior $\overline{\mathscr{E}_\varepsilon}(0)$, there is an arc of curvature $\kappa_i^\varepsilon = \frac{1}{r_i}(1 + o(1))$.

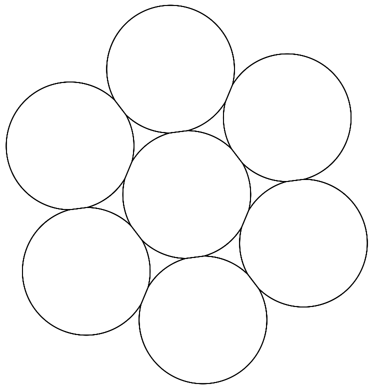


Figure 2.2: A numerical candidate for the minimum 7-bubble of equal areas 4π and with $\varepsilon = 0.02$ obtained with the Surface Evolver by Ken Brakke [Bra92]. The expected second order energy by Theorem 2.2 is $P_\varepsilon = 7 \cdot 4\pi - 12 \cdot 2 \cdot \frac{4}{3} \cdot 0.02^{3/2} = 28\pi - 32 \cdot 0.02^{3/2} \approx 87.8740846325$. The actual energy of the depicted configuration computed numerically is 87.8742016. The rescaled energy $P_\varepsilon^{(1)}$ as defined by (2.4) is ≈ -11.9844, which agrees with the fact that the limit as $\varepsilon \to 0$ is -12, the (negative) total number of contacts.

Remark 2.5. Γ-*convergence.* We decided to state Theorem 2.2 talking about minimizers, but actually a stronger result holds: the rescaled functionals $P_\varepsilon^{(1)}$ given by (2.4) Γ-converge to the tangency functional $\mathscr{T}$ given by (2.5), with respect to the L^1-convergence of clusters (we refer to [Bra02] for the definition and the properties of Γ-convergence). The hard part is the $\liminf$ inequality: to prove it, given any family $\mathscr{E}_\varepsilon$ converging to a cluster of disks $\mathscr{B}$, we can build an improved family with a higher regularity using for instance the density of polygonal clusters among all clusters [BCG17], and then apply Theorem 2.14. The method of looking at the second order behaviour of P_ε is close in spirit to [AB93].

To conclude, we briefly outline the structure of this chapter. In Section 2.1 we introduce the notation, recall basic facts about minimal clusters and prove preliminary results. In Section 2.2 we show the first-order result of Proposition 2.1. In Section 2.3 we prove Theorem 2.2 and Theorem 2.4. In particular we prove that for ε small enough each chamber of a minimizer is connected (Lemma 2.11) and that there is at most one boundary arc between two different chambers (Lemma 2.13). Next we prove an asymptotic version of quantitative isoperimetric inequality, where the isoperimetric deficit controls the "curvature deficit" of the boundary (Theorem 2.14). From this result we deduce the key lower bound for the perimeter of a given cluster converging to a cluster of disks (Proposition 2.18). Finally, we build a *recovery sequence* for Theorem 2.2, that is we prove that the previous lower bound is sharp, and then prove the main theorems. We conclude with some remarks (Section 2.4) and with some partial results on the higher dimensional case (Section 2.5).

2.1 Notation and preliminary results

We use the notation $f(\varepsilon) = O(g(\varepsilon))$ and $f(\varepsilon) = o(g(\varepsilon))$ to mean respectively

$$\limsup_{\varepsilon\to 0^+} \frac{|f(\varepsilon)|}{g(\varepsilon)} < \infty \quad \text{and} \quad \lim_{\varepsilon\to 0^+} \frac{f(\varepsilon)}{g(\varepsilon)} = 0.$$

We denote the area (Lebesgue measure) of a set $E \subset \mathbb{R}^2$ by $|E|$. Recall the L^1 convergence on clusters: $\mathscr{E}_k \to \mathscr{E}$ iff $|\mathscr{E}_k(i) \Delta \mathscr{E}(i)| \to 0$ for every $i = 1, \ldots, N$, where Δ is the symmetric difference of sets (equivalently, the characteristic functions of each chamber converge in L^1). With respect to this convergence, the perimeter given by (2.1) is lower semicontinuous if and only if the following triangle inequalities are satisfied:

$$c_{ij} \leq c_{ik} + c_{kj} \qquad \text{for every choice of distinct } i, j, k\ . \tag{2.6}$$

For a reference see [AB90], in particular Example 2.8 with $\psi \equiv 1$.

We note here for future reference that the functional P_ε can be rewritten in the following equivalent way:

$$P_\varepsilon(\mathscr{E}) = \left(1 - \frac{\varepsilon}{2}\right) \sum_{i=1}^{N} P(\mathscr{E}(i)) + \frac{\varepsilon}{2} P(\mathscr{E}(0)). \tag{2.7}$$

We recall the basic existence and regularity results for minimizing clusters in the plane, which can be found for instance in [Mor98]. The existence of minimal N-clusters for a given area constraint follows by the direct method: by a standard compactness theorem for finite perimeter sets (Theorem 1.2) and the lower semicontinuity of the functional P_ε (which can be proved either checking that the triangle inequalities (2.6) hold, or using (2.7) and the lower semicontinuity of the perimeter on each chamber) we can prove the following:

Theorem 2.6 (Existence). *For every $\varepsilon \in [0,2]$ there is a minimizer of P_ε for any given volume constraint.*

Regarding regularity of minimizers, we have the following theorem:

Theorem 2.7 (Regularity [Mor98, Proposition 4.3]**).** *Any minimizer $\overline{\mathscr{E}_\varepsilon}$ of P_ε has the following properties:*

- *each chamber has a piecewise C^1 boundary made of a finite number of arcs with constant curvature;*
- *these arcs meet in a finite number of vertices, where they satisfy the condition*

$$\sum c_{ij} \tau_{ij} = 0 \tag{2.8}$$

where τ_{ij} is the unit vector starting from the vertex and tangent to $\partial\mathscr{E}(i) \cap \partial\mathscr{E}(j)$, and the sum is extended over all interfaces meeting at the vertex;

- *around any vertex the weighted curvatures sum to zero.*

In the case where all weights are equal, something more can be said: namely that at each vertex exactly three arcs meet forming 120-degree angles. In the general case of minimal weighted clusters there could be also quadruple points (for instance consider four equal squares with a vertex in common, with weights $> \sqrt{2}$ between diagonally-opposite squares and 1 otherwise; this cluster is minimizing among clusters with the same boundary condition. Compare also with the example at the end of [AB90, Section 2.3]). However, for our specific choice of weights given by (2.2), we are able to recover the triple-point property: exactly three arcs meet at each vertex, as the next lemma shows. This property should in principle be inferable from the algebraic conditions that weights have to satisfy at each vertex given in [Mor98, Remark 4.4], however we prefer the following more geometric argument.

Lemma 2.8 (**Triple-point property**). *For ε small enough, at every vertex of a minimizer of P_ε exactly three arcs meet. Moreover at every such vertex exactly one of the chambers is the exterior one $\mathscr{E}(0)$ and the angles are given by $\pi-\theta_\varepsilon, \pi-\theta_\varepsilon, 2\theta_\varepsilon$, where*

$$\theta_\varepsilon = \arccos\left(1-\frac{\varepsilon}{2}\right).$$

Proof. We suppose that there is a vertex at which at least four arcs meet, and prove that the cluster is not minimal since we can modify it to lower the energy. We give the proof under the simplifying assumption that the arcs meeting at the vertex are straight edges; the proof in the general case is almost identical, it suffices to zoom at a sufficiently small scale and apply the same argument.

First we show that there can not be any component of the exterior chamber around such a point:

- if there is only one component of the exterior chamber then, since at least one of the remaining angles is less than 120 degrees, we could put a Steiner configuration inside a small triangle of small lengthscale δ, fixing the area somewhere else (see Figure 2.3);
- if instead there are at least two components of the exterior chamber, then one of the remaining portions is contained in a half-plane. We can modify all the chambers in this half-plane removing completely a small triangle of small lengthscale δ, and fix the area somewhere else (see Figure 2.4).

In both cases, when δ is small enough, we reduce the perimeter since the reduction in perimeter due to the first modification is of order $\approx \delta$, while the change in perimeter due to the area-fixing variations is of order $\approx \delta^2$.

We are therefore left with a configuration in which there is no exterior chamber. But then, since we are supposing to have at least four components, at least one of the angles is less than 120 degrees, and we can lower the energy again by putting a small Steiner configuration inside a small triangle. This proves that there must be exactly three arcs meeting at each vertex. The same proof, as already said, holds even if the arcs are curved, looking at a sufficiently small scale around the vertex and applying similar variations.

Now let us prove that around any vertex exactly two interior and one exterior components meet. If the three chambers meeting at a vertex were all interior chambers, the standard variational argument would

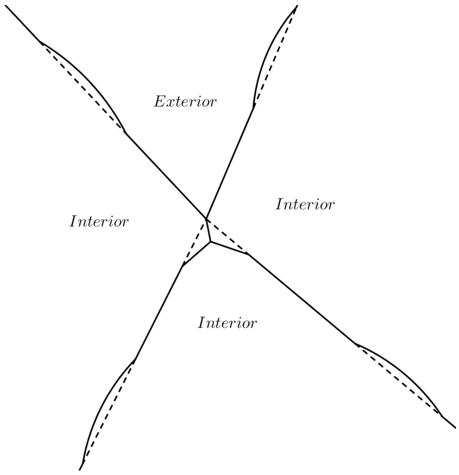


Figure 2.3: If there is only one exterior component, we can put a small Steiner configuration in one of the remaining angles which is less than 120 degrees. We have to fix the area with a slight inflation or deflation.

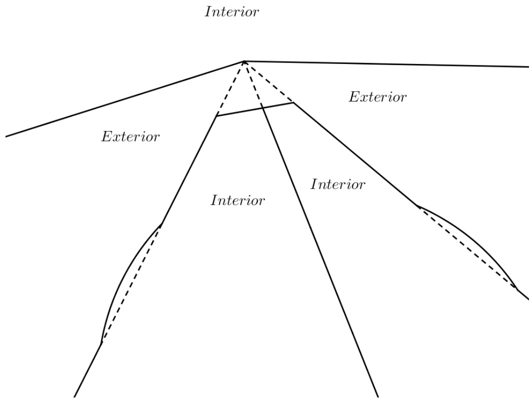


Figure 2.4: If there are at least two exterior components, one of the remaining portions is contained in a half-plane. We can cut and remove a whole triangle, again fixing the area with a slight inflation or deflation.

imply that the angles are 120 degrees; but then we could insert a small triangular hole (a component of the exterior chamber) around the vertex, again adjusting the area somewhere else. The reduction of perimeter is again of order δ, plus corrections of order δ^2 for the area adjustments. The key point is that the perimeter of an equilateral triangle is smaller than the length of its Steiner configuration multiplied by $2-\varepsilon$, for ε sufficiently small. Therefore we conclude that the only components we can have are two interior chambers and one exterior chamber.

Finally, the computation of the angle θ_ε comes directly from condition (2.8). □

2.1.3 Isoperimetric inequality We end this section by stating the isoperimetric inequality in the following form:

Proposition 2.9 (Isoperimetric inequality with signed areas [MFG98]). *A disk B of area $m > 0$ minimizes* length(∂B) *among all oriented rectifiable curves C enclosing net signed area m.*

2.2 First order analysis: convergence to disks

In this section we prove the first-order result that the limit clusters are made of disks. We begin with a simple compactness result:

Lemma 2.10 (Compactness). *Any sequence of minimizers $\overline{\mathscr{E}_\varepsilon}$ has uniformly bounded diameter, that is*

$$\operatorname{diam}(\overline{\mathscr{E}_\varepsilon}) \leq C < +\infty.$$

Proof. The result follows essentially from the fact that for connected sets in the plane the perimeter controls the diameter, namely $\operatorname{diam} E \le \frac{1}{2}P(E)$. Supposing that $E_\varepsilon := \bigcup_{i=1}^N \overline{\mathscr{E}_\varepsilon}(i)$ is connected we indeed obtain

$$2\operatorname{diam} E_\varepsilon \le P(E_\varepsilon) \le P_\varepsilon(\overline{\mathscr{E}_\varepsilon}) \le \sum_{i=1}^N P(B_i)$$

which gives the desired conclusion.

Let us now prove that E_ε is connected. By the regularity result of Theorem 2.7 we know that for every ε each chamber of $\overline{\mathscr{E}_\varepsilon}$ is equivalent to an open set which has piecewise C^1 boundary. If E_ε were disconnected, we could take two connected components and move them until they touch without changing the value of P_ε. The cluster thus created would still be minimal but would have at least a quadruple point, contradicting Lemma 2.8. This concludes the proof. □

We can now prove the first-order result of Proposition 2.1.

Proof of Proposition 2.1. Using N disjoint disks as competitors we obtain that

$$P(\overline{\mathscr{E}_\varepsilon}) \le P_\varepsilon(\overline{\mathscr{E}_\varepsilon}) \le \sum_{i=1}^N \sqrt{4\pi m_i} < +\infty.$$

Moreover by Lemma 2.10 the sequence has uniformly bounded diameter, and thus the following uniform bound holds for minimizers $\overline{\mathscr{E}_\varepsilon}$:

$$\sup_\varepsilon P(\overline{\mathscr{E}_\varepsilon}) + \operatorname{diam}(\overline{\mathscr{E}_\varepsilon}) < \infty.$$

By compactness of finite perimeter sets (Theorem 1.2) this implies that minimizers $\overline{\mathscr{E}_\varepsilon}$ converge, up to subsequence and rigid motions, to a limit cluster $\mathscr{E}_0$ with the same area constraint. By (2.7) we also obtain that

$$P(\overline{\mathscr{E}_\varepsilon}(i)) \le \sqrt{4\pi m_i}(1 + O(\varepsilon)) \tag{2.9}$$

and by lower semicontinuity of perimeter we obtain

$$P(\mathscr{E}_0(i)) \le \sqrt{4\pi m_i}.$$

By the isoperimetric inequality the unique minimizer of perimeter for a given area constraint is the disk and therefore $\mathscr{E}_0(i)$ is a disk of area m_i. □

2.3 Second order analysis: sticky-disk limit

We now want to obtain some more information about minimizers $\overline{\mathscr{E}_\varepsilon}$ as $\varepsilon \to 0$. In the last section we saw that, up to translation, minimal clusters converge to a cluster of disks; this was a simple consequence of the isoperimetric inequality together with a compactness result. However, as already pointed out, we don't expect to see in the limit every cluster of disks: for instance Lemma 2.10 suggests that at least the limit clusters must be connected. To understand what kind of clusters can arise as limits, we will perform a higher order expansion of the perimeter.

Localization of contacts between different chambers

In this subsection we prove a localization result that basically says that each chamber of a minimizer is sandwiched between two concentric disks $(1-o(1))B$ and $(1+o(1))B$, B being a disk with the same area as the chamber. This can be seen as an improvement from the L^1 convergence of Proposition 2.1 to "uniform" convergence, or Hausdorff convergence of the boundaries. A consequence of this is that any pair of chambers whose limit disks are not touching will eventually share no boundary. Moreover we prove that for ε small enough each chamber of a minimizer is connected.

Lemma 2.11 (Localization Lemma). *Suppose that a minimizer $\overline{\mathscr{E}_\varepsilon}$ converges to the cluster of disks $\mathscr{B} = (B_1, \dots, B_N)$. Then, for ε small enough, each chamber $\overline{\mathscr{E}_\varepsilon}(i)$ is connected, and moreover*

$$(1-o(1)))B_i \subset \overline{\mathscr{E}_\varepsilon}(i) \subset (1+o(1))B_i.$$

Proof. We fix a chamber and denote it for simplicity just by E, and the disk by B. We will prove the lemma in four steps:

(i) For ε small enough, E has only one biggest (in terms of area) connected component C_0, which carries almost all the mass, i.e.
$$|C_0| \geq |E|(1-o(1)).$$
In particular, if $\overline{\mathscr{E}_\varepsilon}(i)$ converges to a disk B as $\varepsilon \to 0$, then $|C_0 \Delta B| = o(1)$.

(ii) The convex hull $co(C_0)$ is sandwiched between two disks both converging to B as $\varepsilon \to 0$:
$$(1-o(1))B \subset co(C_0) \subset (1+o(1))B.$$

(iii) For ε small enough the biggest connected component is in fact the only one, i.e. each chamber is connected.

(iv) The same conclusion as in (ii) holds also for $C_0 = E$ itself, namely
$$(1-o(1))B \subset E \subset (1+o(1))B.$$

(i) If there is just one connected component then we are done. Otherwise, denote by $C_0, C_1, \dots$ the connected components of E (indexed by at most countably many indices i, and ordered decreasingly in the area), and set $V_i := |C_i|/|E|$ to be the normalized area of the connected component C_i of E . In this way $\sum_i V_i = 1$. Set $M := \max_i V_i$. If $M \leq \frac{1}{2}$, by the isoperimetric inequality

$$P(E) = \sum_i P(C_i) \geq 2\sqrt{\pi} \sum_i \sqrt{|C_i|} = 2\sqrt{\pi}\sqrt{|E|} \sum_i \sqrt{V_i} \geq 4\sqrt{\pi}\sqrt{|E|}$$

where we used that, since in this case $V_i \leq M \leq 1/2$, we have $\sqrt{V_i} \geq 2V_i$. But by the trivial energy estimate (2.9) we know that $P(E) \leq 2\sqrt{\pi}\sqrt{|E|}(1+o(1))$, so for ε small enough M must be $> \frac{1}{2}$, and in particular there is only one component with maximum area, C_0. In this case for every $i \geq 1$ we have $V_i \leq 1 - M < \frac{1}{2}$, and arguing as above we obtain that

$$P(E) = P(C_0) + \sum_{i \geq 1} P(C_i) \geq 2\pi\sqrt{M} + \sum_{i \geq 1} 2\pi \frac{V_i}{\sqrt{1-M}} = 2\pi\sqrt{M} + 2\pi\sqrt{1-M}.$$

Again from the energy estimate we know that each chamber has an isoperimetric deficit $o(1)$, therefore we obtain the condition

$$\sqrt{M} + \sqrt{1-M} \leq 1 + o(1),$$

which together with the condition $\frac{1}{2} \leq M \leq 1$ easily implies that M must be close to 1, which translates to $|C_0| \geq |E|(1 - o(1))$.

(ii) First we prove that $co(C_0) \supset (1 - o(1))B$. Indeed, given a point $x \in B \backslash co(C_0)$ (if it exists, otherwise we are done), by Hahn-Banach we can find a whole circular cap whose straigth segment passes through x that is contained in $B \backslash co(C_0)$. The area of this circular cap is at least as big as the area of the circular cap whose straight segment is perpendicular to the radius through x. From point (i) this area must be $o(1)$, and this easily imples the desired conclusion.

Next we prove that $co(C_0) \subset (1 + o(1))B$. We use the following two standard facts for planar sets:

(i) the convex hull of an open connected set has smaller perimeter than the original set;

(ii) among convex bodies in the plane, the perimeter is monotone increasing with respect to inclusion.

From the first fact we obtain that $P(co(C_0)) \leq P(B)(1 + o(1))$. Now take any point $x \in co(C_0) \backslash B$. By convexity and since $co(C_0) \supset (1 - o(1))B$, we obtain that $co(C_0) \supset co\big((1 - o(1))B \cup \{x\}\big)$. From the second fact cited above the latter set must have smaller perimeter than $co(C_0)$, and this easily implies that $x \in (1 + o(1))B$.

(iii) Suppose that E has more than one component. From point (ii) we know that all the components except for the biggest one C_0 have a total mass of at most $0 < m = o(1)$. Then by the isoperimetric inequality and the subadditivity of the square root, their total perimeter is bigger than

$$\sum_{i \geq 1} 2\sqrt{\pi}\sqrt{|C_i|} \geq 2\sqrt{\pi}\sqrt{m}.$$

We now remove all the smaller components, and inflate the biggest one, and prove that for ε small enough we find in this way a better competitor, which is incompatible with the supposed minimality of the original cluster. The increase in perimeter due to the inflation can be taken of order of the total removed mass m, see for instance [Mag12, Theorem 29.14]. The net change in perimeter is therefore $-2\sqrt{\pi}\sqrt{m} + bm$ for some constant b, which for $m > 0$ small enough is negative; the same net change holds also for the functional P_ε. This proves that for ε small enough, and therefore m small enough, there can be just one connected component for each chamber.

(iv) The rightmost inclusion follows immediately from $C_0 \subset co(C_0)$ and point (ii). We now prove the other one. From this last inclusion we know that the only obstacle would be the presence of the exterior chamber inside B. To exclude this we argue similarly to point (iii): if there are connected components of the exterior chamber entirely surrounded by E, we can "fill" them with the set E, and then perform a deflation of the set, which for m small enough results in a net decrease in the functional P_ε. If instead there are "tentacles" of the exterior chamber which come from the outside, that is components not entirely surrounded by E, by similar considerations they must be contained in the complement of $(1-o(1))B$, and we are done. □

There is eventually at most one contact between any pair of chambers

Next we shall prove that when ε is small enough, there is at most one arc in common between two different chambers.

Definition 1. *Given a set $E \subset \mathbb{R}^2$, we set B_E as the disk of the same area (say, centered at the origin), $r_E := \sqrt{|E|/\pi}$ as its radius and $\kappa_E = 1/r_E$ as the curvature of ∂B_E.*

Recall that the interface between the chambers $\mathscr{E}_\varepsilon(i)$ and $\mathscr{E}_\varepsilon(j)$ is $\mathscr{E}_\varepsilon(i,j) := \partial\mathscr{E}_\varepsilon(i) \cap \partial\mathscr{E}_\varepsilon(j)$, and that $\overline{\mathscr{E}_\varepsilon}$ denotes a minimizer for P_ε.

Lemma 2.12. *The curvature of the interface arcs $\overline{\mathscr{E}_\varepsilon}(i,j)$ converges up to sign as $\varepsilon \to 0$ to:*

(i) $\kappa_{\mathscr{E}(i)}$ *if* $j = 0$*;*

(ii) $\frac{1}{2}(\kappa_{\mathscr{E}(i)} - \kappa_{\mathscr{E}(j)})$ *if* $i, j \neq 0$.

Proof. By Theorem 2.7 (regularity) we know that the weighted curvatures sum to zero around any vertex:

$$(2-\varepsilon)\kappa_{ij}^\varepsilon + \kappa_{j0}^\varepsilon + \kappa_{0i}^\varepsilon = 0.$$

It is therefore sufficient to prove (i). This follows from the localization lemma 2.11: since each chamber $\overline{\mathscr{E}_\varepsilon}(i)$ is sandwiched between two concentric disks whose radii converge to the same value as $\varepsilon \to 0$, contacts between different chambers can happen in a finite number of zones whose diameter converge to zero. In the complement of these zones there will be only arcs of constant curvature, without triple points. Since each one of these arcs is sandwiched between two concentric disks converging to the same disk, the curvature must converge to the limit curvature $\kappa_{\mathscr{E}_\varepsilon(i)} = \kappa_{\mathscr{B}(i)}$. □

Lemma 2.13.

(i) The length of every interface between any pair of chambers goes to 0 *as* $\varepsilon \to 0$*, that is*

$$\lim_{\varepsilon\to 0} \mathscr{H}^1(\overline{\mathscr{E}_\varepsilon}(i,j)) = 0;$$

(ii) for ε small enough, any pair of chambers of $\overline{\mathscr{E}_\varepsilon}$ share at most one arc, that is $\overline{\mathscr{E}_\varepsilon}(i,j)$ has at most one connected component. If the two chambers converge to non-tangent disks, then they eventually share no boundary.

Proof. (i) This is a consequence of the localization lemma 2.11 and the lower semicontinuity of the perimeter. If two chambers converge to two non tangent disks, then the interface is eventually empty by the localization lemma and we are done. Otherwise, consider the case where the two limit disks have a tangency point p, and suppose by contradiction that for a sequence $\varepsilon_h \to 0$ it holds $\mathscr{H}^1(\overline{\mathscr{E}_{\varepsilon_h}}(i,j)) \geq c > 0$. Notice that again by the localization lemma, the interface is contained in a curved wedge that as $\varepsilon \to 0$ converges to the point p. Since $\overline{\mathscr{E}_\varepsilon}(i) \to B_i$, for every closed neighbourhood K of p we have by semicontinuity

$$P(B_i, K^c) \leq \liminf_{h\to\infty} P(\overline{\mathscr{E}_{\varepsilon_h}}(i), K^c).$$

Adding the inequality

$$c \leq \mathscr{H}^1(\overline{\mathscr{E}_{\varepsilon_h}}(i,j)) \leq \liminf_{h\to\infty} P(\overline{\mathscr{E}_{\varepsilon_h}}(i), K)$$

we obtain

$$\begin{aligned} P(B_i, K^c) + c &\leq \liminf_{h\to\infty} P(\overline{\mathscr{E}_{\varepsilon_h}}(i), K^c) + \liminf_{h\to\infty} P(\overline{\mathscr{E}_{\varepsilon_h}}(i), K) \\ &\leq \liminf_{h\to\infty} P(\overline{\mathscr{E}_{\varepsilon_h}}(i)) \\ &= P(B_i) \end{aligned}$$

which yields a contradiction by choosing the neighbourhood K small enough.

(ii) Suppose there is a component C of the exterior chamber entirely surrounded by two other chambers A and B. We prove that it is more convenient to add this component to one of the chambers and fix its total volume with a slight deflation. Call ℓ_A and ℓ_B the length of the respective interfaces with C, and suppose $\ell_A \leq \ell_B$. Then add C to chamber B, and slightly deflate B far from contact zones (which is always possible for small ε). The contributions to P_ε coming from C change from $\ell_A + \ell_B$ to $(2-\varepsilon)\ell_A$, with a total change of $\ell_A - \ell_B - \varepsilon\ell_A < 0$, while the deflation to fix the total volume of B can be chosen so that the energy decreases; this results in a global decrease in the energy P_ε.

□

An asymptotic quantitative isoperimetric inequality involving curvature

The aim of the following theorem is to prove a particular instance of quantitative isoperimetric inequality in the plane, involving how much the curvature of the boundary of a given set E deviates on small scales from the "ideal" curvature κ_E.

Theorem 2.14. *Let $E \subset \mathbb{R}^2$ be open, of finite area and perimeter and let $\bar\kappa > 0$ be a real number. Suppose the boundary of E contains $m \in \mathbb{N}$ portions made of arcs with constant curvature $\kappa_1, \dots, \kappa_m$, with $\kappa_i \leq \bar\kappa$, each arc having a corresponding chord of length ℓ_i. The curvature is signed, meaning that it is positive if the arc is curved outwards, and negative if it is curved inwards. Then*

$$P(E) \geq \sqrt{4\pi|E|} + \frac{1}{24}\sum_{i=1}^m \ell_i^3(\kappa_i - \kappa_E)^2 - O\left(\sum_{i=1}^m \ell_i^5\right).$$

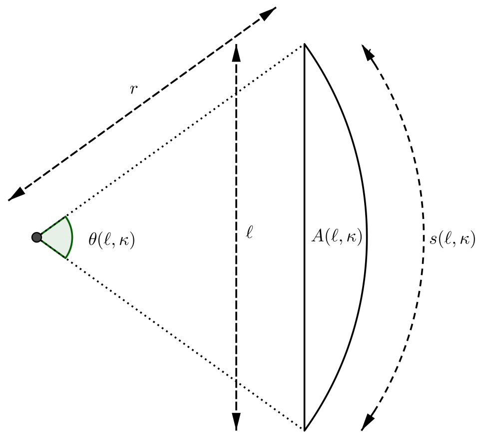


Figure 2.5: Reference figure for Lemma 2.16.

Remark 2.15. In loose terms the previous inequality can be seen as a sort of Taylor expansion of the perimeter functional with base point the disk, in the same spirit as Hales's inequality [Hal01, Theorem 4] can be seen as a Taylor expansion of the perimeter with base point the regular hexagon. It would be interesting to know whether these two inequalities are a particular case of a more general Taylor expansion of the perimeter functional.

We begin with a simple lemma, of which we omit the proof.

Lemma 2.16. *Consider a segment in the plane of length ℓ and an arc of constant curvature κ connecting its endpoints, and let θ and r be the related angle and radius as in Figure 2.5. Then the angle θ, the length s of the arc and the area A of the circular section are given respectively by:*

$$\begin{aligned}
\theta(\ell,\kappa) &= 2\arcsin\frac{\ell\kappa}{2} = \ell\kappa + \frac{1}{24}\ell^3\kappa^3 + O(\ell^5\kappa^5)\\
s(\ell,\kappa) &= \frac{2}{\kappa}\arcsin\left(\frac{\ell\kappa}{2}\right) = \ell + \frac{1}{24}\ell^3\kappa^2 + O(\ell^5\kappa^3)\\
A(\ell,\kappa) &= \frac{\theta r^2}{2} - r^2\cos\frac{\theta}{2}\sin\frac{\theta}{2} = \frac{1}{12}\ell^3\kappa + O(\ell^5\kappa^3).
\end{aligned}$$

We now pass to the proof of Theorem 2.14.

Proof of Theorem 2.14. We inflate or deflate each arc until it reaches curvature κ_E, that is we replace the given arcs of curvature κ_i with an arc of curvature κ_E with the same endpoints, to obtain a new set $\tilde{E}$ with area $A(\tilde{E}) = A(E) + \Delta A$ and perimeter $P(\tilde{E}) = P(E) + \Delta P$; then we apply the isoperimetric inequality of Proposition 2.9 to the new set $\tilde{E}$ and draw the consequences for the original set E, exploiting the explicit fomulas given by the previous lemma. We set for simplicity $\ell = \sum_{i=1}^{m} \ell_i$.

By Lemma 2.16 we can compute explicitly

$$\begin{aligned}
\Delta P &= \sum_{i=1}^{m} \left(s(\ell_i, \kappa_E) - s(\ell_i, \kappa_i)\right) \\
&= \sum_{i=1}^{m} \frac{1}{24} \ell_i^3 (\kappa_i^2 - \kappa_E^2) + O\left(\ell^5\right) \\
\Delta A &= \sum_{i=1}^{m} \left(A(\ell_i, \kappa_E) - A(\ell_i, \kappa_i)\right) \\
&= \sum_{i=1}^{m} \frac{1}{12} \ell_i^3 (\kappa_E - \kappa_i) + O\left(\ell^5\right).
\end{aligned}$$

The isoperimetric inequality applied to $\tilde{E}$ gives $P(\tilde{E}) \geq \sqrt{4\pi|\tilde{E}|}$. Therefore

$$\begin{aligned}
P(E) = P(\tilde{E}) - \Delta P &\geq \sqrt{4\pi}\sqrt{|E| + \Delta A} - \Delta P \\
&= \sqrt{4\pi|E|}\sqrt{1 + \frac{\Delta A}{|E|}} - \Delta P \\
&= \sqrt{4\pi|E|}\left(1 + \frac{1}{2}\frac{\Delta A}{|E|}\right) + O\left(\frac{\Delta A}{|E|}\right)^2 - \Delta P \\
&= \sqrt{4\pi|E|} + \kappa_E \Delta A - \Delta P + O(\ell^6).
\end{aligned}$$

Inserting now the asymptotic expansions for ΔA and ΔP we obtain

$$\begin{aligned}
P(E) &\geq \sqrt{4\pi|E|} + \sum_{i=1}^{m} \left(\kappa_E \frac{1}{12} \ell_i^3 (\kappa_E - \kappa_i) - \frac{1}{24} \ell^3 (\kappa_e - \kappa_i)^2\right) - O\left(\ell^5\right) \\
&= \sqrt{4\pi|E|} + \sum_{i=1}^{m} \frac{1}{24} \ell_i^3 (\kappa_i - \kappa_E)^2 - O\left(\ell^5\right).
\end{aligned}$$

$\square$

Consequences for the N-bubble: lower-bound inequality

In this section we will derive the consequences of Theorem 2.14 in the general case of weighted clusters with possibly different areas, obtaining the lower bound for the energy P_ε given by Proposition 2.18. We find it useful, however, to examine first the simpler case of a double bubble with equal areas, to explain the idea behind it. In particular, we will obtain the asymptotics given by (2.3) as a lower bound, without using the explicit shape of minimizers.

Proposition 2.17. *For every 2-cluster $\mathscr{E} = (E_1, E_2)$ with both areas equal to π we have*

$$P_\varepsilon(\mathscr{E}) \geq 4\pi - \frac{4}{3}\varepsilon^{3/2} - O(\varepsilon^{5/2}).$$

Proof. It is clearly sufficient to prove the statement when $\mathscr{E}$ is a minimizer of P_ε under the same volume constraint. By Lemma 2.13 we know that the chambers will have at most one single arc in common. Suppose this arc has length s and curvature κ, and that the chord of this arc has length ℓ . Then writing

$$P_\varepsilon(\mathscr{E}) = P(E_1) + P(E_2) - \varepsilon s,$$

recalling Lemma 2.16 and applying Theorem 2.14 to both chambers we obtain

$$\begin{aligned}
P_\varepsilon(\mathscr{E}) &\geq 4\pi + \frac{1}{24}\ell^3\left((1-\kappa)^2 + (1+\kappa)^2\right) - \varepsilon\left(\ell + \frac{1}{24}\ell^3\kappa^2 + O(\ell^5)\right) - O(\ell^5) \\
&= 4\pi + \frac{1}{12}\ell^3 - \varepsilon\ell + \frac{1}{12}\kappa^2\ell^3\left(1 - \frac{\varepsilon}{2}\right) - O(\ell^5) \\
&\geq 4\pi + \frac{1}{12}\ell^3 - \varepsilon\ell - O(\ell^5)
\end{aligned}$$

where the key fact is that the curvature κ appears in the first line once with a positive sign and once with a negative sign, and where the last inequality follows from $\varepsilon \leq 2$. We now optimize in $\ell \geq 0$ the expression $\frac{1}{12}\ell^3 - \varepsilon\ell$ to obtain the minimum point $\ell = 2\varepsilon^{1/2}$, and thus obtaining

$$P_\varepsilon(\mathscr{E}) \geq 4\pi - \frac{4}{3}\varepsilon^{3/2} - O(\varepsilon^{5/2})$$

as wanted. □

We will now perform a computation similar to the previous one, but this time for a general number N of chambers and possibly different areas, to obtain a lower bound for the energy P_ε.

Proposition 2.18. *Let $\mathscr{E} = \{E_1, \dots, E_N\}$ be a planar cluster whose chambers have areas $|E_i| = m_i = \pi r_i^2$ and therefore ideal curvature $\kappa_{E_i} = 1/r_i$ (see Definition 1), and whose boundaries have piecewise constant curvature. Suppose that every pair of chambers shares at most one arc. Then*

$$P_\varepsilon(\mathscr{E}) \geq \sum_{i=1}^N P(B_{E_i}) - \frac{4}{3}\varepsilon^{3/2}\sum_{1\leq i<j\leq N}\sigma_{ij}\frac{2r_ir_j}{r_i+r_j} + O(\varepsilon^{5/2}) \tag{2.10}$$

where σ_{ij} is one if the chambers E_i and E_j share some boundary, and zero otherwise.

Proof. Call κ_{ij} the curvature of the arc between chambers i and j, s_{ij} its length and ℓ_{ij} the length of the relative chord (we omit for simplicity the dependence on ε), and set $\ell = \sum_{i,j}\ell_{ij}$. We apply Theorem 2.14 to each chamber to obtain

$$\begin{aligned}
P_\varepsilon(\mathscr{E}) &= \sum_{i=1}^N P(E_i) - \varepsilon\sum_{1\leq i<j\leq N} s_{ij} \\
&\geq \sum_{i=1}^N\left(P(B_{E_i}) + \frac{1}{24}\sum_{j\neq i}\ell_{ij}^3(\kappa_{ij} - \kappa_{E_i})^2 - O(\ell^5)\right) - \varepsilon\sum_{1\leq i<j\leq N} s_{ij} \\
&= \sum_{i=1}^N P(B_{E_i}) + \sum_{1\leq i<j\leq N}\left(\frac{1}{24}\ell_{ij}^3\left((\kappa_{ij} - \kappa_{E_i})^2 + (\kappa_{ij} + \kappa_{E_j})^2\right)\right. \\
&\qquad\qquad \left. -\varepsilon\left(\ell_{ij} + \frac{1}{24}\ell_{ij}^3\kappa_{ij}^2\right)\right) - O(\ell^5).
\end{aligned}$$

Now we first optimize in κ_{ij} each term in the sum, i.e. the quadratic polynomial in κ_{ij} given by

$$\begin{aligned}&\frac{1}{24}\ell_{ij}^3\left((\kappa_{ij}-\kappa_{E_i})^2+(\kappa_{ij}+\kappa_{E_j})^2\right)-\varepsilon\left(\ell_{ij}+\frac{1}{24}\ell_{ij}^3\kappa_{ij}^2\right)\\ =&\frac{1}{24}\ell_{ij}^3\left((2-\varepsilon)\kappa_{ij}^2+2(\kappa_{E_j}-\kappa_{E_i})\kappa_{ij}+\kappa_{E_i}^2+\kappa_{E_j}^2\right)-\varepsilon\ell_{ij}.\end{aligned}$$

The minimum point is easily seen to be

$$\kappa_{ij}=\frac{\kappa_{E_i}-\kappa_{E_j}}{2-\varepsilon} \tag{2.11}$$

giving the expression a minimum value of

$$\begin{aligned}&\frac{1}{24}\ell_{ij}^3\left(\kappa_{E_i}^2+\kappa_{E_j}^2+\frac{(\kappa_{E_i}-\kappa_{E_j})^2}{2-\varepsilon}\right)-\varepsilon\ell_{ij}\\ =&\frac{1}{24}\ell_{ij}^3\left(\frac{1}{2}(\kappa_{E_i}+\kappa_{E_j})^2-\frac{\varepsilon}{4-2\varepsilon}(\kappa_{E_i}-\kappa_{E_j})^2\right)-\varepsilon\ell_{ij}.\end{aligned} \tag{2.12}$$

We now optimize in ℓ_{ij}: setting the derivative in ℓ_{ij} equal to zero we find

$$\begin{aligned}\ell_{ij}^2&=\frac{8\varepsilon}{\frac{1}{2}(\kappa_{E_i}+\kappa_{E_j})^2-\frac{\varepsilon}{4-2\varepsilon}(\kappa_{E_i}-\kappa_{E_j})^2}\\ &=\frac{16\varepsilon}{(\kappa_{E_i}+\kappa_{E_j})^2}+O(\varepsilon^2)\end{aligned}$$

which implies

$$\ell_{ij}=\frac{4}{\kappa_{E_i}+\kappa_{E_j}}\varepsilon^{1/2}+O(\varepsilon^{3/2}). \tag{2.13}$$

Substituting this back into (2.12) and observing that by the previous computation $O(\ell^5)=O(\varepsilon^{5/2})$, we obtain that the expression is greater than

$$-\frac{8}{3}\varepsilon^{3/2}\frac{1}{\kappa_{E_i}+\kappa_{E_j}}+O(\varepsilon^{5/2})$$

and now summing among all pairs (i,j) we obtain

$$P_\varepsilon(\overline{\mathscr{E}_\varepsilon})\geq\sum_{i=1}^N P(B_{E_i})-\frac{4}{3}\varepsilon^{3/2}\sum_{1\leq i<j\leq N}\sigma_{ij}\frac{2}{\kappa_{E_i}+\kappa_{E_j}}+O(\varepsilon^{5/2})$$

which is the desired result.

□

As a consequence of the previous inequality and Lemmas 2.11 and 2.13 we obtain the following:

Corollary 2.19. *Suppose minimizers $\overline{\mathscr{E}_\varepsilon}$ converge as $\varepsilon \to 0$ to the cluster of disks $\mathscr{B}$. Then*

$$P(\overline{\mathscr{E}_\varepsilon}) \geq P(\mathscr{B}) - \frac{4}{3}\varepsilon^{3/2}\mathscr{T}(\mathscr{B}) + O(\varepsilon^{5/2})$$

where $\mathscr{T}$ is the tangency functional (2.5).

Remark 2.20 (Non-optimal lower bound for P_ε)**.** Viewing an N-cluster as a "superposition" of 2-clusters we can obtain a worse lower bound than equation (2.10), but with the same order of $\varepsilon^{3/2}$ for the second term. We notice that for $N \geq 2$ we can rewrite

$$P_\varepsilon(\mathscr{E}) = \frac{1}{N-1}\sum_{1\leq i<j\leq N} P_{\delta(\varepsilon)}\big((\mathscr{E}(i),\mathscr{E}(j))\big)$$

where $\delta(\varepsilon) = (N-1)\varepsilon$ and $P_\delta((\mathscr{E}(i),\mathscr{E}(j))) = P(\mathscr{E}(i)) + P(\mathscr{E}(j)) - \delta\mathscr{H}^1(\mathscr{E}(i,j))$ is the weighted perimeter of the 2-cluster $(\mathscr{E}(i),\mathscr{E}(j))$. From the solution of the double bubble (for simplicity in the case of equal volumes $|\mathscr{E}(i)| = \pi$) we know that $P_\delta((E_i,E_j)) \geq 4\pi - \frac{4}{3}\delta^{3/2} + O(\delta^{5/2})$ from which

$$\begin{aligned}
P_\varepsilon(\mathscr{E}) &= \frac{1}{N-1}\sum_{1\leq i<j\leq N} P_{\delta(\varepsilon)}((E_i,E_j)) \\
&\geq \frac{1}{N-1}\sum_{1\leq i<j\leq N}\left(4\pi - \sigma_{ij}(\mathscr{E})\frac{4}{3}\delta^{3/2} + O(\delta^{5/2})\right) \\
&= 2N\pi - \frac{4}{3}\sqrt{N-1}\,\mathscr{C}(\mathscr{E})\varepsilon^{3/2} + O(\varepsilon^{5/2})
\end{aligned}$$

where $\mathscr{C}(\mathscr{E}) = \sum_{i<j}\sigma_{ij}(\mathscr{E})$ is the number of pairs (i,j) such that E_i and E_j share some boundary. This is the estimate we are looking for, except for the factor $\sqrt{N-1}$ which makes the inequality worse. Observe that we can not obtain in this way the optimal inequality we are aiming to: indeed each double-bubble inequality is optimal when there is just one contact between two disks and the remaining portion of boundary is circular, which can not be simultaneously true for all pairs of bubbles.

Sharpness of lower bound (recovery sequence)

We now want to show that the inequality proved in Corollary 2.19 is essentially sharp, which means that, given a cluster of disks $\mathscr{B} = (B_1\dots,B_N)$, we can actually find a sequence of clusters $\mathscr{E}_\varepsilon$ converging to $\mathscr{B}$ for which the reverse inequality holds. We think that there should be a simpler way to do this other than the way proposed in the following, analyzing the sharpness of the inequality of Theorem 2.14, which is used to prove Proposition 2.18. However we were not able to follow this route and instead propose in the following a quite explicit and tedious computation for the polar equation of each chamber of an approximating sequence.

The idea is to construct between any pair of tangent disks B_i, B_j in the limit cluster $\mathscr{B}$ an arc whose constant curvature is $\frac{1}{2}(\kappa_{E_i} - \kappa_{E_j})$ (which is the right asymptotic value given by condition (ii) in Lemma 2.12), of length $\ell_{ij}^\varepsilon = 4\varepsilon^{1/2}/(\kappa_{E_i} + \kappa_{E_j})$ (which is up to $O(\varepsilon^{3/2})$ the optimal value found in (2.13)). In the remaining portion of the boundaries of the chambers $\mathscr{E}_\varepsilon(i)$ we can pretty much put any interface which, in polar coordinates w.r.t. the center of B_i, has $W^{1,\infty}$ norm at most $O(\varepsilon^2)$; we achieve this by a simple two-piece piecewise linear interpolation in the angle variable. Recall that the total area must be $|B_i|$ to satisfy the area constraint, hence the need for an interpolation.

We start with a couple of simple lemmas regarding the area and perimeter of small perturbations of a circle. We parametrize $\mathscr{S}^1$ by $\gamma : [-\pi, \pi] \to \mathbb{R}^2$,

$$\gamma(t) = \begin{pmatrix} \cos t \\ \sin t \end{pmatrix}$$

and consider a normal perturbation with magnitude $u : [-\pi, \pi] \to (-1, \infty)$, which gives a variation

$$\gamma_u(t) = \gamma(t) + u(t)\nu(t) = (1 + u(t))\gamma(t)$$

where $\nu(t) = \gamma(t)$ is the outer normal. Using the formula for the area in polar coordinates we obtain the following result.

Lemma 2.21 (Variation of area).

$$Area(\gamma_u) = \pi + \int_{-\pi}^{\pi} u(t)dt + \frac{1}{2}\int_{-\pi}^{\pi} u(t)^2 dt. \tag{2.14}$$

Lemma 2.22 (Variation of perimeter). *If $u(t) \geq -\frac{1}{2}$ for every t and $\|u\|_{W^{1,\infty}} \leq 1$, then the length $L(\gamma_u)$ of the curve γ_u satisfies*

$$L(\gamma_u) = 2\pi + \int_{-\pi}^{\pi} u(t)dt + \frac{1}{2}\int_{-\pi}^{\pi} u'(t)^2 dt + O\big(\|u\|^3_{W^{1,\infty}}\big). \tag{2.15}$$

Proof. We have

$$\gamma_u'(t) = (1 + u(t))\gamma'(t) + u'(t)\gamma(t)$$

and by the orthogonality of γ and γ' we obtain

$$|\gamma_u'(t)| = \sqrt{(1+u(t))^2 + u'(t)^2} = \sqrt{1 + 2u(t) + u(t)^2 + u'(t)^2}.$$

By the Taylor expansion with Lagrange remainder

$$\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + r(x)$$

with $r(x) = \frac{1}{16(1+\xi)^{5/2}}x^3$ and ξ between 1 and x. Set $x = 2u(t) + u(t)^2 + u'(t)^2$. From $u(t) \geq -\frac{1}{2}$ we obtain $x \geq -\frac{3}{4}$, and then also $\xi \geq -\frac{3}{4}$, thus $|r(x)| \leq C|x|^3$ for every $x \geq -\frac{3}{4}$. Therefore

$$\begin{aligned} L(\gamma_u) &= \int_{-\pi}^{\pi} |\gamma_u'(t)| dt \\ &= \int_{-\pi}^{\pi} \left(1 + u + \frac{1}{2}(u^2 + u'^2) - \frac{1}{8}(2u + u^2 + u'^2)^2 + r(u)\right) dt \\ &= 2\pi + \int_{-\pi}^{\pi} u + \frac{1}{2}\int_{-\pi}^{\pi} u'^2 + O\big(\|u\|^3_{W^{1,\infty}}\big). \end{aligned}$$

□

Remark 2.23. In particular consider a variation u which preserves the area, that is

$$\int u = -\frac{1}{2}\int u^2.$$

Then plugging this into (2.15) we obtain that for an area-preserving variation, the perimeter is

$$2\pi + \frac{1}{2}\int (u'^2 - u^2) + O\big(\|u\|^3_{W^{1,\infty}}\big).$$

Lemma 2.24. *Consider a circle of radius r centered at the origin and given $R \in \mathbb{R}$ consider a circle of radius $|R|$ tangent to the first one whose center has cartesian coordinates $(r+R,0)$, (so that if R is positive it is on the opposite side with respect to the tangent line, if R is negative it is on the same side). Then the polar coordinates of the second circumference in a neighbourhood of the tangency point are given by:*

$$\rho(\theta) = (R+r)\cos\theta - R\sqrt{1-\left(1+\frac{r}{R}\right)^2 \sin^2\theta},$$

and the Taylor expansion for small θ is

$$\rho(\theta) = r + \frac{r}{2}\left(1+\frac{r}{R}\right)\theta^2 + O(\theta^4).$$

Proof. The polar equation of a circumference of radius R whose center has polar coordinates (r_0,ϕ) is given by

$$\rho^2 + r_0^2 - 2\rho r_0 \cos(\theta-\phi) = R^2.$$

In our case $(r_0,\phi) = (r+R,0)$. Inserting this into the previous equation and solving for ρ (and choosing the right sign) gives the desired conclusion. □

Theorem 2.25 (Recovery sequence). *For every cluster of disks $\mathscr{B} = (B_1,\dots,B_N)$ with radii $r_1,\dots,r_N$ we can construct a recovery sequence $\mathscr{E}_\varepsilon$, namely a sequence such that $\mathscr{E}_\varepsilon \to \mathscr{B}$ in the convergence of clusters and such that*

$$P_\varepsilon(\mathscr{E}_\varepsilon) = \sum_{i=1}^N 2\pi r_i - \frac{4}{3}\varepsilon^{3/2}\sum_{1\le i<j\le N}\sigma_{ij}\frac{2r_ir_j}{r_i+r_j} + O(\varepsilon^{5/2})$$

where

$$\sigma_{ij} = \begin{cases} 1 & \text{if } B_i \text{ and } B_j \text{ touch} \\ 0 & \text{otherwise} \end{cases}.$$

Proof. We build, for each disk in the limit configuration, a "dented" disk, inserting small arcs of constant curvature $\kappa_{ij} = \frac{1}{2}\left(\frac{1}{r_j}-\frac{1}{r_i}\right)$ between two tangent disks B_i and B_j. The length of the corresponding chord is set to be $\ell^\varepsilon_{ij} = \frac{4r_ir_j}{r_i+r_j}\varepsilon^{1/2}$ (these are the asymptotically optimal values given by the optimizations in (2.11) and (2.13)).

We describe the boundary of $\mathscr{E}_\varepsilon(i)$ in polar coordinates w.r.t. the center of B_i by the function $\rho_i(\theta)$. Around any contact point $p_{ij} = (r_i, \theta_{ij})$, thanks to the previous lemma, the parametrization is given by

$$\rho_i(\theta) = r_i + \frac{r_i}{2}\left(1 + \frac{r_i}{R_{ij}}\right)(\theta - \theta_{ij})^2 + O((\theta - \theta_{ij})^4)$$

where $R_{ij} = 1/\kappa_{ij}$. We now suppose for simplicity $\theta_{ij} = 0$ (we are interested in computing only lengths, which are rotation invariant) and compute the polar coordinates of the endpoints of the (i, j)-arc, whose chord has length ℓ^ε_{ij}: they are given by $(\rho_i(\Delta\theta_i), \Delta\theta_i)$ and $(\rho(-\Delta\theta_{ij}), -\Delta\theta_{ij})$ where $\Delta\theta_{ij}$ is implicitly given by

$$2\rho_i(\Delta\theta_{ij}) \sin \Delta\theta_{ij} = \ell^\varepsilon_{ij}.$$

We now invert this expression to obtain the Taylor expansion of $\Delta\theta_{ij}$ in terms of ℓ^ε_{ij}: first insert the Taylor expansions of $\rho_i(\theta)$ and $\sin\theta$ to obtain

$$2\left(r_i + \frac{r_i}{2}\left(1 + \frac{r_i}{R_{ij}}\right)\Delta\theta^2_{ij} + O(\Delta\theta^4_{ij})\right)\left(\Delta\theta_{ij} - \frac{1}{6}\Delta\theta^3_{ij} + O(\Delta\theta^5_{ij})\right) = \ell^\varepsilon_{ij}.$$

Then a simple computation yields

$$\Delta\theta_{ij} = \frac{\ell^\varepsilon_{ij}}{2r_i} + O(\varepsilon^{3/2}).$$

Using Lemma 2.22 and a rescaling, setting $(1 + u(\theta))r_i = \rho_i(\theta)$, and observing that we can set the total area to be $|B_i|$ with $\rho_i(\theta)$ being piecewise linear between two consecutive arcs and having there $W^{1,\infty}$-norm bounded by a constant times ε^2, we find that

$$\begin{aligned}
P(\mathscr{E}_\varepsilon(i)) &= r_i\left(2\pi + \frac{1}{2}\int (u'(t)^2 - u(t)^2)dt + O(\varepsilon^{5/2})\right) \\
&= r_i\left(2\pi + \frac{1}{2}\int_{-\Delta\theta_{ij}}^{\Delta\theta_{ij}} u'(t)^2 dt + O(\varepsilon^{5/2})\right) \\
&= r_i\left(2\pi + \frac{1}{2}\int_{-\Delta\theta_{ij}}^{\Delta\theta_{ij}} \left(1 + \frac{r_i}{R_{ij}}\right)^2 t^2 dt + O(\varepsilon^{5/2})\right) \\
&= 2\pi r_i + \frac{r_i}{2}\frac{(r_i + R_{ij})^2}{R^2_{ij}}\frac{2}{3}\Delta\theta^3_{ij} + O(\Delta\theta^5_{ij}) \\
&= 2\pi r_i + \frac{1}{3}\frac{r_i R_{ij}}{r_i + R_{ij}}\varepsilon^{3/2} + O(\varepsilon^{5/2})
\end{aligned}$$

where we used that the only relevant term up to $O(\varepsilon^{5/2})$ in the integral is $u'(t)^2$ between $-\Delta\theta_{ij}$ and $\Delta\theta_{ij}$. Moreover, recalling Lemma 2.16, we have

$$s(\ell^\varepsilon_{ij}, \kappa_{ij}) = \ell^\varepsilon_{ij} + O(\varepsilon^{3/2}).$$

Therefore summing among all the arcs of the chamber $\mathscr{E}_\varepsilon(i)$ we obtain

$$P(\mathscr{E}_\varepsilon(i)) - \frac{\varepsilon}{2}\sum_j s(\ell^\varepsilon_{ij}, \kappa_{ij}) = 2\pi r_i - \frac{2}{3}\varepsilon^{3/2}\sum_j \frac{r_i R_{ij}}{r_i + R_{ij}} + O(\varepsilon^{5/2}).$$

Now summing among all i's, and recalling that $\frac{1}{R_{ij}} = \frac{1}{2}\left(\frac{1}{r_j} - \frac{1}{r_i}\right)$, each arc (i, j) is counted with a weight given by

$$\begin{aligned} & -\frac{2}{3}\varepsilon^{3/2}\left(\frac{1}{\frac{1}{R_{ij}}+\frac{1}{r_i}} - \frac{1}{\frac{1}{R_{ij}}-\frac{1}{r_j}}\right) \\ = & -\frac{4}{3}\varepsilon^{3/2}\frac{2r_ir_j}{r_i+r_j} \end{aligned}$$

which is the desired result. □

Proof of the main theorems

We now put together the previously obtained results to prove Theorem 2.2 and Theorem 2.4.

Proof of Theorem 2.2. Given a family of minimizing clusters $\overline{\mathscr{E}_\varepsilon}$ converging to $\mathscr{B}$, by the regularity Theorem 2.7 they have boundary of piecewise constant curvature. By Lemma 2.13 all curvatures are bounded, and every pair of chambers $\overline{\mathscr{E}_\varepsilon}(i)$ and $\overline{\mathscr{E}_\varepsilon}(j)$ shares at most one arc, and shares no arc if the limit disks B_i and B_j are not tangent. Applying Corollary 2.19 we obtain that

$$P_\varepsilon(\overline{\mathscr{E}_\varepsilon}) \geq \sum_{i=1}^N P(B_i) - \frac{4}{3}\mathscr{T}(\mathscr{B})\varepsilon^{3/2} + O(\varepsilon^{5/2}), \tag{2.16}$$

or equivalently (recalling definition (2.4)) that

$$P_\varepsilon^{(1)}(\overline{\mathscr{E}_\varepsilon}) \geq -\mathscr{T}(\mathscr{B}) + O(\varepsilon).$$

By Theorem 2.25 we can actually find a recovery sequence, that is a sequence $\mathscr{E}_\varepsilon$ converging to $\mathscr{B}$ and such that

$$P_\varepsilon(\mathscr{E}_\varepsilon) = \sum_{i=1}^N P(B_i) - \frac{4}{3}\mathscr{T}(\mathscr{B})\varepsilon^{3/2} + O(\varepsilon^{5/2}),$$

which shows the other inequality in (2.16). In particular,

$$P_\varepsilon^{(1)}(\overline{\mathscr{E}_\varepsilon}) = -\mathscr{T}(\mathscr{B}) + O(\varepsilon),$$

and in order to minimize P_ε for ε small enough, it is necessary that the limit cluster $\mathscr{B}$ maximizes $\mathscr{T}(\mathscr{B})$, the number of weighted tangencies.

□

Proof of Theorem 2.4. Theorem 2.7 implies that there are a finite number of arcs of constant curvature, meeting in a finite number of vertices. By Lemma 2.8 at every vertex exactly three arcs meet, one of the chambers is the exterior one and the angle θ_ε is given by $\theta_\varepsilon = \arccos(1-\varepsilon/2)$. By Lemma 2.12 the curvatures of the arcs are converging to the desired values. By Lemma 2.13 there is at most one arc between any pair of chambers whose limit disks are tangent, and none otherwise. Moreover, it follows from Proposition 2.18 that in the former case, for ε small enough there is *exactly* one arc, otherwise we would get a worse inequality from Proposition 2.18, that is $\lim_{\varepsilon\to 0} P^{(1)}_\varepsilon(\overline{\mathscr{E}_\varepsilon}) > -\mathscr{T}(\mathscr{B})$. Finally, the length ℓ^ε_{ij} of the arc between $\overline{\mathscr{E}_\varepsilon}(i)$ and $\overline{\mathscr{E}_\varepsilon}(j)$ must be $o(\varepsilon^{1/2})$-close to the optimal value given by (2.13), otherwise again we would obtain a worse inequality.

□

2.4 Remarks

(i) *Higher dimension.* A natural question is whether an analogous result holds for minimizing clusters in $\mathbb{R}^n$, where the weights are given by 2.2 and the length is replaced by the Hausdorff measure $\mathscr{H}^{n-1}$. This will be the object of the last section of this chapter. The first-order results of Section 2.2 are true in any dimension. The proof of compactness is however more subtle, as in dimension $n \geq 3$ such a strong regularity result as Theorem 2.7 is not available, and moreover perimeter does not control diameter even for connected smooth sets. The proof follows the lines of [Mag12, Theorem 29.1]. The localization lemma 2.11 is still true but requires a different proof, see Proposition 2.32. The second-order results of Section 2.3 seem more difficult to extend, mainly because of the lack of a strong regularity result. In the planar case we are able to make explicit computations thanks to the fact that we are dealing with arcs of constant curvature.

(ii) *The case $\varepsilon \to 2$.* The other natural asymptotic behaviour we could consider is for $\varepsilon \to 2$, which is the limit for the triangle inequalities (2.6) to hold. In this case for minimal clusters the union of all chambers $\bigcup_{i=1}^N \overline{\mathscr{E}_\varepsilon}(i)$ converges to a disk (by the isoperimetric inequality) and the cluster converges up to subsequence and rigid motions to an optimal partition of the disk. This is much simpler to prove than the main result of this paper: in this case, setting $\alpha = 2-\varepsilon$, the relevant rescaled functionals are

$$G_\alpha(\mathscr{E}) = \frac{P_{2-\alpha}(\mathscr{E}) - (1-\alpha)2\pi\sqrt{N}}{\alpha}$$

which Γ-converge to $P(\mathscr{E})$.

The $\liminf$ inequality is an immediate consequence of the rewriting

$$G_\alpha(\mathscr{E}) = P(\mathscr{E}) + \frac{1-\alpha}{\alpha}(P(\mathscr{E}(0)) - 2\pi\sqrt{N}) \geq P(\mathscr{E})$$

while the recovery sequence is given by the constant sequence.

(iii) *Higher order expansion.* Even though Theorem 2.2 highly restricts the class of possible clusters of disks we can see in the limit $\varepsilon \to 0$, it doesn't completely characterizes them because of a general lack of uniqueness of minimizers for the tangency functional $\mathscr{T}$ in 2.5: in the case of equal radii already for $N = 6$ there are three distinct minimizers, see Figure 2.6; see also [DLF17] for the characterization of those N which admit a unique minimizer for the sticky disk potential. For those N that admit many minimizers, a way to select among them would be to go beyond the order $\varepsilon^{3/2}$ and look at the subsequent order in the expansion of perimeter. However this seems quite difficult

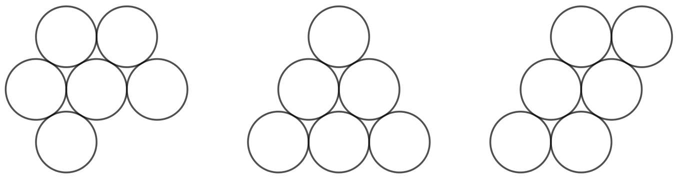


Figure 2.6: For $N = 6$ and equal radii there are three distinct minimizers of the tangency functional $\mathscr{T}$.

and apparently involves some "non-local" terms. A computation in the case of equal areas seems to suggest that the relevant quantity to be maximized at the next order is the total number of paths of length 2 in the *bond graph* associated to $\mathscr{B}$, that is the graph where vertices are the centers of the disks and edges are drawn when two disks touch (notice that the tangency functional is exactly the number of paths of length 1, i.e. edges, in the same graph). However there are no rigorous results in this direction. This leaves a question which could be of some interest:

Open problem (maximizing k-paths in subgraphs of the triangular lattice) Among finite subgraphs of order N of the triangular lattice, find those which maximize the total number of k-paths contained in them.

Here the number of k-paths of a graph G is the total number of distinct discrete paths of length k which at each step move from a vertex to one of its neighbours. The central limit theorem this time suggests that, as k goes to infinity, a circular global shape could be the preferred one.

2.5 Higher dimension

We now consider tha analogue of (2.2) in general dimension. We thus consider N-clusters $\mathscr{E} = (\mathscr{E}(1), \dots, \mathscr{E}(N))$ in $\mathbb{R}^n$, and minimize the perimeter

$$P_\varepsilon(\mathscr{E}) = \frac{1}{2} \sum_{\substack{0 \le i,j \le N \\ i \ne j}} c_{ij}(\varepsilon) \mathscr{H}^{n-1}(\partial^* \mathscr{E}(i) \cap \partial^* \mathscr{E}(j)) \tag{2.17}$$

where as in the previous sections

$$c_{ij}(\varepsilon) = \begin{cases} 1 & \text{if } i = 0 \text{ or } j = 0 \\ 2 - \varepsilon & \text{if } i, j \ne 0 \end{cases}. \tag{2.18}$$

The goal is to prove a *sticky-disk limit* result analogous to Theorem 2.2. However we are not able to prove a lower-bound inequality analogous to Corollary 2.19, because we lack the strong regularity results that are available in dimension 2. In the following we will partially extend the results of the previous sections to gneeral dimension. In particular we will prove the analogue of the Localization Lemma 2.11.

We begin by proving the Truncation Lemma, which is then used to prove the Localization Lemma.

First variation of volume and perimeter

Given an open set $\Omega \subset \mathbb{R}^n$, we consider the following family of diffeomorphisms: fix a smooth vectorfield $T \in C_c^\infty(\Omega, \mathbb{R}^n)$, and consider

$$\Phi_t(x) := x + tT(x).$$

Then, for $t < \varepsilon$ with ε sufficiently small, Φ_t is a smooth diffeomorphism such that $\{x : \Phi_t(x) \neq x\} \subset\subset \Omega$. We call the family $\{\Phi_t\}_{t<\varepsilon}$ a **local variation** in Ω.

Given a finite perimeter set $E \subset \mathbb{R}^n$, we now consider its first variation of volume and perimeter, that is a formula to compute $P(\Phi_t(E))$ and $|\Phi_t(E)|$ for small t.

Theorem 2.26 (**First variation of volume** [Mag12, Theorem 17.8]). *Given a set of finite perimeter $E \subset \mathbb{R}^n$, given a local variation $\{\Phi_t\}_{t<\varepsilon}$ as defined above, we have*

$$|\Phi_t(E)| = |E| + t\int_{\partial * E} T \cdot \nu_E d\mathscr{H}^{n-1} + O(t^2) = |E| + t\int_E \operatorname{div} T + O(t^2). \tag{2.19}$$

where the constants involved in O depend only on T and $|E|$.

Theorem 2.27 (**First variation of perimeter** [Mag12, Theorem 17.5]). *If E is a set of finite perimeter in $\mathbb{R}^n$ and $\{\Phi_t\}_{t<\varepsilon}$ is a local variation as defined above, then*

$$P(\Phi_t(E)) = P(E) + t\int_{\partial^* E} \operatorname{div}^\tau T d\mathscr{H}^{n-1} + O(t^2) \tag{2.20}$$

where $\operatorname{div}^\tau T(x) = \operatorname{div} T(x) - \nu_E(x) \cdot (\nabla T(x)\nu_E(x))$ is the ***tangential divergence*** *of T, and where the constants involved in O depend only on T and $P(E)$.*

Truncation Lemma

The Truncation Lemma could be roughly summarized as "upgrading L^1 convergence to uniform convergence", and it's an intermediate result towards the analogue in higher dimension of Lemma 2.11. We named it *truncation* lemma (instead of *localization*, as in the planar case) because of the different method involved in the proof: truncation and volume-fixing variations. In particular we use a standard method which involves writing a differential inequality that involves the function $m(r) := |E \cap B_r|$. We reserve the name *localization lemma* for Proposition 2.32, which is really the analogue of Lemma 2.11.

We begin with a simplified version of the Truncation Lemma to explain the idea behind the proof, even though this simplified version could be proved in a much simpler way thorugh a calibration argument (see Remark 2.29); then we will prove the full version. In the simplified version the result is the following: if a finite perimeter set E is sufficiently close (in measure) to a ball B_1 with the same volume, then we can decrease the perimeter of E by truncating it with a ball B_{1+r}, with $r > 0$ sufficiently small depending on δ.

The idea of the proof is a more or less standard method in minimal surfaces problems: obtaining a differential inequality that involves the volume of E inside a ball of radius r (see [Mag12, Remark 15.16]). For instance it is similar in spirit to the following result for minimal clusters, which excludes "infiltrations" of a third fluid between two main ones [Leo01]: if in a certain ball B_r most of the volume is filled by just two chambers, then in $B_{r/2}$ there are no other chambers.

We begin by recalling a few results. Given a finite perimeter set E define $m(r) := |E \cap B_{1+r}|$. Then for a.e. $r > 0$ by (1.4) we have that

$$m'(r) = \mathscr{H}^{n-1}(E \cap \partial B_{1+r}) \tag{2.21}$$

and by (1.5)

$$P(E \cap B_{1+r}) = P(E, B_{1+r}) + \mathscr{H}^{n-1}(E \cap \partial B_{1+r}) = P(E, B_{1+r}) + m'(r). \tag{2.22}$$

Lemma 2.28 (Truncation simplified). *Let E be a finite perimeter set in $\mathbb{R}^n$, with $|E| = |B| = \omega_n$. Suppose $|E \Delta B| \le \delta$. Then there exists $r \in [0, \Delta r]$ such that*

$$P(E \cap B_{1+r}) \le P(E),$$

where $\Delta r = 2\left(\frac{\delta}{\omega_n}\right)^{1/n}$.

Proof. Suppose by contradiction this is not the case, and in particular that $m(r) < \omega_n$ for every $r \in [0, \Delta r]$. Then for a.e. r in the interval, by (2.22) we have

$$P(E, B_{1+r}) + m'(r) = P(E \cap B_{1+r}) \ge P(E) = P(E, B_{1+r}) + P(E, B^c_{1+r})$$

and therefore $m'(r) \ge P(E, B^c_{1+r})$. Now we use that for a.e. r

$$P(E, B^c_{1+r}) = P(E \cap B^c_{1+r}) - \mathscr{H}^{n-1}(E \cap B_{1+r}) = P(E, B^c_{1+r}) - m'(r)$$

to deduce that $2m'(r) \ge P(E \cap B^c_{1+r})$. By the isoperimetric inequality we have that

$$P(E \cap B^c_{1+r}) \ge n\omega_n^{1/n} |E \cap B^c_{1+r}|^{\frac{n-1}{n}} = n\omega_n^{1/n} (\omega_n - m(r))^{\frac{n-1}{n}}.$$

If we define $g(r) := \omega_n - m(r)$, putting together the last inequalities we can write

$$-2g'(r) \ge n\omega_n^{1/n} g(r)^{\frac{n-1}{n}}$$

and since $g(r) > 0$ we cand divide by $g(r)$ obtaining

$$-\left(g(r)^{1/n}\right)' \ge \frac{1}{2}\omega_n^{1/n}.$$

Integrating between 0 and Δr we obtain

$$g(\Delta r)^{1/n} \le g(0)^{1/n} - \frac{1}{2}\omega_n^{1/n}\Delta r \le \delta^{1/n} - \frac{1}{2}\omega_n^{1/n}\Delta r \le 0$$

which is a contradiction because we assumed $m(r) < \omega_n$ in the interval, that is $g(r)\,0$. $\square$

Remark 2.29. As already pointed out the previous result follows from a simpler calibration argument which does not need the differential inequality. We used the differential inequality to explain the method that we will use to prove the general result. We now explain what is the aforementioned calibration argument. The result is the following: for any set E of finite perimeter and any ball B, $P(E\cap B)\le P(E)$. Actually we can obtain the same for any convex set K replacing B, see also [Mag12, Exercise 15.14]. In particular in Lemma 2.28 we can choose *any* $r>0$ without assummptions on the smallness of $|E\Delta B|$.

Proof. Consider for simplicity as B the unit ball centered at the origin, and consider as a calibration the gradient of the fundamental solution of the Laplacian

$$\eta(x) := \frac{x}{|x|^{n+1}}.$$

Then $\operatorname{div}\eta = 0$ in $\mathbb{R}^n\setminus\{0\}$ and $|\eta(x)|\le 1$ for $x\in B^c$. Moreover

$$\mathscr{H}^{n-1}(E\cap\partial B) = \int_{E\cap\partial B} 1 d\mathscr{H}^{n-1} = \int_{E\cap\partial B} \eta\cdot\nu_B d\mathscr{H}^{n-1}$$

and

$$P(E,\overline{B}^c) = \int_{\partial^*E\cap\overline{B}^c} 1 d\mathscr{H}^{n-1} \ge \int_{\partial^*E\cap\overline{B}^c} \eta\cdot\nu_E d\mathscr{H}^{n-1}.$$

Therefore by the divergence theorem for finite perimeter sets 1.6 we have

$$\begin{aligned} P(E)-P(E\cap B) &= P(E,\overline{B}^c) - \mathscr{H}^{n-1}(E\cap\partial B) \\ &\ge \int_{\partial^*E\cap B^c} \eta\cdot\nu_E \, d\mathscr{H}^{n-1} - \int_{E\cap\partial B} \eta\cdot\nu_B \, d\mathscr{H}^{n-1} \\ &= \int_{E\cap B^c} \operatorname{div}\eta \, dx = 0. \end{aligned}$$

□

We now pass to the stronger statement. Given a finite perimeter set E with $|E|=|B|=\omega_n$, and given a $0<r<1$, we truncate it with B_{1+r} and fill it inside B_{1-r}, that is we consider

$$E_r := (E\cap B_{1+r})\cup B_{1-r}.$$

Proposition 2.30 (Truncation & volume-fixing variation). *Let $B\subset\mathbb{R}^n$ be the ball of radius 1 centered at the origin, and let $B(x_0,R)$ be a ball of radius R with center in $x_0\in\partial B$. Let $E\subset\mathbb{R}^n$ be a set of finite perimeter of volume $|E|=|B|=\omega_n$, and fix a parameter $\lambda>0$. If $|E\Delta B|=\delta\le\left(\frac{\lambda n}{2C}\right)^n\omega_n$ then there exists a radius $r\in[0,\Delta r]$ where*

$$\Delta r = \frac{4}{\lambda\,\omega_n^{1/n}}\delta^{1/n}$$

and a diffeomorphism ϕ which is the identity outside $B(x_0,R)$ such that the set $\tilde{E}_r := \phi(E_r)$ satisfies $|\tilde{E}_r|=|E|$ and

$$P(\tilde{E}_r) \le P(E,B_{1+r}) + \lambda P(E,B^c_{1+r}). \tag{2.23}$$

In particular for small δ the set $\tilde{E}_r$ is contained in $B_{1+2\Delta r}$.

The set $\tilde{E}_r$ is obtained by first truncating E obtaining E_r; and then by restoring the volume through a diffeomorphism supported in the ball B_R. The proposition says that we can find a value of r (sufficiently small, depending on λ, δ and R) such that the final set $\tilde{E}_r$ not only has less perimeter than the original set E, but we can also gain a bit on the perimeter in B^c_{1+r} if $\lambda < 1$.

In order to prove the previous proposition we first prove in the following lemma that, after the truncation, we can put the volume back to the original one with a change in perimeter proportional to the change in volume. The lemma is similar to [Mag12, Lemma 17.21], but we need a constant independent of the set E, and therefore we have to make some additional assumptions, namely that the class of sets we consider are sufficiently close to a fixed ball $B = B(0,1)$. Nevertheless the proof is very similar.

Lemma 2.31 (Volume-fixing variations). *Let E be a finite perimeter set in $\mathbb{R}^n$ such that $B_{1-\rho} \subset E \subset B_{1+\rho}$. Fix $R > 0$. There is a constant $\delta = \delta(n,\rho,R)$ such that if $\big||E| - |B|\big| \leq \delta$ then there is a diffeomorphism $\phi : \mathbb{R}^n \to \mathbb{R}^n$ which is the identity outside $B(x_0,R)$ such that*

- $|\phi(E)| = |B|$;
- $|P(\phi(E)) - P(E)| \leq C(n,\rho,R)P(E)\big||\phi(E)| - |E|\big|$.

Proof. Fix a vectorfield $\eta \in C^\infty_c(\mathbb{R}^n,\mathbb{R}^n)$, and let $\phi_t(x) = x + t\eta(x)$ be the associated family of diffeomorphisms for sufficiently small t. In particular $\nabla\phi_t = Id + t\eta(x)$. By the volume and perimeter variations (2.19) and (2.20) we have

$$\begin{aligned}
|\phi_t(E)| &= |E| + t\int_{\partial^* E} \eta \cdot \nu_E d\mathscr{H}^{n-1} + O(t^2) \\
P(\phi_t(E)) &= P(E) + t\int_{\partial^* E} \operatorname{div}^\tau \eta \, d\mathscr{H}^{n-1} + O(t^2)
\end{aligned}$$

where $O(t^2)$ depends only on η, $|E|$ and $P(E)$. If we choose η such that the flux

$$\Phi(\eta) := \int_{\partial^* E} \eta \cdot \nu_E \, d\mathscr{H}^{n-1}$$

is non zero, then for $|t|$ small enough the function $t \mapsto |\phi_t(E)|$ is injective and such that e.g.

$$\big||\phi_t(E)| - |E|\big| \geq \frac{\Phi(\eta)}{2}|t|.$$

It follows that we can obtain any volume sufficiently close to $|E|$, and for t small enough

$$\begin{aligned}
|P(\phi_t(E)) - P(E)| &\leq 2|t|\left|\int_{\mathscr{F}E} \operatorname{div}^\tau \eta d\mathscr{H}^{n-1}\right| \\
&\leq 2|t|P(E)\|\nabla\eta\|_{L^\infty(B_{1+\rho}\setminus B_{1-\rho})} \\
&\leq \frac{4}{\Phi(\eta)}P(E)\|\nabla\eta\|_{L^\infty(B_{1+\rho}\setminus B_{1-\rho})}\big||\phi_t(E)| - |E|\big|
\end{aligned}$$

since $\partial^* E \subset B_{1+\rho} \backslash B_{1-\rho}$. As of now the choice of η and the value of $\Phi(\eta)$ depend on the specfic set E. Let us show that we can make a universal choice. The basic observation is that

$$n|E| = \int_E \operatorname{div} x\, dx = \int_{\partial^* E} x \cdot \nu_E \, d\mathscr{H}^{n-1}$$

so that $\eta(x) = x$ gives a positive value to $\Phi(\eta)$ depending only on $|E|$. Since we want a perturbation supported in B_R we can choose

$$\eta(x) = x\psi\left(\frac{x}{|x|}\right)$$

where $\psi \in C^\infty(\mathbb{S}^{n-1})$ is a positive cutoff function. If we consider the circular cone $C(x_0, R)$ with vertex in the origin constructed over $B(x_0, R)$ we obtain

$$\begin{aligned}
\int_{\partial^* E} \eta \cdot \nu_E \, d\mathscr{H}^{n-1} &= \int_{\partial^* E \cap C(x_0,R)} \eta \cdot \nu_E \, d\mathscr{H}^{n-1} \\
&= \int_{\partial^*(E \cap C(x_0,R))} \eta \cdot \nu_E \, d\mathscr{H}^{n-1} \\
&= \int_{E \cap C(x_0,R)} \operatorname{div} \eta \, dx \\
&= \int_{E \cap C(x_0,R)} (\psi \operatorname{div} x + x \cdot \nabla \psi) dx \\
&= n \int_{E \cap C(x_0,R)} \psi(x) dx
\end{aligned}$$

since ψ is $0-$*homogeneous* and thus $x \cdot \nabla \psi = 0$. Since by assumption $E \supset B_{1-\rho}$, the last term is positive and bounded below by $n\|\psi\|_{L^1(B_{1-\rho} \cap C(x_0,R))}$. We therefore conclude

$$|P(\phi_t(E)) - P(E)| \leq \frac{4\|\nabla \eta\|_{L^\infty(B_{1+\rho} \backslash B_{1-\rho})}}{n\|\psi\|_{L^1(B_{1-\rho} \cap C(x_0,R))}} P(E) \big| |\phi_t(E)| - |E| \big|.$$

$\square$

Proof of Proposition 2.30. Suppose by contradiction that for every $r \in [0, \Delta r]$ the opposite inequality holds:

$$P(\tilde{E}_r) > P(E, B_{1+r}) + \lambda P(E, B^c_{1+r})$$

where $E_r = (E \cap B_{1+r}) \cup B_{1-r}$. Define the function $m(r) := |E \cap B^c_{1+r}| + |E^c \cap B_{1-r}|$. Then m is nonincreasing and for a.e. $r > 0$

$$m'(r) = -\mathscr{H}^{n-1}(E \cap \partial B_{1+r}) - \mathscr{H}^{n-1}(E^c \cap \partial B_{1-r}).$$

By the isoperimetric inequality we thus have that for a.e. $r > 0$

$$\begin{aligned}
P(E, B^c_{1+r}) + \mathscr{H}^{n-1}(E \cap \partial B_{1+r}) &= P(E \cap B^c_{1+r}) \\
&\geq n\omega_n^{1/n} |E \cap B^c_{1+r}|^{\frac{n-1}{n}}
\end{aligned}$$

and

$$\begin{aligned}P(E^c, B_{1-r}) + \mathscr{H}^{n-1}(E^c \cap \partial B_{1-r}) &= P(E^c \cap B_{1-r})\\ &\geq n\omega_n^{1/n}|E^c \cap B_{1-r}|^{\frac{n-1}{n}}.\end{aligned}$$

Since by the previous lemma for a.e. r we have $|P(\tilde{E}_r) - P(E_r)| \leq C||\tilde{E}_r| - |E_r|| = C|m(r) - \omega_n|$ we obtain that for a.e. $r \in [0, \Delta r]$

$$\begin{aligned}&P(E) + \mathscr{H}^{n-1}(E \cap \partial B_{1+r}) - P(E, B^c_{1+r}) + \mathscr{H}^{n-1}(E^c \cap \partial B_{1-r}) - P(E^c, B_{1-r})\\ &= P(E_r) > P(E, B_{1+r}) + \lambda P(E, B^c_{1+r}) - C|\omega_n - |E_r||\end{aligned}$$

that is (writing $P(E) = P(E, B_{1+r}) + P(E, B^c_{1+r})$ and erasing equal terms)

$$-m'(r) > \lambda P(E, B^c_{1+r}) + P(E^c, B_{1-r}) - C|\omega_n - |E_r||.$$

We now observe that

$$|\omega_n - |E_r|| = ||E| - |E_r|| = ||E \cap B^c_{1+r}| - |E^c \cap B_{1-r}|| \leq m(r).$$

Using that $\lambda < 1$ and the subadditivity of $s \mapsto s^{\frac{n-1}{n}}$ it follows that

$$-2m'(r) \geq \lambda n\omega_n^{1/n} m(r)^{\frac{n-1}{n}} - Cm(r).$$

Since by assumption $m(r) \leq m(0) \leq \left(\frac{\lambda n}{2C}\right)^n \omega_n$, we have that $Cm(r) \leq \frac{1}{2} n\omega_n^{1/n} m(r)^{\frac{n-1}{n}}$. Moreover

$$m(r) \neq 0 \text{ for } r \text{ in } [0, \Delta r], \tag{2.24}$$

otherwise $\tilde{E}_r = E$ and the inequality (2.23) is trivially satisfied. Therefore we obtain

$$\frac{d}{dr} m(r)^{1/n} < -\frac{\lambda\,\omega_n^{1/n}}{4}$$

for a.e. r. We therefore obtain

$$m(r)^{1/n} - m(0)^{1/n} < -\frac{\lambda\,\omega_n^{1/n}}{4} r$$

which for $r = \Delta r$ becomes

$$m(\Delta r)^{1/n} < m(0)^{1/n} - \frac{\lambda\,\omega_n^{1/n}}{4}\Delta r = \delta^{1/n} - \frac{\lambda\,\omega_n^{1/n}}{4}\Delta r \leq 0$$

by the definition of Δr, which contradicts (2.24).

Finally, we prove that $\tilde{E}_r$ is contained in $B_{1+2\Delta r}$ if δ is sufficiently small. This is trivial because the truncation makes the set contained in $B_{1+\Delta r}$, while the volume-fixing variation given by Lemma 2.31 expands by a quantity (called $|t|$ in the proof of the Lemma) of order δ (the volume to be fixed). Therefore for δ small enough $\delta \ll \delta^{\frac{1}{n}} \approx \Delta r$ and the claim is proved. □

Localization Lemma

The following result is the extension of Lemma 2.11 to any dimension.

Proposition 2.32 (Localization Lemma). *Suppose that $\overline{\mathscr{E}_\varepsilon}$ are N-clusters in $\mathbb{R}^n$, minimizing P_ε given by (2.17) with a volume constraint $|\mathscr{E}_\varepsilon(i)| = m_i$. Suppose that $\overline{\mathscr{E}_\varepsilon} \to \mathscr{B} = (B_1, \dots B_n)$, where B_i are balls. Then for ε sufficiently small, we have that*

$$(1 - r(\varepsilon))B_i \subseteq \overline{\mathscr{E}_\varepsilon}(i) \subseteq (1 + r(\varepsilon))B_i \tag{2.25}$$

where $r(\varepsilon) \to 0$ as $\varepsilon \to 0$.

Proof. In short, we apply the Truncation Lemma given by Proposition 2.30 with $\lambda = 1 - 2\varepsilon$ to each chamber, noting that we can choose the ball B_{R_i} for each chamber so that B_{R_i} stays far from the other balls B_j, $j \neq i$. The only care has to be taken to control the interfaces between different chambers.

We suppose that (2.25) does not hold, and we prove that the truncated and volume-fixed clusters $\tilde{\mathscr{E}}_\varepsilon$, obtained by applying Proposition 2.30 to each chamber, have lower P_ε-perimeter. Consider therefore the truncated and volume-fixed clusters $\tilde{\mathscr{E}}_\varepsilon$. We call for simplicity $\mathscr{E}_\varepsilon^{old}$ the original cluster and $\mathscr{E}_\varepsilon^{new}$ the modified cluster. Then

$$P_\varepsilon(\mathscr{E}_\varepsilon^{new}) = \sum_{i=1}^{N} P(\mathscr{E}_\varepsilon^{new}(i)) - \varepsilon \sum_{1 \le i < j \le N} \mathscr{H}^{n-1}(\mathscr{E}_\varepsilon^{new}(i, j)).$$

Applying Proposition 2.30 with $\lambda = 1 - 2\varepsilon$ to each chamber we obtain

$$\begin{aligned} P(\mathscr{E}_\varepsilon^{new}(i)) - P(\mathscr{E}_\varepsilon^{old}(i)) &= P(\mathscr{E}_\varepsilon^{new}(i)) - P(\mathscr{E}_\varepsilon^{old}(i), (1+r)B_i) - P(\mathscr{E}_\varepsilon^{old}(i), ((1+r)B_i)^c) \\ &\le -2\varepsilon P(\mathscr{E}_\varepsilon^{old}(i), ((1+r)B_i)^c). \end{aligned}$$

On the other hand the only contributions to

$$\varepsilon \mathscr{H}^{n-1}(\mathscr{E}_\varepsilon^{old}(i, j)) - \varepsilon \mathscr{H}^{n-1}(\mathscr{E}_\varepsilon^{new}(i, j))$$

can come from pieces of $\mathscr{E}_\varepsilon^{old}(i)$ outside $(1 + r)B_i$ or pieces of $\mathscr{E}_\varepsilon^{old}(j)$ outside of $(1 + r)B_j$. In any case the sum of all these contributions is at most $\varepsilon P(\mathscr{E}_\varepsilon^{old}, ((1 + r)\mathscr{B})^c)$, so that

$$P_\varepsilon(\mathscr{E}_\varepsilon^{new}) - P(\mathscr{E}_\varepsilon^{old}) \le -\varepsilon P(\mathscr{E}^{old}, ((1 + r)\mathscr{B})^c) < 0$$

by the initial assumption. This contradicts the minimality of $\overline{\mathscr{E}_\varepsilon}$. □

Chapter 3

Global shape of planar clusters

In this chapter we prove the existence of a limit global shape E_∞ for minimizing planar N-clusters with equal areas as $N \to \infty$. We prove also some basic regularity results for E_∞, and that the perimeter density is asymtptotically uniform.

Contents

In this Chapter our focus is the *global shape* of planar N-clusters $\mathscr{E}_N$, that is

$$E_N := \bigcup_{i=1}^{N} \mathscr{E}_N(i) = \mathbb{R}^2 \setminus \mathscr{E}_N(0). \tag{3.1}$$

Our aim is understanding the shape of E_N when $\mathscr{E}_N$ are minimizing N-clusters with chambers of equal area, in particular when $N \to \infty$. To avoid that the total area of the clusters goes to infinity, we rescale E_N by a factor $\frac{1}{\sqrt{N}}$.

The question of what is the limit of $\frac{1}{\sqrt{N}} E_N$ when $N \to \infty$ was considered by many authors; among them we can cite Cox, Graner, Heppes and Morgan [CG03], [HM05], [CMG13]. We quote Frank Morgan from [Mor09, Figure 13.1.4]

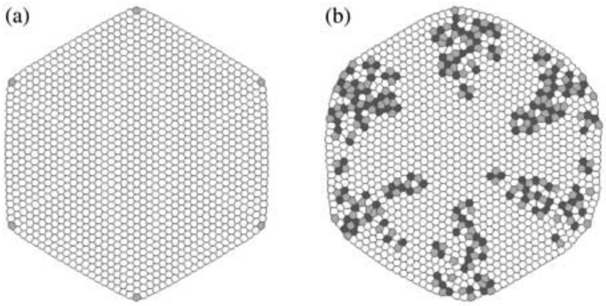


Figure 3.1

> "For a large number N of unit bubbles (here 200 and 1000), Cox et al. conjecture that the whole cluster will be approximately one big regular hexagon. The author, however, predicts that for N very large, the cluster will be approximately circular."

and also [Mor09, p. 123]

> "[...] I think that for very large N the whole cluster should become circular, to minimize the unshared outer perimeter, despite the cost of dislocations in the underlying hexagonal structure."

See also [HM05, 3.2 Remarks]:

> We, however, conjecture that very large clusters can become roughly circular with negligible additional internal cost [...]

and [CMG13]

> For larger N, the optimal cluster is less likely to be hexagonal in shape, even for N a hexagonal number, and we find that for $N \geq 4447$ the perfect hexagonal cluster is no longer best even for a hexagonal number of bubbles.

We say that the clusters $\mathscr{E}_N$ converge in shape or **shape-converge** to a set E_∞ if $\frac{1}{\sqrt{N}}E_N \to E_\infty$ in measure, or equivalently if the correpsonding characteristic functions converge in L^1.

Disclaimer We will often omit the subscript N when it is clear from the context, writing simply $\mathscr{E}$ instead of $\mathscr{E}_N$.

3.1 Three formulations of the problem

We begin by describing three different settings to study the asymptotic behaviour of minimal clusters. In short, they are essentially: exact constraint on the area (area of each chamber $\frac{1}{N}$, $N \to \infty$); loose constraint

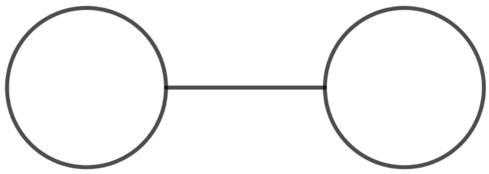


Figure 3.2: For problem $(\mathscr{P}_N^c)$ we consider connected chambers in the sense that each of them is enclosed by a single closed Lipschitz curve. In the case depicted here the middle curve is crossed twice and thus is counted twice in the perimeter energy.

on the area (area of each chamber $\leq \varepsilon^2$, fixed *total* area, $\varepsilon \to 0$); relaxed problem with connectedness constraint (area of each chamber $= \frac{1}{N}$, $N \to \infty$, if two chambers disconnect in the limit we still count the disappeared interface that connects them). More precisely we have the following problems:

$(\mathscr{P}_N)$ We consider N-clusters $\mathscr{E}_N$ made of chambers with area $\frac{1}{N}$, and we put no constraint on the connectedness of each chamber. We minimize the perimeter $P(\mathscr{E}_N)$.

$(\mathscr{P}_\varepsilon)$ We consider clusters $\mathscr{E}_\varepsilon$ with total area 1 and whose (possibly countably many) chambers have area $\leq \varepsilon^2$, and for simplicity we will count each connected component as a single chamber (this is always possible up to a relabeling).

$(\mathscr{P}_N^c)$ We consider N-clusters whose chambers have area $\frac{1}{N}$ and each of which is the set enclosed by a closed Lipschitz curve; the perimeter of a chamber is the length of the curve, which means that in the case of a single chamber with two components as in Figure 3.2 we count the middle curve twice.

The first problem is the classical one. The second is more suitable to apply cut and paste arguments because we do not care about an exact area constraint for each chamber. The third simplifies the first one.

The existence of a minimizer for each problem (for fixed N or ε) follows by the direct method. For problem $(\mathscr{P}_N)$ we use the compactness provided by Theorem 1.2. For problem $(\mathscr{P}_N^c)$ we parametrize the boundary of each chamber as a Lispchitz curve with unit speed and use Ascoli-Arzelà (see [Mor94, Corollary 3.3]). For problem $(\mathscr{P}_\varepsilon)$ we use the compactness result for Caccioppoli partitions (Theorem 1.6). We omit the details.

We recall the basic regularity result given by Theorem 2.7: each minimizer for problem $(\mathscr{P}_N)$ is identified by a finite number of segments and pieces of circles that meet forming 120 degree angles.

3.2 Existence of the limit global shape

In this Section we will prove the existence of a limit global shape for minimizing N-clusters, that is a limit up to subsequence and rigid motions of $\frac{1}{\sqrt{N}}\bar{E}_N$ when $N \to \infty$. The precise convergence is the one given by the compactness theorem of finite perimeter sets (Theorem 1.2).

We can prove the existence of the global shape for problem $(\mathscr{P}_N^c)$; for problem $(\mathscr{P}_N)$ we have a conditional result that relies on an improved version of Hales inequality (3.6), which has not been proved. Somehow the original Hales inequality is barely insufficient to prove the existence of a global shape, and an improved version by a tiny margin would suffice.

We will first recall Hales inequality (Theorem 3.1), which is the key tool that was employed by Hales in [Hal01] to prove the *honeycomb conjecture* (to which we will refer also as *honeycomb inequality*), which in one of its forms could be rephrased as follows: for every N-cluster $\mathscr{E}_N$ with chambers of unit area,

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}N. \tag{3.2}$$

A consequence of this inequality is that the regular hexagonal partition of the plane, also called *honeycomb*, provides in a suitable sense the optimal partition of the plane in equal-area cells. Indeed, (3.2) says that the average perimeter per chamber is at least $\sqrt[4]{12}$, the semiperimeter of a regular hexagon of area 1. We also mention [Car11, Teorema 5.10] (in italian) for a detailed exposition of Hales inequality.

Then we will see how Hales inequality can be used to prove a refined version of (3.2), in the form

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}N + cP(E_N) \tag{3.3}$$

where $c > 0$ and $E_N = \bigcup_{i=1}^N \mathscr{E}(i)$ is the global shape of $\mathscr{E}_N$ (see Lemma 3.6). Actually we need to assume either that a slightly improved Hales inequality is true (Conjecture 3.4) or a lower bound on the area of each connected component of a minimizer (which is satisfied if e.g. all chambers are connected). We discuss this issue in the following, see in particular the Subsection *An improved Hales inequality?* and Section 3.3.

Finally we will see how the inequality above, together with the trivial upper bound $P(\mathscr{E}_N) \leq \sqrt[4]{12}N + \mathscr{O}(\sqrt{N})$ given by Lemma 3.7 and the compactness of finite perimeter sets, will ensure the existence of a global shape (in the sense of finite perimeter sets) for minimizing N-clusters as $N \to \infty$.

Hales inequality

We recall here the setting outlined in [Hal01] in order to state Hales inequality.

Let Γ be a closed piecewise simple rectifiable curve in the plane, on which we consider the orientation given by the parametrization, and let $L(\Gamma)$ be its length. The signed area of Γ is

$$A(\Gamma) = \int_\Gamma x dy.$$

Let $V := (v_1, \ldots, v_k)$, $k \geq 2$ be a collection of points on Γ, in the order provided by the parametrization of Γ. We join v_i and v_{i+1} with a directed segment f_i, where $v_{k+1} := v_1$. We call $A(V)$ the signed area of the polygon with vertices v_i bounded by the directed chords f_i. Let moreover e_i be the piece of Γ between v_i and v_{i+1}. Let $x(e_i)$ be the signed area of the region bounded by e_i and f_i^*, where f_i^* is f_i with the reversed orientation. In this way we have that

$$A(\Gamma) = A(V) + \sum_e x(e)$$

where the sum is among $e = e_1, \dots e_k$. Let also $\alpha(\Gamma) := \min\{1, A(\Gamma)\}$. Define a truncation function $\tau : \mathbb{R} \to \mathbb{R}$ by $\tau(x) := \max\{-\frac{1}{2}, \min\{\frac{1}{2}, x\}\}$, and set

$$T(\Gamma) := \sum_e \tau(x(e)) \tag{3.4}$$

to be the sum of the truncated areas of $x(e)$.

Theorem 3.1 (**Hales inequality** [Hal01, Theorem 4]). *Consider a curve Γ as above, together with a partition with $k \geq 2$ points $v_1, \dots, v_k$, and define $L(\Gamma)$, $A(\Gamma)$, $T(\Gamma)$ as above. Assume the lower bound on the area*

$$A(\Gamma) \geq \frac{2\pi\sqrt{3}}{3k^2}. \tag{3.5}$$

Then

$$L(\Gamma) \geq 2\sqrt[4]{12}\alpha(\Gamma) - a(k-6) - \sqrt[4]{12}T(\Gamma) \tag{3.6}$$

where $a = 0.0505$. Equality is attained if and only if Γ is the boundary of a regular hexagon of area 1.

Set now $\alpha(\mathscr{E}_N) := \sum_{i=1}^N \alpha(\mathscr{E}_N(i))$. Using the previous inequality, Hales is able to prove the following honeycomb inequality:

Theorem 3.2 (**Honeycomb inequality** [Hal01, Theorem 2]). *For every planar N-cluster $\mathscr{E}_N$ we have*

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}\alpha(\mathscr{E}_N).$$

In particular, for every planar N-cluster $\mathscr{E}_N$ with chambers of area ≥ 1 we have

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}N.$$

Remark 3.3. We stress the difference between the *Hales* and the *honeycomb* inequalities: the first one concerns a single chamber (or rather, a single connected component) and involves the signed areas included between the curve and the polygon associated to the partition of the boundary (we could also call it *isoperimetric inequality for curvilinear polygons*); the second one instead concerns the whole N-cluster and involves only the perimeter. To prove the honeycomb inequality we essentially have to sum Hales inequality among all chambers, as we will see in the proof of Lemma 3.6.

An improved Hales inequality?

In order to unconditioinally prove the existence of the global shape for problem $(\mathscr{P}_N)$ we would need an improved Hales inequality in the following sense: we would need the same conclusion of Theorem 3.1 but with a slightly weaker lower bound on the area enclosed by the curve Γ, namely

$$A(\Gamma) \geq \frac{2\pi\sqrt{3}}{3k^2}(1-\delta)$$

for any fixed $\delta > 0$.

We state this as:

Conjecture 3.4 (**Improved Hales inequality**). *Consider a curve Γ as above, together with a partition with $k \geq 2$ points $v_1, \dots, v_k$, and define $L(\Gamma)$, $A(\Gamma)$, $T(\Gamma)$ as above. Assume the lower bound on the area*

$$A(\Gamma) \geq \frac{2\pi\sqrt{3}}{3k^2}(1-\delta) \tag{3.7}$$

for some fixed $\delta > 0$. Then

$$L(\Gamma) \geq 2\sqrt[4]{12}\alpha(\Gamma) - a(k-6) - \sqrt[4]{12}T(\Gamma)$$

for some constant a. Equality is attained if and only if Γ is the boundary of a regular hexagon of area 1.

Without this result to prove the existence of a global shape for problem $(\mathscr{P}_N)$ we have to require that the lower bound (3.5) is satisfied by every connected component of minimizers. The validity of this lower bound is not known in general, but an even stronger result is conjectured:

Conjecture 3.5 (Problem 5 in [SM96]). *For every N, every chamber of a minimizing N-cluster is connected.*

We will now carry on the proof of the existence of the global shape with the assumption (3.5). In Section 3.3 we will discuss how we could remove this assumption if we knew that Conjecture 3.4 holds.

An improved honeycomb inequality

The following inequality was already observed by Heppes and Morgan [HM05, Theorem 3.1], but somehow they do not take into consideration the assumption (3.5) on the lower bound on the area of each connected component of the chambers. Since to us it is not clear how to remove this assumption we have to assume it.

Lemma 3.6 (**Improved Honeycomb inequality**). *Consider an N-cluster $\mathscr{E}_N$ whose chambers have area 1, and with each connected component of every chamber having area at least $\frac{2\pi\sqrt{3}}{3k^2}$, where k is the number of distinct components of other chambers touching it. Then*

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}|E_N| + c_1 P(E_N) + c_2 K_0 \tag{3.8}$$

for positive constants c_1, c_2, where K_0 is the number of arcs on the boundary ∂E_N, that is the number of arcs in the boundary of $\mathscr{E}_N(0)$. In particular we can choose $c_1 = \frac{1}{8}$ and $c_2 = \frac{a}{2} = 0.02525$.

Proof. Up to relabeling each connected component as a separate chamber, we can assume that all the chambers except at most for $\mathscr{E}(0)$ are connected, and that they satisfy the bound on the area

$$\frac{2\pi\sqrt{3}}{3K_i^2} \le |\mathscr{E}(i)| \le 1$$

where K_i is the number of distinct chambers sharing some boundary with the chamber $\mathscr{E}(i)$.

We sum the various Hales inequalities (3.6) for each chamber, as in the proof of the honeycomb conjecture [Hal01], but we are slightly more careful and at the last line we save a portion of $P(E_0)$ in Dido's inequality. More precisely we have that

$$\begin{aligned} P(\mathscr{E}) &= \frac{1}{2}\sum_{i=0}^{N} P(\mathscr{E}(i)) \\ &\ge \frac{1}{2}P(\mathscr{E}(0)) + \frac{1}{2}\sum_{i=1}^{N}\left(2\sqrt[4]{12}|\mathscr{E}(i)| - a(K_i-6) - \sqrt[4]{12}T(\Gamma_i)\right) \\ &\ge \frac{1}{2}P(\mathscr{E}(0)) + \sqrt[4]{12}|\mathscr{E}| - \frac{a}{2}\sum_{i=1}^{N}(K_i-6) - \frac{\sqrt[4]{12}}{2}\sum_{i=1}^{N}T(\Gamma_i). \end{aligned} \tag{3.9}$$

Now the term involving the K_i's reflects just the combinatorics of the graph, and thanks to Euler's formula and the regularity of minimizers we can conclude that

$$-\sum_{i=1}^{N}(K_i-6) \ge 6 + K_0 \tag{3.10}$$

Indeed, by Euler's formula we have that

$$F - E + V = 1$$

where F is the number of faces of the graph (without the exterior one), E the number of edges and V the number of vertices. We have that $F = N$, and since the degree at each vertex is 3, we also have

$$3V = 2E = \sum_{i=0}^{N} K_i.$$

Therefore

$$1 = N - E + \frac{2}{3}E = N - \frac{1}{3}E = N - \frac{1}{6}\sum_{i=0}^{N}K_i = -\frac{1}{6}K_0 + \sum_{i=1}^{N}\left(1 - \frac{K_i}{6}\right)$$

and we obtain (3.10) with equality just by rearranging terms. Note that for problem $(\mathscr{P}_N^c)$ the degree of vertices could be ≥ 3, but the same proof yields (3.10).

As for the second sum of (3.9), recall from (3.4) that each term $T(\Gamma_i)$ is the sum of the (truncated and signed) areas enclosed between each curvilinear edge and the correspoding chord. Therefore, whenever an edge of the graph is shared between two interior chambers, the two contributions exactly cancel out, because one area has positive sign and the other one has negative sign. The only terms surviving in the sum are the signed areas that are associated to the curvilinear edges that form the boundary of $\mathscr{E}(0)$, that is we are left with

$$\sum_{e\subset\partial\mathscr{E}(0)} \tau(x(e))$$

where the sum is among all edges constituting $\partial\mathscr{E}(0)$. In conclusion, (3.9) becomes

$$P(\mathscr{E}) \geq \sqrt[4]{12}|\mathscr{E}| + \frac{a}{2}(K_0+6) + \frac{1}{2}P(\mathscr{E}(0)) - \frac{\sqrt[4]{12}}{2}\sum_{e\subset\partial\mathscr{E}(0)} \tau(x(e)).$$

We now examine the last two terms, that we can write together as

$$\frac{1}{2}\sum_{e\subset\partial\mathscr{E}(0)} \left(L(e) - \sqrt[4]{12}\tau(x(e))\right)$$

where $L(e)$ is the length of the edge e. We use Dido's inequality (1.8) (that is the relative isoperimetric inequality in a half plane) to conclude that the length of the edge $L(e)$ and the signed area $x(e)$ satisfy

$$L(e) \geq \sqrt{\pi|x(e)|} \geq \sqrt{\pi|\tau(x(e))|} \geq \sqrt{\pi}\sqrt{2}|\tau(x(e))| \geq \sqrt{2\pi}\tau(x(e)).$$

and therefore

$$\frac{1}{2}\sum_{e\subset\partial\mathscr{E}(0)} \left(L(e) - \sqrt[4]{12}\tau(x(e))\right) \geq \frac{1}{2}\sum_{e\subset\partial\mathscr{E}(0)} \left(1-\frac{\sqrt[4]{12}}{\sqrt{2\pi}}\right)L(e) = \frac{1}{2}\left(1-\frac{\sqrt[4]{12}}{\sqrt{2\pi}}\right)P(\mathscr{E}(0))$$

and the factor before $P(\mathscr{E}(0))$ is approximately $0.1287... \geq \frac{1}{8}$.

In conclusion, since the total area of the cluster is N, we have proved that

$$P(\mathscr{E}) \geq \sqrt[4]{12}N + \frac{a}{2}(6+K_0) + \frac{1}{8}P(\mathscr{E}(0)).$$

$\square$

Proof of the existence of the global shape

Lemma 3.7 (Upper bound for the energy). *For every $N\in\mathbb{N}$ we can build a cluster $\mathscr{E}_N^{hex}$ whose chambers are regular hexagons of area 1 and such that*

$$P(\mathscr{E}_N^{hex}) \leq \sqrt[4]{12}N + C_1\sqrt{N}.$$

In the setting of problem $(\mathscr{P}_\varepsilon)$ there is a similar competitor such that

$$P(\mathscr{E}_\varepsilon^{hex}) \leq \frac{1}{\varepsilon}\sqrt[4]{12} + C_1$$

Proof. We could consider any configuration of N hexagonal chambers which has an outer perimeter of order $\sqrt{N}$, but for simplicity we refer to the spiral configurations of Figure 4.2. A simple calculation shows that the sidelength of a hexagon of area 1 is $\ell_0 = \frac{1}{3}\sqrt[4]{12}$. The total number of exterior edges is (Lemma 4.4)

$$2\lceil\sqrt{12N-3}\rceil$$

while the number of inner edges is

$$3N - \lceil\sqrt{12N-3}\rceil.$$

The total perimeter of the cluster is thus

$$\ell_0(3N + \lceil\sqrt{12N-3}\rceil) \leq \sqrt[4]{12}N + \frac{1}{3}\sqrt[4]{12}(\sqrt{12N}+1)$$

and we can choose $C_1 = \frac{1}{3}\sqrt[4]{12}(\sqrt{12}+1) \approx 2.7695\ldots$.

In the case of problem $(\mathscr{P}_\varepsilon)$ it is sufficient to set $N := \lfloor\frac{1}{\varepsilon^2}\rfloor$ and consider the rescaled competitor $\varepsilon\mathscr{E}_N^{hex}$. If $\frac{1}{\varepsilon^2}$ is not an integer we can add a spare chamber with circular shape. □

A slightly better upper bound is given in [HM05], where it is proven that there is a competitor $\mathscr{E}_N$ such that

$$P(\mathscr{E}_N) \leq \sqrt[4]{12}N + \frac{\pi\sqrt[4]{12}}{3}\sqrt{N} + \sqrt[4]{12}$$

and thus we can choose $C_1 = \sqrt[4]{12}(\pi+1)/3 \approx 2.5694\ldots$. However the specific constant is not important for our purposes, that is to prove compactness.

We now come to the main theorem, that is the existence of a global shape for problem $(\mathscr{P}_N)$. We can prove it under the assumption that each connected component of each chamber in a minimizing N-cluster satisfies the bound (3.5) (which is automatically true for problem $(\mathscr{P}_N^c)$). As already stated this could be avoided in the case we knew that the improved Hales inequality as per Conjecture 3.4 holds (see Section 3.3).

Theorem 3.8 (**Existence of a global shape**). *Under the assumption* (3.5) *for the areas of each connected component, up to subsequence and rigid motions minimal clusters $\mathscr{E}_N$ shape-converge to a finite perimeter set E_∞, in the sense that the rescaled sets $\frac{1}{\sqrt{N}}E_N$ converge in L^1 to E_∞.*

Proof. By Lemma 3.7 we know that there is a competitor $\mathscr{E}_\varepsilon^{hex}$ such that

$$P(\mathscr{E}_N^{hex}) \leq \sqrt[4]{12}N + C_1\sqrt{N}$$

while the improved honeycomb inequality of Lemma 3.6 gives

$$P(\mathscr{E}_N) \geq \sqrt[4]{12}N + c_1 P(E_N).$$

We deduce that for a minimizer $P(\overline{E}_N) \leq \frac{C_1}{c_1}\sqrt{N}$. In particular the rescaled sets $\frac{1}{\sqrt{N}}E_N$ have equibounded perimeter. We conclude by the compactness theorem for finite perimeter sets (Theorem 1.2) that, up to rigid motions and up to subsequence, $\frac{1}{\sqrt{N}}E_N$ converge to a finite perimeter set E_∞, and moreover $P(E_\infty) \leq \frac{C_1}{c_1}$. The confinement of the supports, that is assumption (ii) of the cited theorem, comes from the fact that minimizers are connected, and for connected sets in the plane the perimeter controls the diameter. □

3.3 Removing the lower bound on the areas

We now discuss more in detail the role of Conjecture 3.4 and how it can be used to prove the existence of a global shape for problem $(\mathscr{P}_N)$ without assuming the bound (3.5). In particular the aim of this Section is to prove a conditional result: we can remove the assumption on the lower bound on the cells' areas in Lemma 3.6 (and therefore in Theorem 3.8), provided that a slightly better version of the Hales inequality (3.6) holds; namely, provided that the bound on the area can be improved by any factor less than 1:

$$A(\Gamma) \geq \frac{2\pi\sqrt{3}}{3k^2}(1-\delta)$$

for some positive δ.

Lemma 3.9. *Suppose that Hales inequality* (3.6) *holds under the assumption that*

$$A(\Gamma) \geq \frac{2\pi\sqrt{3}}{3k^2}(1-\delta) \tag{3.11}$$

that is suppose Conjecture 3.4 holds. Then for any cluster $\mathscr{E}$

$$P(\mathscr{E}) \geq \sqrt[4]{12}A(\mathscr{E}) + cP(\mathscr{E}(0)), \tag{3.12}$$

with the constant c sufficiently small depending on δ.

Proof. Define the functional F on the space of all clusters by

$$F(\mathscr{E}) = P(\mathscr{E}) - \sqrt[4]{12}A(\mathscr{E}) - cP(\mathscr{E}(0)).$$

Then equation (3.12) is equivalent to

$$F(\mathscr{E}) \geq 0 \text{ for every cluster } \mathscr{E}.$$

If all connected components of the chambers of $\mathscr{E}$ satisfy the bound (3.11) then we can argue as in the proof of Lemma 3.6 and we are done. If otherwise assumption (3.11) is not satisfied for at least one connected component, we prove that we can "pop" an edge of this component and merge it with one of its neighbours so that the value of F decreases. In this way we keep on merging the components until the area bound is satisfied for all of them.

We consider for notational simplicity a cluster with connected chambers (this is always possible up to relabeling each connected component as a standalone chamber). Consider then a cluster $\mathscr{E}$ and suppose that there exists a chamber, say $\mathscr{E}(1)$, that touches k other chambers and such that

$$A(\mathscr{E}(1)) < \frac{2\pi\sqrt{3}}{3k^2}(1-\delta).$$

Then by the isoperimetric inequality we have

$$P(\mathscr{E}(1)) \geq \sqrt{4\pi A(\mathscr{E}(1))} = \sqrt{\frac{4\pi}{A(\mathscr{E}(1))}} A(\mathscr{E}(1)) \geq \sqrt[4]{12} \frac{1}{\sqrt{1-\delta}} kA(\mathscr{E}(1))$$

and therefore there must be a neighbouring chamber such that the common interface has length ℓ at least

$$\ell \geq \frac{P(\mathscr{E}(1))}{k} \geq \sqrt[4]{12} \frac{1}{\sqrt{1-\delta}} A(\mathscr{E}(1)). \tag{3.13}$$

We now remove this interface and merge $\mathscr{E}(1)$ with the neighbouring chamber, obtaining a new cluster $\widetilde{\mathscr{E}}$, and prove that $F(\widetilde{\mathscr{E}}) \leq F(\mathscr{E})$. There are two cases:

- the neighbouring chamber is not the exterior chamber; say it is $\mathscr{E}(2)$.

  Then the functional F decreases because $P(\mathscr{E}(0))$ remains unchanged, while $P(\mathscr{E}) - \sqrt[4]{12}A(\mathscr{E})$ decreases by (3.13).

- the neighbouring chamber is $\mathscr{E}(0)$, the exterior one.

  In this case $P(\mathscr{E}(0))$ can decrease at most by ℓ; therefore

$$\begin{aligned} F(\widetilde{\mathscr{E}}) &= P(\widetilde{\mathscr{E}}) - \sqrt[4]{12}A(\widetilde{\mathscr{E}}) - cP(\widetilde{\mathscr{E}}(0)) \\ &\leq \big(P(\mathscr{E}) - \ell\big) - \sqrt[4]{12}\big(A(\mathscr{E}) - A(\mathscr{E}(1))\big) - c\big(P(\mathscr{E}(0)) - \ell\big) \\ &= F(\mathscr{E}) - \ell + \sqrt[4]{12}A(\mathscr{E}(1)) + c\ell \\ &< F(\mathscr{E}) \end{aligned}$$

  if c is sufficiently small, namely if

$$\frac{1-c}{\sqrt{1-\delta}} > 1.$$

In conclusion, we proved that if there is a component which does not satisfy the bound (3.11), then we can merge two components and lower the value of F. Continuing in this way, we reach the case in which each chamber satisfy the bound (3.11), and F has decreased. Therefore to prove (3.12) for all clusters, it suffices to prove it for clusters satisfying the area bound (3.11). But this is true by the same proof of Lemma 3.6. □

As a corollary under the assumption that Conjecture 3.4 holds we can remove the assumption on the lower bound of the areas in Theorem 3.8 (existence of a global shape).

Corollary 3.10. *Suppose that Hales inequality* (3.6) *holds under the assumption that*

$$A(\Gamma) \geq \frac{2\pi\sqrt{3}}{3k^2}(1-\delta),$$

that is suppose Conjecture 3.4 holds. Then there is a limit global shape of minimal clusters $\mathscr{E}_N$ for the problem $(\mathscr{P}_N)$.

3.4 Basic regularity of the global shape

After having established existence of a global shape, the natural following is to characterize it, or at least find some of its properties. This is a more delicate issue than it could appear at first. We will establish a really basic regularity result for E_∞, which can be stated as follows: the set of points of zero Lebesgue density $E_\infty^{(0)}$ is open (see (1.7) for the definition of density). We actually expect a much stronger regularity:

Conjecture 3.11. *The global shape E_∞ is a convex set.*

For simplicity we consider problem $(\mathscr{P}_\varepsilon)$, that is we consider clusters with areas $\leq \varepsilon^2$ and total area 1. In particular we denote the global shape by

$$E_\varepsilon := \bigcup_{i=1}^{m} \mathscr{E}_\varepsilon(i)$$

and call $E_0 := \lim_{\varepsilon \to 0} E_\varepsilon$. We also say that $\mathscr{E}_\varepsilon$ **shape-converge** to E_0. We again assume that either Conjecture 3.4 holds or the lower bound (3.5) is satisfied, in which case the existence of the limit shape E_0 follows the same proof as for the problem $(\mathscr{P}_N)$.

Lemma 3.12 (**Most chambers have diameter $\mathscr{O}(\varepsilon)$**)**.** *There is a constant C_2 such that the number of chambers with diameter greater than $C_2\varepsilon$ is at most C_2/ε:*

$$\#\{i : diam(\mathscr{E}_\varepsilon(i)) \geq C_2\varepsilon\} \leq \frac{C_2}{\varepsilon}. \tag{3.14}$$

In particular their total area is at most $C_2\varepsilon$.

Proof. Let $\mathscr{G}_\varepsilon$ be the subcluster of $\mathscr{E}_\varepsilon$ composed by the good chambers with diameter less than $C_2\varepsilon$, and $\mathscr{F}_\varepsilon$ the complementary subcluster whose chambers have diameter at least $C_2\varepsilon$. Define $\Sigma_\varepsilon = \partial\mathscr{F}_\varepsilon \cap \partial\mathscr{G}_\varepsilon$ to be the portion of boundary in common between $\mathscr{F}_\varepsilon$ and $\mathscr{G}_\varepsilon$, and let M be the number of chambers of $\mathscr{F}_\varepsilon$.

We first prove that $P(\mathscr{F}_\varepsilon) \geq C_2 M\varepsilon$. Indeed, since the diameter of each chamber is at least $C\varepsilon$, their perimeter is at least $2C_2\varepsilon$. Therefore

$$P(\mathscr{F}_\varepsilon) = \frac{1}{2}\sum_{i=0}^{M} P(\mathscr{F}_\varepsilon(i)) \geq C_2 M\varepsilon.$$

We observe also that, since the chambers have area at most ε^2, the total area of $\mathscr{F}_\varepsilon$ is at most $M\varepsilon^2$ and therefore $|\mathscr{G}_\varepsilon| \geq 1 - M\varepsilon^2$. Now we consider two cases:

Case I $\mathscr{H}^1(\Sigma_\varepsilon) \leq \frac{1}{2}P(\mathscr{F}_\varepsilon)$.

Then

$$\begin{aligned}P(\mathscr{E}_\varepsilon) &= P(\mathscr{G}_\varepsilon) + P(\mathscr{F}_\varepsilon) - \mathscr{H}^1(\Sigma_\varepsilon)\\ &\geq P(\mathscr{G}_\varepsilon) + \frac{1}{2}P(\mathscr{F}_\varepsilon)\\ &\geq \frac{1}{\varepsilon}\sqrt[4]{12}|\mathscr{G}_\varepsilon| + \frac{C_2}{2}M\varepsilon\\ &\geq \frac{1}{\varepsilon}\sqrt[4]{12} + \left(\frac{C_2}{2} - \sqrt[4]{12}\right)M\varepsilon.\end{aligned}$$

From the upper bound of Lemma 3.7 we conclude.

Case II $\mathscr{H}^1(\Sigma_\varepsilon) \geq \frac{1}{2}P(\mathscr{F}_\varepsilon)$.

Then we observe that $P(G_\varepsilon) \geq \mathscr{H}^1(\Sigma_\varepsilon) \geq \frac{C_2}{2}M\varepsilon$ and apply the improved honeycomb inequality (Lemma 3.6) to obtain

$$\begin{aligned}P(\mathscr{E}_\varepsilon) \geq P(\mathscr{G}_\varepsilon) &\geq \frac{1}{\varepsilon}\sqrt[4]{12}|\mathscr{G}_\varepsilon| + cP(G_\varepsilon)\\ &\geq \frac{1}{\varepsilon}\sqrt[4]{12} + \left(\frac{C_2}{2}c - \sqrt[4]{12}\right)M\varepsilon\end{aligned}$$

and we conclude again using the upper bound of Lemma 3.7. In particular we can choose $C_2 = 2\frac{1+\sqrt[4]{12}}{c}$.

□

Restriction lemma

Given an open set $U \subset \mathbb{R}^2$ with locally finite perimeter and a cluster $\mathscr{E}_\varepsilon = (\mathscr{E}_\varepsilon(0), \ldots, \mathscr{E}_\varepsilon(N))$, we define the notion of "the portion of $\mathscr{E}_\varepsilon$ inside U" in two ways:

- the *truncation* $\mathscr{E}_\varepsilon \cap U$ is obtained intersecting the chambers with U, that is we consider the cluster whose chambers are $\mathscr{E}_\varepsilon(i) \cap U$;
- the *restriction* $\mathscr{E}_\varepsilon^U$ is obtained considering the subcluster composed by all the chambers which are entirely contained in U. We set $E_\varepsilon^U = \bigcup_{i=1}^N \mathscr{E}_\varepsilon^U(i)$.

We now prove in the next lemma that if a family of clusters $\mathscr{E}_\varepsilon$ has a convergent global shape $E_\varepsilon \to E_0$ and satisfies the diameter bound (3.14), then also the restriction subclusters for any given regular open set U shape-converge: $E_\varepsilon^U \to E_0 \cap U$. In the following we will just need this for U equal to a disk, but the proof works assuming that $|I_r(\partial U)| \leq Cr$ where I_r denotes the r-neighbourhood. This is true for instance if U is a Lipschitz domain.

Lemma 3.13 (Stability of shape convergence under restrictions). *Given clusters $\mathscr{E}_\varepsilon$ that shape-converge to E_0 and satisfy the diameter bound (3.14), and given any regular open set U with locally finite perimeter, the restriction clusters $\mathscr{E}_\varepsilon^U$ also shape-converge to $E_0 \cap U$. The same result for the truncation clusters $\mathscr{E}_\varepsilon \cap U$ is also trivially true.*

Proof. Given a positive r, define

$$U_r := \{x \in U : \operatorname{dist}(x, U^c) > r\}$$

If $r > C\varepsilon$ then by Lemma 3.12

$$|E_\varepsilon^U| \geq |E_\varepsilon \cap U_r| - C_2\varepsilon \geq |E_\varepsilon \cap U| - Cr - C_2\varepsilon$$

because $|E_\varepsilon \cap U| = |E_\varepsilon \cap U_r| + |E_\varepsilon \cap (U \setminus U_r)| \leq |E_\varepsilon \cap U_r| + Cr$ (here we are using the regularity of U, in particular $|U \setminus U_r| \leq Cr$). Therefore

$$|E_\varepsilon^U \Delta (E_\varepsilon \cap U)| = |(E_\varepsilon \cap U) \setminus E_\varepsilon^U| = |E_\varepsilon \cap U| - |E_\varepsilon^U| \leq Cr + C_2\varepsilon$$

and choosing a family $r(\varepsilon) \to 0$ as $\varepsilon \to 0$ and such that $r > C_2\varepsilon$ (C_2 being the constant of Lemma 3.12; e.g. to stay safe we can choose $r(\varepsilon) = \sqrt{\varepsilon}$) we obtain that

$$|E_\varepsilon^U \Delta (E_0 \cap U)| \leq |E_\varepsilon^U \Delta (E_\varepsilon \cap U)| + |(E_\varepsilon \cap U) \Delta (E_0 \cap U)|$$

goes to zero, which means $E_\varepsilon^U \to E_0 \cap U$. $\square$

Corollary 3.14. *Shape convergence is stable under restrictions for sequences of minimizing clusters $\mathscr{E}_\varepsilon$: the restriction subclusters $\mathscr{E}_\varepsilon^U$ converge in shape to $E_0 \cap U$.*

Proof. Apply Lemma 3.13. The assumption on the diameter bound is satisfied by Lemma 3.12. $\square$

We will use the previous result to prove the result of the next section (Theorem 3.17).

Basic regularity of E_0

We now prove the basic regularity result for the global shape E_0, namely that the measure-theoretic exterior $E_0^{(0)}$ is an open set.

Theorem 3.15 (Basic regularity of E_0). *The limit global shape E_0 is equivalent to a closed set: more precisely, the set $E_0^{(0)}$ of points of Lebesgue density* 0 *is an open set.*

Proof. We take a point of density 0 (wlog the origin), and prove that for a sufficiently small radius r we have $|B_r \cap E_0| = 0$. Suppose by contradiction this is not true. In particular for any radius s, $0 < s < r$, we have that $\mathscr{E}_\varepsilon \cap B_s \neq \emptyset$ for sufficiently small ε. By the density assumption for any positive η there is r_0 such that $|E_0 \cap B_s| \leq \eta s^2$ for every $0 \leq s \leq r_0$. We construct a competitor $\widetilde{\mathscr{E}}_\varepsilon$ by cutting the cluster $\mathscr{E}_\varepsilon$ with a ball B_r and replacing the cut part somewhere else with a cluster $\mathscr{E}^{hex}$ as in Lemma 3.7. Call $m(r) := |E_0 \cap B_r|$. Then

$$P(\widetilde{E}_\varepsilon) \leq P(\mathscr{E}_\varepsilon) - P(\mathscr{E}_\varepsilon, B_r) + \mathscr{H}^1(E_\varepsilon \cap \partial B_r) + \frac{\sqrt[4]{12}}{\varepsilon} m(r) + C_1\sqrt{m(r)}. \tag{3.15}$$

By the improved Hales inequality 3.12 we have

$$P(\mathscr{E}_\varepsilon) \geq \frac{\sqrt[4]{12}}{\varepsilon} m(r) - \mathscr{H}^1(E_\varepsilon \cap \partial B_r) + cP(E_\varepsilon \cap B_r) \tag{3.16}$$

and moreover since minimizers are connected we know that for sufficiently small ε we have $P(\mathscr{E}_\varepsilon, B_r) \geq r$. Therefore by (3.15), (3.16) and the minimality of $\mathscr{E}_\varepsilon$ we obtain

$$0 \leq P(\widetilde{\mathscr{E}}_\varepsilon) - P(\mathscr{E}_\varepsilon) \leq 2\mathscr{H}^1(E_\varepsilon \cap \partial B_r) - 2cr + C_1\sqrt{m(r)}.$$

By Fubini for a.e. $r > 0$ we have that

$$\mathscr{H}^1(E_\varepsilon \cap \partial B_r) \to \mathscr{H}^1(E_0 \cap \partial B_r) \quad \text{as } \varepsilon \to 0$$

and in particular for a.e. r and sufficiently small ε we have

$$\mathscr{H}^1(E_\varepsilon \cap \partial B_r) \leq 2H^1(E_0 \cap \partial B_r) = 2m'(r).$$

Therefore we obtain

$$4m'(r) - 2cr + C\sqrt{m(r)} \geq 0.$$

By the density assumption we can choose η so that $C\sqrt{m(r)} \leq cr$ for every sufficiently small radius r. But then

$$m'(r) \geq \frac{1}{2}cr$$

and thus

$$m(r) \geq m(0) + \frac{1}{4}cr^2 = \frac{1}{4}cr^2$$

which is a contradiction if we also choose $\eta < \frac{1}{4}c$. We therefore conclude by contradiction that for some $r > 0$ we have $|E_0 \cap B_r| = 0$. □

Remark 3.16. The analogous result for the measure-theoretic interior, i.e. that $E_0^{(1)}$ is an open set, can not be obtained so easily. Instead of a cut-type argument we would need a filling-type argument: for instance find the optimal way to fill the empty region between two different honeycombs without creating too much energy. This is a much harder task.

3.5 Asymptotic energy distribution in minimal clusters

After having extablished the existence of a limit global shape in the space of finite perimeter sets by forgetting about the interior structure of the clusters, we now see what happens to the interior structure. To this aim we define the measures $\nu_\varepsilon := \varepsilon\mathscr{H}^1 \llcorner \partial\mathscr{E}_\varepsilon$ and the goal is to find the (weak) limit of ν_ε as $\varepsilon \to 0$.

The next theorem says that the perimeter density is asymptotically uniform (and equal to the energy of a hexagonal partition).

Theorem 3.17 (Equipartition of the limit density). *Given a family of minimizers $\mathscr{E}_\varepsilon$ that shape-converge to E_0, the measures defined above satisfy*

$$\nu_\varepsilon \overset{*}{\rightharpoonup} \sqrt[4]{12}\mathscr{L}^2 \llcorner E_0.$$

Proof. (i) *Upper bound on the total mass.* The improved honeycomb inequality of Lemma 3.6 and the upper bound given by Lemma 3.7 imply

$$\sqrt[4]{12} \le \|\nu_\varepsilon\| \le \sqrt[4]{12} + \mathscr{O}(\varepsilon)$$

where $\|\cdot\|$ is the total mass. Therefore up to subsequence $\nu_\varepsilon \overset{*}{\rightharpoonup} \nu$ and $\|\nu\| \le \liminf_{\varepsilon\to 0} \|\nu_\varepsilon\| = \sqrt[4]{12}$.

(ii) *Pointwise lower bound on balls:* for any ball B, $\nu(\bar{B}) \ge \sqrt[4]{12}|B \cap E_0|$.

Indeed, consider the restrictions $\mathscr{E}_\varepsilon^B$ inside B to obtain a subcluster $\mathscr{E}_\varepsilon^B$. By Lemma 3.13 $E_\varepsilon^B \to B \cap E_0$ in L^1. By the honeycomb inequality (3.2) (suitably rescaled by ε) we obtain that $\nu_\varepsilon(B) \ge \varepsilon P(\mathscr{E}_\varepsilon^B) \ge \sqrt[4]{12}|E_\varepsilon^B|$. Therefore by the weak convergence and by Lemma 3.13

$$\nu(\bar{B}) \ge \limsup_{\varepsilon\to 0} \nu_\varepsilon(\bar{B}) \ge \limsup_{\varepsilon\to 0} \sqrt[4]{12}|E_\varepsilon^B| = \sqrt[4]{12}|B \cap E_0|.$$

(iii) *Pointwise lower bound on open sets:* for any open set U, $\nu(U) \ge \sqrt[4]{12}|U \cap E_0|$.

We use a covering argument. Given any open set U we consider the fine cover given by

$$\mathscr{F} := \{\bar{B}(x,r) : x \in U, 0 < r < \operatorname{dist}(x, \partial U)\}.$$

By the Besicovitch-Vitali covering theorem [AFP00, Theorem 2.19] applied to the measure $\nu + \mathscr{L}^2$ there is a subfamily $\mathscr{F}' \subset \mathscr{F}$ such that

$$(\nu + \mathscr{L}^2)\left(U \setminus \bigcup \mathscr{F}'\right) = 0.$$

Therefore using part (ii)

$$\begin{aligned}
\nu(U) &= \nu\left(U \setminus \bigcup \mathscr{F}'\right) + \nu\left(\bigcup \mathscr{F}'\right) \\
&= \sum_{\bar{B} \in \mathscr{F}'} \nu(\bar{B}) \\
&\ge \sum_{\bar{B} \in \mathscr{F}'} \sqrt[4]{12}|\bar{B} \cap E_0| \\
&= \sqrt[4]{12}\left|\bigcup_{\bar{B} \in \mathscr{F}'} \bar{B}\right| \\
&= \sqrt[4]{12}|U \cap E_0|.
\end{aligned}$$

(iv) *Pointwise lower bound on Borel sets:* for any Borel set A, $\nu(A) \geq \sqrt[4]{12}|A \cap E_0|$.

By the regularity of the measures ν and $\mathscr{L}^2$, for any Borel set A we have

$$\begin{aligned}\nu(A) &= \inf\{\nu(U) : U \text{ open}, U \supset A\}\\ &\geq \inf\{\sqrt[4]{12}|U \cap E_0| : U \text{ open}, U \supset A\}\\ &= \sqrt[4]{12}|A \cap E_0|.\end{aligned}$$

□

Open problem (Next-order energy density) Define $\mu_\varepsilon = \mathscr{H}^1 \llcorner \partial\mathscr{E}_\varepsilon - \frac{1}{\varepsilon}\sqrt[4]{12}\mathscr{L}^2 \llcorner E_\varepsilon = \frac{1}{\varepsilon}(\nu_\varepsilon - \mathscr{L}^2 \llcorner E_\varepsilon)$. Is there a limit $\lim_{\varepsilon\to 0} \mu_\varepsilon$ in a suitable space? Is this limit supported on the boundary ∂E_0?

3.6 Relation to weighted clusters of Chapter 2

We now briefly discuss what we can say about the asymptotic global shape of *weighted* clusters, as those considered in Chapter 2.

Some results of this chapter hold also in the case where we put different weights. Consider for instance the case of the functional P_ε as defined in (2.2), which we recall here for convenience

$$P_\varepsilon(\mathscr{E}) = \frac{1}{2}\sum_{\substack{0\leq i,j\leq N\\ i\neq j}} c_{ij}(\varepsilon)\mathscr{H}^1(\partial\mathscr{E}(i) \cap \partial\mathscr{E}(j)),$$

$$c_{ij}(\varepsilon) = \begin{cases} 1 & \text{if } i = 0 \text{ or } j = 0\\ 2-\varepsilon & \text{if } i,j \neq 0\end{cases}.$$

For any $\varepsilon > 1$ (i.e. the weigth between bubbles is lower than the weight with the exterior) the existence of a global shape for P_ε-minimizers when $N \to \infty$ follows immediately, even without assuming Conjecture 3.4 or the lower bound on the areas (3.5). Indeed we can write

$$P_\varepsilon(\mathscr{E}_N) = (2-\varepsilon)P(\mathscr{E}_N) + (\varepsilon - 1)P(\mathscr{E}_N(0)) \geq (2-\varepsilon)\sqrt[4]{12}N + \sqrt{N}(\varepsilon-1)P(\mathscr{E}_N(0))$$

and use the same upper bound of Lemma 3.7 to obtain equiboundedness of $\frac{1}{\sqrt{N}}P(\mathscr{E}_N(0))$.

In the case when $\varepsilon < 1$ we could obtain the existence of a limit global shape assuming Conjecture 3.4, and the values of admissible ε would depend on the constant δ of the conjecture. However we can not expect this to hold for $\varepsilon > 0$ small. Indeed there is a competitor which creates holes and is better than the honeycomb as soon as $2-\varepsilon > \sqrt{3}$ (it is sufficient to insert a small triangular hole at each vertex of the honeycomb; a first variation argument shows that this improves the situation if $2-\varepsilon > \sqrt{3}$). This is in agreement with the results of Chapter 2, where for really small ε and fixed N we obtain many holes between the bubbles, which are almost disks.

There is an issue which we mentioned already in Remark 2.3, and which consists in understanding if we can exchange the order of the limits for $\varepsilon \to 0$ and for $N \to \infty$, and similarly in the case $\varepsilon \to 2$, which

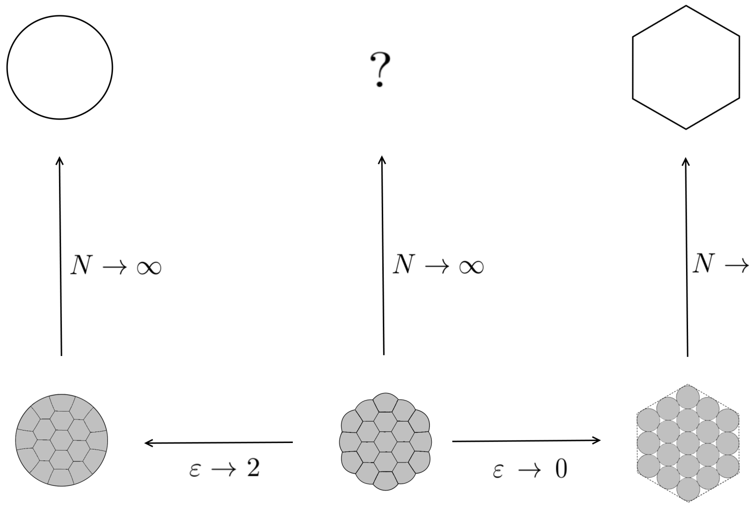


Figure 3.3: For a fixed number N of chambers, as $\varepsilon \to 0$ we obtain minimal configurations for the sticky disk (Theorem 2.2). As $\varepsilon \to 2$ we obtain an optimal partition of the disk (Section 2.4, Remark (ii)). If we then send $N \to \infty$ we obtain in the first case a hexagonal global shape ([AYFS12], [DPS17], see also Chapter 4, Section 4.1), while in the second case a circular global shape (trivial). This indicates that the global shape as $N \to \infty$ for minimizers of the classical perimeter could be intermediate and neither a hexagon nor a circle.

has been already mentioned in Section 2.4(ii). If we fix N we know that in the two cases the global shape is respectively a hexagon and a circle. Exchanging the order of the limits would give information on the limit global shape when ε is close to 0 or 2. We can actually do this in the case $\varepsilon \to 2$ and prove that for any fixed ε close to 2, the limit global shape as $N \to \infty$ of P_ε-minimizing clusters is close to a disk. Set for convenience $\alpha := 2 - \varepsilon$.

Proposition 3.18. *For any fixed α suppose $\mathscr{E}_\alpha^N$ are minimizing N-clusters with chambers of unit area for*

$$P_{2-\alpha}(\mathscr{E}) := \alpha P(\mathscr{E}) + (1-\alpha)P(\mathscr{E}(0)).$$

Then $\frac{1}{\sqrt{N}}\mathscr{E}_\alpha^N$ shape-converge (up to subsequence and rigid motions) to a finite perimeter set E_α^∞ which satisfies

$$A(E_\alpha^\infty) \le C\sqrt{\alpha}.$$

Recall that $A(E)$ is the asymmetry index introduced in (1.11) and measures the distance of E from a disk. We put for simplicity

$$E_\alpha^N := \frac{1}{\sqrt{N}} \bigcup_{i=1}^{N} \mathscr{E}_\alpha^N(i).$$

Proof. From Hales inequality (3.6) we have

$$P_{2-\alpha}(\mathscr{E}^N) \geq \alpha N \sqrt[4]{12} + (1-\alpha)P(\mathscr{E}^N(0)).$$

Moreover we can build a competitor which satisfies

$$P_\alpha(\mathscr{E}^N) \leq \alpha N \sqrt[4]{12} + C\alpha\sqrt{N} + (1-\alpha)2\sqrt{\pi}\sqrt{N}.$$

Indeed it suffices to consider an (almost-)optimal partition of a disk of area N. For instance, given a disk of radius $R = \sqrt{N/\pi}$, put a honeycomb inside the disk of radius $R-10$ and the on the annulus $B_R \setminus B_{R-10}$ put any partition such that each chamber has perimeter bounded by a constant C.

Then we conclude that for a minimizer $\bar{\mathscr{E}}_\alpha^N$ we have

$$P(E_\alpha^N) \leq 2\sqrt{\pi} + C\alpha$$

and therefore the isoperimetric deficit satisfies

$$\delta(E_\alpha^N) \leq C\alpha.$$

Since minimizers are connected we conclude by compactness of finite perimeter sets that E_α^N converge in L^1 to a finite perimeter set E_α^∞. By lower semicontinuity of perimeter

$$\delta(E_\alpha^\infty) \leq C\sqrt{\alpha}$$

and by the quantitative isoperimetric inequality (Theorem (1.5)) we conclude

$$A(E_\alpha^\infty) \leq C\sqrt{\alpha}.$$

$\square$

Chapter 4

Variants

We analyze some variants of the problem of minimizing N-clusters. In the first variant (Section 4.1) we consider clusters whose chambers are equal *regular* hexagons, and prove that minimizers are crystallized, that is they lie in the same honeycomb. By known results [AYFS12], [DPS17] it follows that in this case the asymptotic global shape is a regular hexagon. In the second variant (Section 4.2) we consider anisotropic clusters with cubic Wulff shape. Thanks to the quantitative anisotropic isoperimetric inequality [FMP10] we prove that in this case in any dimension the asymptotic global shape is a cube, with a precise rate of convergence. Then in Section 4.3 we look at square clusters made of equal-area square chambers and prove a Γ-convergence result for low energy configurations that gives rise to *polycrystals*. Finally in Section 4.4 we analyze the sticky-disk model and prove a compactness result for the orientation of low energy configurations.

Contents

4.1 Hexagonal clusters

We now consider **hexagonal clusters**, that is N-clusters whose chambers are *regular* hexagons of side-length 1. We again look at minimizing clusters and ask what is the global shape as $N \to \infty$. The situation here is very rigid, since any pair of hexagons with non-parallel sides share no boundary. Still, the problem of characterizing minimizers is not completely obvious, and bears a close resemblance to the *sticky disk* problem: maximize the number of tangencies among N disjoint disks of unit radius in the plane. In fact, the proof of the main result will follow the lines of the proof of the crystallization for the sticky disk [HR80].

For this section, an admissible hexagonal N-cluster is thus a cluster $\mathscr{E}_N$ whose chambers are closed regular hexagons of sidelength 1. A minimal hexagonal N-cluster $\bar{\mathscr{E}}_N$ is a cluster that minimizes the usual perimeter $P(\mathscr{E}_N)$. As always, we could at times omit the subscript N.

First we will show that minimal N-clusters are *oriented*, that is all hexagons have the same orientation. Then we will prove that minimal hexagonal N-clusters are *crystallized*, that is they coincide (up to a rigid motion) with a portion of the *honeycomb* (4.2). To this aim, to every hexagonal N-cluster $\mathscr{E}$ we associate a graph $G(\mathscr{E})$, called bond graph, where the vertices are the centers $\{x_i\}$ of the hexagons, and two vertices are connected by a straight edge if and only if the corresponding hexagons have nonempty intersection. We prove some properties of graphs associated to N-clusters, and then obtain the crystallization result by adapting the proof by R.C. Heitmann and C. Radin used in [HR80] to prove crystallization for ground states of the sticky disk. A similar proof has been used by Radin in [Rad81] to prove crystallization for a special type of potential called *soft disk*. At their turn, Heitmann and Radin took inspiration from a proof by H. Harborth in [Har74], which concerned the maximum number of edges in a subgraph of the triangular lattice with a fixed number of vertices.

Finally, having proved crystallization of minimal N-clusters, we are left with finding the least perimeter configurations among all subsets of fixed cardinality of the infinite honeycomb. We can also restate this equivalently as the following minimization problem: among all subsets X_N of N points of the infinite triangular lattice $\mathscr{A}_2$ (the dual of the hexagonal lattice, see (4.1)), minimize the total energy

$$E(X_n) = \frac{1}{2}\sum_{i\neq j} V(|x_i - x_j|)$$

where $V : [0,\infty) \to \mathbb{R}\cup\{\infty\}$ is the **sticky disk potential**:

$$V(r) = \begin{cases} +\infty & \text{if } 0 \le r < 1 \\ -1 & \text{if } r = 1 \\ 0 & \text{if } r > 1 \end{cases} .$$

In this way the problem of minimizing the total perimeter of crystallized N-clusters becomes completely equivalent to the problem of minimizing the energy of crystallized configurations of particles. As we will see, the global shape converges to an hexagon. We can conclude this using two approaches: the first one, from [DPS17], gives a precise estimate on the rate of convergence of minimizers to a hexagonal global shape; the second one, from [AYFS12] gives a weaker estimate for the convergence, but it could possibly be adapted to more general settings (namely, to study configurations with *low* energy, not just minimizers, and moreover with more general potentials instead of the *sticky disk*). A variant of the second approach, using the quantitative anisotropic isoperimetric inequality for the cubic anisotropy, will be explained later in Section 4.2.

Minimal N-clusters are oriented

Given a hexagonal N-cluster $\mathscr{E}$, for every chamber $\mathscr{E}(i)$ consider its vertices $v_i^1,\dots,v_i^6$ and the set $V_i := \{v_i^k - x_i\}$ of the positions of the vertices relative to the center x_i of $\mathscr{E}(i)$. We say that two hexagons $\mathscr{E}(i),\mathscr{E}(j)$ have the same orientation, or are parallel, if $V_i = V_j$.

Lemma 4.1 (**Minimal N-clusters are oriented**). *If $\mathscr{E} = \{\mathscr{E}(1),\dots,\mathscr{E}(N)\}$ minimizes the perimeter among all admissible N-clusters, then the hexagons $\mathscr{E}(i)$ have the same orientation, i.e. $V_i = V_j$ for every $i, j = 1,\dots,N$.*

Proof. We divide the hexagons in equivalence classes with respect to the equivalence relation of having the same direction, i.e. $\mathscr{E}(i) \sim \mathscr{E}(j) \iff V_i = V_j$. The key simple point is that the perimeter is additive with respect to these equivalence classes, since two of them can intersect only in a finite number of points.

Suppose now that there are at least two nonempty equivalence classes. Then move all the classes far away from each other (which preserves the perimeter by the above observation), and rotate them all in the same direction, and then glue back two of them along the sides of two hexagons, thus decreasing the perimeter. This shows that the original configuration was not minimal, and this shows that in a minimal cluster there can be only one equivalence class. □

The next aim is to prove that in minimal N-clusters **crystallization** occurs, that is all chambers are part of the same hexagonal honeycomb. Let $\mathscr{A}_2 \subset \mathbb{R}^2$ be the **triangular lattice** of sidelength 1:

$$\mathscr{A}_2 := \left\{ m\begin{pmatrix}1\\0\end{pmatrix} + n\begin{pmatrix}1/2\\ \sqrt{3}/2\end{pmatrix} : m,n \in \mathbb{Z} \right\}. \tag{4.1}$$

Given $x \in \sqrt{3}\mathscr{A}_2$ define its **Voronoi cell** $\mathscr{V}(x)$ as the set of points whose distance from x is less or equal than the distance from any other point of $\sqrt{3}\mathscr{A}_2$:

$$\mathscr{V}(x) := \left\{ y \in \mathbb{R}^2 : |x-y| \le |y-z| \; \forall z \in \sqrt{3}\mathscr{A}_2 \right\}.$$

It is easy to check that

$$\mathscr{H}_2 := \{V(x) : x \in \sqrt{3}\mathscr{A}_2\} \tag{4.2}$$

is a family of closed regular hexagons with unit sidelength, which we will refer to as the *honeycomb* in this Section. Notice the difference with the honeycomb in the other chapters, whose hexagons have unit *area*.

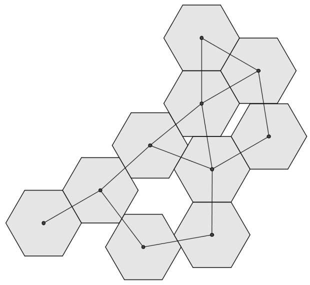


Figure 4.1: An oriented cluster and its bond graph.

Bond graph

We fix from now on a cluster $\mathscr{E}_N$ of hexagons having the same orientation, and we associate to every chamber $\mathscr{E}_N(i)$ its center $x_i^{(N)} \in \mathbb{R}^2$. We construct a planar graph $G = G(\mathscr{E}_N)$ associated to $\mathscr{E}_N$, called **bond graph**, in this way: the vertices of the graph are the centers $x_i^{(N)}$ of the hexagons, and two distinct vertices $x_i^{(N)}, x_j^{(N)}$ are connected with a straight edge if and only if the two hexagons $\mathscr{E}_N(i), \mathscr{E}_N(j)$ have nonempty intersection (recall that interiors are disjoint by hypothesis, but boundaries can overlap since we are considering closed hexagons). Call $\mathrm{Edge}(G)$ the set of all undirected edges of G (also called bonds), that is of all unordered pairs of vertices that are connected by an edge. Call two chambers bonded if their centers are connected by a bond. The edges identify a finite number of *inner* faces, that is bounded regions surrounded by edges, and one *exterior* unbounded face.

Observe that, if we call $P_{ij} = \mathscr{H}^1(\mathscr{E}_N(i) \cap \mathscr{E}_N(j))$ the common perimeter between chambers $\mathscr{E}_N(i)$ and $\mathscr{E}_N(j)$ (which is always ≤ 1), then we can rewrite the total perimeter as

$$P(\mathscr{E}_N) = 6N - \sum_{i<j} P_{ij} \geq 6N - \sum_{\substack{i<j \\ P_{ij} \neq 0}} 1 = 6N - \#\mathrm{Edge}(G).$$

Therefore if we want to minimize the perimeter we may try to:

(i) maximize the number of edges in the graph G;

(ii) maximize the common perimeter P_{ij} between each pair of bonded cells.

As we will show it turns out that doing both things simultaneously is possible (for example with the *spiral* configurations, see Figure 4.2), and this will imply that every pair of bonded chambers must share an entire side; this in turn implies crystallization provided that the graph is connected, which can be trivially seen to be true.

More precisely, denoting by $B(N)$ the maximum value of $\#\mathrm{Edge}(G)$ among all graphs $G(\mathscr{E}_N)$, we will show that

$$B(N) = \lfloor 3N - \sqrt{12N - 3} \rfloor \tag{4.3}$$

following the proof by Heitmann and Radin [HR80], and that the maximum is attained by the spiral (although this is not the only minimizer, see Remark 4.5).

Maximum number of edges in the bond graph

We now first derive some properties that the bond graph G associated to an oriented cluster must satisfy in order to maximize the number of bonds. Then we will prove the bound (4.3).

Lemma 4.2 (**Properties of** $G(\mathscr{E}_N)$)**.** *Let $G(\mathscr{E}_N)$ be the graph associated to an oriented N-cluster with the maximum number of bonds, $N \geq 3$. Then:*

- *G is connected;*
- *the angle between every pair of edges sharing one vertex is at least $\pi/3$;*
- *every vertex has degree between 2 and 6;*
- *every edge belongs to at least one inner face.*

Proof. If G had at least two connected components, we could translate on of them until it touches another one, thus increasing the number of bonds, which contradicts the fact that G had the maximum number of bonds.

The fact that the minimum angle between two consecutive edges is at least $\pi/3$ is self-evident from a picture.

If a vertex has degree zero then the graph is disconnected. If a vertex has degree one, we could slide the corresponding hexagon along the side of its neighbouring hexagon until it touches another one, contradicting maximality of bonds. If we can make a whole 2π angle without touching another hexagon then the hexagon must lie in a connected component of size 2, and the graph must be disconnected, contradiction.

From the bound on the angle between consecutive edges it follows that every vertex has at most six edges.

If there were an edge belonging to no inner face, by removing it we would disconnect the graph, obtaining two components and lowering by one the total number of edges. Now we can always put together the two components by creating at least two new edges, contradicting the minimality of the original graph. □

Proposition 4.3. *Let G be the graph associated to an oriented N-cluster. Then the maximum number $B(N)$ of edges that G can have satisfies*

$$B(N) \leq \lfloor 3N - \sqrt{12N-3} \rfloor .$$

Proof. We prove the theorem by induction on the number N of vertices of G. The cases $N = 1,2$ are true by inspection. We thus consider $N \geq 3$. Take a graph of order N realizing the maximum number of edges. Let us define the following quantities:

- F is the total number of faces excluding the external one;
- F_j is the number of faces having exactly j sides; thus $F = \sum_j F_j$;

- a is the number of vertices on the boundary of the graph, i.e. the vertices touching the external face;

- k_j is the number of vertices in the boundary with degree j; thus $a = \sum_j k_j$.

Then:

(i) From the lower bound on the angle between consecutive edges we obtain that, for a boundary vertex with j edges, the exterior angle is $\pi - \sum \alpha_{int} \leq \pi - (j-1)\pi/3$.

Summing among all boundary vertices, the exterior angles α_{ext}^j add up to 2π, and so:

$$2\pi = \sum_j \alpha_{ext}^j \leq \sum_j k_j \left(\pi - (j-1)\frac{\pi}{3}\right) = \pi a - \sum_j k_j (j-1)\frac{\pi}{3}$$

which can be rewritten as:

$$3a - 6 \geq \sum_j k_j (j-1). \tag{4.4}$$

(ii) The number of edges $B(N)$ can be also obtained by summing over the faces the number of edges per face:

$$\sum_j jF_j = 2B(N) - a$$

since every boundary edge is counted once and the others are counted twice. Now we use the fact that every face has at least three sides and Euler's identity $F + V - E = 1$ to get

$$\sum_j jF_j \geq 3F = 3(B(N) - N + 1)$$

and combining this with the previous identity we obtain

$$N - a \geq B(N) - 2N + 3. \tag{4.5}$$

(iii) We now remove the boundary vertices of G and all the edges connected to them, obtaining a graph G' of order $N - a$. This is equivalent to remove the boundary hexagons of the original N-cluster and to consider the bond graph G' of the new cluster. If $a = N$, then by (4.5) we obtain $B(N) \leq 2N - 3 \leq 3N - \sqrt{12N - 3}$, and we are done. If instead $a < N$, by definition G' has at most $B(N - a)$ edges. The total number of removed edges to obtain G' from G is at most $\sum_j k_j (j-1)$. Therefore if $a < N$

$$B(N - a) \geq B(N) - \sum_j k_j (j-1)$$

and from equation (4.4) we obtain the key relation

$$B(N) \leq B(N - a) + 3a - 6. \tag{4.6}$$

We are now ready to prove the induction step. Suppose that the theorem is true for every $m = 1, \dots, N-1$. From inequality (4.6), induction hypothesis and equation (4.5) we get

$$\begin{aligned} B(N) &\leq 3(N-a) - \sqrt{12(N-a)-3} + 3a - 6 \\ &= (3N-6) - \sqrt{12(N-a)-3} \\ &\leq (3N-6) - \sqrt{12(B(N)-2N+3)-3} \end{aligned}$$

from which it follows

$$\sqrt{12B(N)-36N+33} \leq (3N-6) - B(N)$$

and squaring both sides

$$B(N)^2 - 6NB(N) + (9N^2 - 12N + 3) \geq 0.$$

The left term is a second degree polynomial in $B(N)$. The solutions of the associated equation are

$$\frac{6N \pm \sqrt{36N^2 - 4(9N^2 - 12N + 3)}}{2} = 3N \pm \sqrt{12N-3},$$

but since $B(N) \leq 3N$ (because every vertex has degree at most 6) and since $B(N)$ is an integer we obtain

$$B(N) \leq \lfloor 3N - \sqrt{12N-3} \rfloor.$$

□

The next lemma gives the exact number of edges in a special *spiral* configuration, which is built nestling hexagons around a spiraling path and which we denote by Sp_N (see Figure 4.2). This construction can essentially be found in [HR80], but we reproduce it here adding the details of the computation. The same configuration is called *daisy* in [DPS17].

Lemma 4.4 (Spiral configurations). *The upper bound $\lfloor 3N - \sqrt{12N-3} \rfloor$ is attained by the spiral configurations Sp_N, thus giving*

$$B(N) = \lfloor 3N - \sqrt{12N-3} \rfloor.$$

Proof. We follow closely the construction in [HR80], adding some details. Consider three fixed integers $s \geq 0$, $0 \leq k \leq 5$, and $0 \leq j \leq s$. Consider a big "hexagon of points", with $s+1$ points per side, and then place an incomplete layer of points by filling k of the six sides and by placing a further j points. We refer to figure 4.2 for the construction, which is easier to visualize than to explain. Then it is easy to check that the total number of points is $N = (3s^2 + 3s + 1) + (s+1)k + j$, and we can obtain any positive integer with this construction. We claim that the total number $H(n)$ of bonds in this spiraling configuration is exactly $\lfloor 3N - \sqrt{12N-3} \rfloor$.

To enumerate the bonds, we sum the degree of each vertex and divide by two:

$$H(N) = \frac{1}{2}\sum_v e_v = \frac{1}{2}\sum_v (6 - m_v) = 3N - \frac{1}{2}\sum_v m_v$$

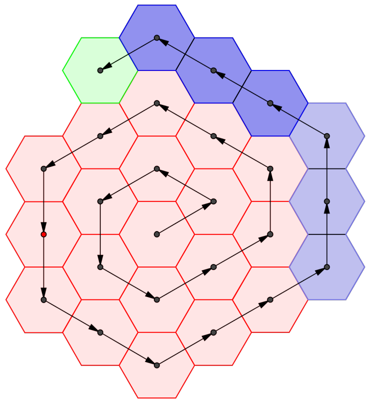


Figure 4.2: A spiral configuration with $s = 2$, $k = 2$, $j = 1$. Both the vertices and their Voronoi cells are pictured. In general $s+1$ is the "sidelength" (i.e. the number of cells, or vertices, per side) of the big hexagon (in red); $0 \leq k \leq 5$ is the number of entirely filled sides on the last layer (in blue); j is the number of remaining vertices (in green).

where v is a vertex, e_v its degree and $m_v = 6 - e_v$ the number of missing edges (to reach a total of 6) of v. Now, the only missing edges occur on the boundary.

If $j = k = 0$ then it is easy to see that for every of the three possible directions for the edges there are $2(2s+1)$ missing edges, giving a total of $6(2s+1)$ missing edges, so that

$$H(N) = 9s^2 + 3s.$$

If instead $j \neq 0$ or $k \neq 0$ then for each of the three possible directions for the edges, the missing edges with that direction are the sum of: $2(2s+1)$ due to the hexagon of side $s+1$ (as before); $2(k+1)$ due to the last layer. In total there are $12s+6+2(k+1)$ missing edges. Therefore

$$\begin{aligned} H(N) = 3N - \frac{1}{2}\sum_v m_v &= 3(3s^2+3s+1) - \frac{1}{2}(12s+6+2k+2) \\ &= 9s^2+3s+(3s+2)k+3j-1. \end{aligned}$$

In summary

$$H(n) = \begin{cases} 9s^2+3s & \text{if } j = k = 0 \\ 9s^2+3s+(3s+2)k+3j-1 & \text{if } j \neq 0 \text{ or } k \neq 0. \end{cases}$$

The statement of the lemma can be rewritten as

$$H(N) - 3N = \lfloor -\sqrt{12N-3} \rfloor = -\lceil \sqrt{12N-3} \rceil$$

which is equivalent to

$$(3N - H(N) - 1)^2 < 12N - 3 \leq (3N - H(N))^2.$$

The case $j = k = 0$ (a complete hexagon of side $s+1$) is simple since in this case $N = 3s^2 + 3s + 1$ and $H(N) = 9s^2 + 3s$, and thus

$$\sqrt{12N-3} = \sqrt{36s^2 + 36s + 9} = 6s + 3 = 3N - H(N).$$

If instead $j + k > 0$ we have

$$\begin{aligned} 3N - H(N) &= 3(3s^2 + 3s + 1 + (s+1)k + j) - (9s^2 + 3s + (3s+2)k + 3j - 1) \\ &= 6s + k + 4. \end{aligned} \tag{4.7}$$

and

$$12n - 3 = (6s+3)^2 + 12\big((s+1)k + j\big) = \big((6s+3) + k\big)^2 - k^2 + 6k + 12j. \tag{4.8}$$

Putting together the last two estimates the thesis becomes then

$$(6s + k + 3)^2 < (6s + k + 3)^2 - k^2 + 6k + 12j \leq (6s + k + 4)^2.$$

As for the first inequality we have

$$k^2 - 6k - 12j = k(k-6) - 12j < 0$$

since $k \leq 5$ and $j \geq 0$, and they can not be both zero.

As for the second inequality, it is equivalent to

$$k^2 - 4k + 7 + 12(s - j) \geq 0$$

which is true since $12(s-j) \geq 0$ and $k^2 - 4k + 7 = (k-2)^2 + 3 > 0$. □

Remark 4.5. While for $j = k = 0$ the big hexagon given by the spiral configuration is the uninque minimizer, in general the spiral configurations are not the unique minimizers. Instead, for some values of N there is a high non-uniqueness, see [Sch13] for a construction of many minimizers, which differ among them by $\approx N^{3/4}$ vertices, and also [DLF17] for a characterization of those N which admit a unique minimizer.

Crystallization of minimal N-clusters

We now collect the results proven until now to obtain the crystallization of minimal N-clusters.

Theorem 4.6. *Every minimal hexagonal N-cluster is crystallized, i.e. it coincides up to rotations and translations with a subfamily of N cells of the hexagonal infinite honeycomb* (4.2).

Proof. From Lemma 4.1 we know that a minimal cluster must be oriented. From Lemmas 4.3 and 4.4 we know that the maximum number of bonds is $B(N) = \lfloor 3N - \sqrt{12N-3} \rfloor$, and that there exists a

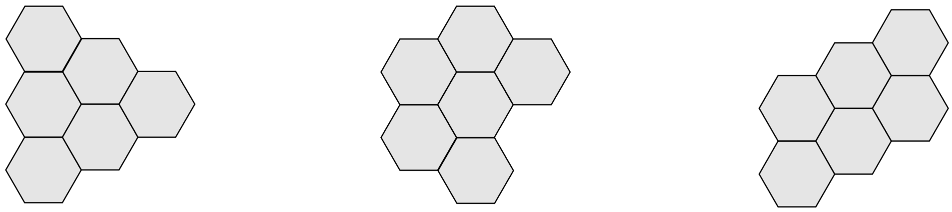


Figure 4.3: All depicted configurations are minimal for $N = 6$, showing non-uniqueness in minimizers.

configuration (the spiral) that not only realizes this maximum but also maximizes the common perimeter between every pair of bonded cells. This implies that for any N-cluster $\mathscr{E}_N$

$$P(\mathscr{E}_N) = 6N - \sum_{i<j} P_{ij} \geq 6N - \sum_{\substack{i<j \\ P_{ij}\neq 0}} 1 = 6N - \#\mathrm{Edge}(G)$$
$$\geq 6N - B(N) = P(Sp_N) \geq \min P.$$

In particular this is true when $\mathscr{E}_N$ is any minimal n-cluster, for which all inequalities become equalities. This implies that every two touching hexagons must share an entire side, and that the number of these bonds must be $B(n)$. The former, together with the connectedness of G, implies that the cluster is crystallized. □

Global shape of minimal N-clusters

After obtaining crystallization, we can prove that the asymptotic global shape when $N \to \infty$ is hexagonal. We mention two approaches.

The first approach comes from a work by Davoli, Piovano and Stefanelli [DPS17], where they prove an edge-isoperimetric inequality in the triangular lattice. Given an N-point subset C_N of the triangular lattice $\mathscr{A}_2$, its edge boundary Θ is the set

$$\Theta(C_N) := \{(x_i, x_j) : |x_i - x_j| = 1, x_i \in C_N, x_j \in \mathscr{A}_2 \backslash C_N\},$$

and the **edge perimeter** is its cardinality $|\Theta(C_N)|$. Call

$$\theta_N := \min\{\Theta(C_N)\}$$

where the minimum is taken among all possible N-point subsets of $\mathscr{A}_2$. It is easy to see that, given a crystallized configuration X_N of N particles, and considered the hexagonal N-cluster $\mathscr{E}_N = \mathscr{E}(X_N)$ given by the Voronoi hexagons of each particle, the perimeter of the cluster and the edge perimeter of X_N are closely related, namely

$$P(\mathscr{E}_N) = 3N + \frac{1}{2}|\Theta_N|.$$

Therefore minimizing the edge perimeter of X_N is the same as minimizing the perimeter of $\mathscr{E}(X_N)$, and minimal configurations are in correspondence. Associate to any configuration X_N its **empirical measure**

$$\mu_{X_N} := \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i/\sqrt{N}}.$$

We now invoke the following theorem to obtain the convergence to the hexagonal shape.

Theorem 4.7 ([DPS17, Theorem 1.2]). *For every sequence of minimizers M_N in $\mathscr{A}_2$ there exists a sequence of suitable translations M'_N such that*

$$\mu_{M'_N} \overset{*}{\rightharpoonup} \frac{2}{\sqrt{3}}\chi_H$$

weakly in the sense of measures, where χ_H is the characteristic function of the regular hexagon H defined as the convex hull of the vectors*

$$\left\{\pm\frac{1}{\sqrt{3}}e_1, \pm\frac{1}{\sqrt{3}}e_2, \pm\frac{1}{\sqrt{3}}(e_2-e_1)\right\}.$$

Furthermore, the following assertions hold true:

$$|M_N \backslash H_{r_{M_N}}| \leq KN^{3/4} + o(N^{3/4}) \tag{4.9}$$

$$\left\| \mu_{M_N} - \mu_{H_{r_{M_N}}} \right\| \leq KN^{-1/4} + o(N^{-1/4}) \tag{4.10}$$

$$\left\| \mu_{M'_N} - \frac{2}{\sqrt{3}}\chi_H \right\|_F \leq KN^{-1/4} + o(N^{-1/4}), \tag{4.11}$$

where $H_{r_{M_N}}$ is the maximal spiral configuration that can be fit inside M_N, $K := \frac{2}{3^{1/4}}$ and $\|\cdot\|_F$ is the flat norm (1.1).

The second approach involves the work by Au Yeung, Friesecke and Schmidt [AYFS12] where they prove that the limiting global shape as $N \to \infty$ is a regular hexagon in the following sense: associate again to a minimal N-cluster $\mathscr{E}_N$ its empirical measure

$$\mu_N = \frac{1}{n}\sum_{i=1}^{N} \delta_{x_i^{(N)}/\sqrt{N}}$$

where $x_i^{(N)}$ are the centers of the hexagons $\mathscr{E}_N(i)$. Then up to rigid motions, $\mu_N \overset{*}{\rightharpoonup} \rho\chi_H\mathscr{L}^2$, where H is a regular hexagon of side 1, $\rho = 2/3\sqrt{3}$ and $\mathscr{L}^2$ is the Lebesgue measure on $\mathbb{R}^2$. In particular this is a consequence of the following Γ-convergence result. Define the functionals

$$I_N(\mu) = \begin{cases} \displaystyle\int_{\mathbb{R}^4\backslash \mathrm{diag}} NV(\sqrt{N}|x-y|)d\mu\otimes d\mu & \text{if } \mu = \frac{1}{N}\sum_{i=1}^{N}\delta_{x_i/\sqrt{N}} \\ & \text{for some distinct } x_i \in \mathscr{A}_2; \\ +\infty & \text{otherwise} \end{cases}$$

where V is the sticky-disk potential.

Theorem 4.8 ([AYFS12, Theorem 5.1]). *The sequence of functionals I_N Γ-converges, with respect to the weak* convergence of probability measures, to the limit functional*

$$I_\infty(\mu) := \begin{cases} \displaystyle\int_{\partial^* E} \Gamma(\nu_E) d\mathscr{H}^1 & \text{if } \mu = \frac{2}{\sqrt{3}} \mathbb{1}_E \text{ for some set} \\ & E \text{ of finite perimeter;} \\ +\infty & \text{otherwise} \end{cases}$$

where Γ is the hexagonal anisotropy explicitly given by

$$\Gamma(\nu) = 2\left(\nu_2 - \frac{\nu_1}{\sqrt{3}}\right) \text{ for } \nu = \begin{pmatrix} -\sin\phi \\ \cos\phi \end{pmatrix}, \phi \in [0, \tfrac{2\pi}{6}]$$

etended $\frac{2\pi}{6}$-periodically.

4.2 Anisotropic clusters

By using the anisotropic perimeter P_K defined in (1.9) we can define an anisotropic version of the perimeter of an N-cluster $\mathscr{E}$ simply by

$$P_K(\mathscr{E}) := \frac{1}{2} \sum_{i=0}^{N} P_K(\mathscr{E}(i)). \tag{4.12}$$

The anisotropic global shape problem is: given a convex set K, what is the global shape of N-clusters minimizing P_K as $N \to \infty$? While for general convex K the problem has at least the same difficulty as the isotropic one, we expect some simplifications in the case when K tiles the space, that is when there is a partition of $\mathbb{R}^n$ (up to a $\mathscr{L}^n$-negligible set) by translated copies of K. This happens for instance for the cube in any dimension, and for the hexagon in the planar case.

Cubic anisotropy

We will see how the quantitative anisotropic isoperimetric inequality can be used to conclude that, when K is a cube in $\mathbb{R}^n$, then the global shape is itself a cube, with an estimate for the rate of convergence to the cube. The same approach, however, does not work when K is a hexagon in the plane, essentially due to the following key fact: while it is possible to partition a cube in many equal cubes, it is not possible to partition a hexagon in many equal hexagons. However, if we impose a priori that all cells are exactly hexagons, then the method works (see Section 4.1).

As a corollary we will recover an $N^{3/4}$-law for the square lattice, originally proved by Schmidt in the planar case for the triangular lattice [Sch13], and obtain its analogue in higer dimension: among subsets S with cardinality N of the square lattice $\mathbb{Z}^2$ (or $\mathbb{Z}^n$), minimizers of the edge-perimeter $\Theta(S)$ differ from a square (cube) at most by $N^{3/4}$ points ($N^{1-\frac{1}{2n}}$). Here the **edge-perimeter** is the total number of unit-length segments connecting a point in S with a point in $\mathbb{Z}^n \setminus S$. Actually Schmidt proves more in the planar case, namely the sharpness of the estimate, constructing a sequence of planar minimizers with N_k points, for a certain sequence with $N_k \to \infty$, which really differ from a hexagon by $\approx N_k^{3/4}$ points.

Let $Q = [-1,1]^n \subset \mathbb{R}^n$, and consider the anisotropic perimeter P_Q as defined above. Equivalently, we weight the normal with the ℓ^1-norm:

$$P_Q(E) = \int_{\partial^* E} \|\nu_E(x)\|_1 d\mathscr{H}^{n-1}(x).$$

Let also $Q_0 = [0,1]^n$ in $\mathbb{R}^n$, so that $P_Q(Q_0) = 2n$. Given an N-cluster $\mathscr{E}_N$, define its anisotropic perimeter by (4.12) and define its global shape as $E_N := \bigcup_{i=1}^N \mathscr{E}(i)$.

Theorem 4.9 (**Cubic global shape with rate of convergence**). *As $N \to \infty$, the global shape of P_Q-minimizing N-clusters $\bar{\mathscr{E}}_N$ converge to a cube. More precisely, for every minimizer $\bar{\mathscr{E}}_N$ with unit chambers' areas there is a translation vector τ such that*

$$\frac{1}{N}|E_N \Delta(\tau + \sqrt{N} Q_0)| \leq C(n) \frac{1}{N^{\frac{1}{2n}}}.$$

Proof. (i) Lower bound: for any competitor $\mathscr{E}_N$, by the anisotropic isoperimetric inequality applied to the chambers $\mathscr{E}(1), \ldots, \mathscr{E}(N)$ (but not $\mathscr{E}(0)$), we have that

$$P_Q(\mathscr{E}_N) \geq \frac{1}{2}(N P_Q(Q_0) + P_Q(E_N)).$$

(ii) Upper bound: we build a competitor $\widetilde{\mathscr{E}}_N$ with reasonably low energy. Write $N = m^n + k$ where $m := \lfloor N^{1/n} \rfloor$, $0 \leq k \leq (m+1)^n - m^n - 1$. Then the competitor is made of a big cube of side m partitioned in unit cubes, plus an additional layer of k cubes, reasonably laid. We will take for granted that this competitor can be chosen to have perimeter at most equal to that of a big cube of sidelength $m+1$, that is

$$P_Q(\widetilde{\mathscr{E}}_N) \leq \frac{1}{2}\left(N P_Q(Q_0) + 2n(m+1)^{n-1}\right).$$

(iii) Isoperimetric deficit of $\bar{E}_N$: putting together (i) and (ii) we obtain that for a minimizer $\bar{\mathscr{E}}$

$$P_Q(\bar{E}_N) \leq 2n(m+1)^{n-1}$$

and therefore we can estimate the isoperimetric deficit of $\bar{E}_N$

$$\begin{aligned}
\delta_Q(\bar{E}_N) &= \frac{P_Q(\bar{E}_N)}{N^{\frac{n-1}{n}} P(Q_0)} - 1 \\
&\leq \frac{2n(m+1)^{n-1}}{N^{\frac{n-1}{n}} 2n} - 1 \\
&\leq \left(\frac{N^{\frac{1}{n}} + 1}{N^{\frac{1}{n}}}\right)^{n-1} - 1 \\
&\leq (2^{n-1} - 1)\frac{1}{N^{\frac{1}{n}}}.
\end{aligned}$$

because $(1+x)^{n-1} \leq 1 + (2^{n-1} - 1)x$ for $0 \leq x \leq 1$.

(iv) Conclusion: by the quantitative anisotropic isoperimetric inequality [FMP10] we obtain that there is $\tau \in \mathbb{R}^n$ such that

$$\frac{|\bar{E}_N \Delta(\tau + N^{1/n} Q_0)|}{|N^{1/n} Q_0|} \leq C(n)\sqrt{\delta P(\bar{E}_0)} \leq C(n)\sqrt{2^{n-1}-1}\frac{1}{N^{1/2n}}.$$

□

$N^{3/4}$-law for edge-perimeter minimizers in $\mathbb{Z}^2$

We now obtain as a Corollary the upper $N^{1-\frac{1}{2n}}$-law for edge-perimeter minimizers. Given a subset S with cardinality N of the lattice $\mathbb{Z}^n$, associate to each point $x \in S$ its **Voronoi cell** $V(x) := \{y \in \mathbb{R}^n : |y-x| \leq |y-z| \forall z \in \mathbb{Z}^n\}$, which is a unit cube. Define moreover the characteristic function $f_S := \sum_{x \in S} \chi_{V(x)}$.

Corollary 4.10 (**Upper $N^{1-\frac{1}{2n}}$-law for edge-perimeter minimizers in $\mathbb{Z}^n$**). *Given a subset S with cardinality N of $\mathbb{Z}^n$, minimizers for the edge-perimeter differ from a big cube of sidelength $N^{1/n}$ by at most $\approx N^{1-\frac{1}{2n}}$ points, that is a translation of f_S satisfies $\|f_S - \chi_{N^{1/n}Q_0}\|_1 \leq CN^{1-\frac{1}{2n}}$.*

Proof. Associate to each point $x \in S$ its Voronoi cell and apply the previous theorem to the union of these cells, noting that the edge-perimeter of S equals exactly the anisotropic perimeter of the union of the cells. Then a suitable translation of a cube of sidelength $N^{1/n}$ verifies the estimate of Theorem 4.9. □

Remark 4.11. The previous Corollary actually sets an upper bound for the discrepancy from a cube; it remains to prove whether it is sharp, that is to construct a sequence of minimizers S_{N_j}, with $N_j \to \infty$, that really differ from a cube by $\approx N_j^{1-\frac{1}{2n}}$ points. As we will show next, this is possible in the planar case. In the case of $\mathbb{Z}^3$, this is false: it has been proved in [Mai+18] that the same $N^{3/4}$ law holds for the dicrepancy in the cubic shape for a minimizer (and not $N^{5/6}$). This is quite surprising since the same behaviour is witnessed in two and three dimensions. However, it does not seem the case that the same $N^{3/4}$ law continues to hold in general dimension n: it is reasonable to expect at least a discrepancy of the order of the surface area, that is $N^{\frac{n-1}{n}}$, which for $n \geq 5$ is worse than $N^{3/4}$. Anyway, the case $n \geq 4$ remains open.

In order to prove the sharpness in the planar case we cite the following result :

Theorem 4.12 ([HH76]). *Among planar unions of N unit squares with sides parallel to the axes and with centers lying in $\mathbb{Z}^2$, the minimal perimeter is $2\lceil 2\sqrt{N}\rceil$.*

Associate as above to any subset S of $\mathbb{Z}^2$ the union of its Voronoi cells, and the function $f_S = \sum_{x \in S} \chi_{V(x)}$.

Lemma 4.13 (**Lower $N^{3/4}$-law for edge-perimeter minimizers in $\mathbb{Z}^2$**). *There exists a sequence $N_j \to \infty$ and minimizers S_{N_j} of the edge-perimeter that differ from a square by at least $\approx N_j^{3/4}$ points, that is $\|f_S - \sqrt{N}Q_0\| \gtrsim N_j^{3/4}$ for every translation of f_S. In particular, we can choose $N_j = j^4 + 2j^3 + 2j^2 + 2j + 1$.*

Proof. Observe that $N_j = (j^2+j+1)^2+1 = (j^2+2j+2)(j^2+1)$. We claim that a rectangle of sides $a_j = j^2+2j+2$ and $b_j = j^2+1$ is a minimizer among configurations of cardinality $N_j = a_j b_j$. Indeed, N_j is of the form m_j^2+1, $m_j = j^2+j+1$, and therefore

$$\begin{gathered} m_j^2 < N_j < \left(m_j + \frac{1}{2}\right)^2 \\ 2m_j < 2\sqrt{N_j} < 2m_j+1 \end{gathered}$$

and the minimal cardinality given by Theorem 4.12 is $2\lceil 2\sqrt{N_j}\rceil = 4m_j+2 = 4j^2+4j+6$, which coincides with the perimeter of the rectangle $2(a_j+b_j)$.

In particular, the two sides differ by $2j+1 \approx N^{1/4}$, and thus the area of the discrepancy from a square is $\approx N^{1/2}N^{1/4} \approx N^{3/4}$. □

By Corollary 4.10 and Lemma 4.13 we obtain:

Corollary 4.14 (Sharp $N^{3/4}$-law for edge-perimeter minimizers in $\mathbb{Z}^2$). *Minimizers for the edge perimeter in $\mathbb{Z}^2$ differ from a square by at most $\approx N^{3/4}$ points, and there is a sequence N_j and minimizers S_{N_j} that really differ by $\approx N_j^{3/4}$ points.*

Remark 4.15. The same $N^{3/4}$ law could be proved for the triangular lattice in a similar way, but some care has to be taken in considering to which set the anisotropic isoperimetric inequality has to be applied. Indeed, rather than to the union of the Voronoi cells, it has to be applied to a slightly modified polygon that eliminates the oscillations at a microscopic level. Referring to [AYFS12] the right sets to take into consideration are the sets called H'_N.

4.3 Square clusters: Γ-convergence to a polycrystal

We now describe a model for polycrystals that arises from perimeter-minimizing square clusters. For every natural number N we consider all families $\mathcal{Q}_N = (Q_1^N, \ldots, Q_N^N)$ composed by N squares in $\mathbb{R}^2$ with area $\frac{1}{N}$ and with pairwise disjoint interiors. We consider the perimeter of their union

$$F(\mathcal{Q}_N) := P\left(\bigcup_{i=1}^{N} Q_i^N\right)$$

and look for sequences of configurations $\mathcal{Q}_N$ minimizing F. Observe that F as defined above does not coincide with the perimeter of $\mathcal{Q}_N$ seen as a cluster, but it is strictly related: $P(\mathcal{Q}_N) = \frac{1}{2}(4\sqrt{N} + F(Q_N))$ and thus minimizing one or the other functional is the same. Actually we will be interested in configurations with *bounded energy*, that is sequences $(\mathcal{Q}_N)_N$ such that

$$\sup_{N\in\mathbb{N}} F(\mathcal{Q}_N) < \infty.$$

We define the space of orientations as

$$K := \{(x,y) \in \mathbb{R}^2 : x^2 + y^2 = 1, x \geq 0 \wedge y \geq 0\},$$

that is, identifying $\mathbb{R}^2$ wth $\mathbb{C}$, K is the set of all unit vectors $e^{i\theta}$ with $\theta \in [0, \frac{\pi}{2}]$, and we define also

$$\widetilde{K} := K \setminus e_2$$

with $e_2 = (0,1) = e^{i\frac{\pi}{2}}$. Define now a **polycrystal** to be a Caccioppoli partition of $\mathbb{R}^2$ together with an orientation for each set in the partition, that is a collection $\mathscr{E}_I = (E_i, t_i)_{i \in I}$ with I at most countable such that each E_i is a finite perimeter set, $\sum_{i \in I} P(E_i) < \infty$ and where $t_i \in \widetilde{K}$ and where moreover $\sum_{i \in I} |E_i| = 1$. Define the polycrystal perimeter as

$$P(\mathscr{E}_I) = \sum_{i \in I} P_{t_i}(E_i)$$

where P_{t_i} is the perimeter having as Wulff shape a unit square with sides either parallel or perpendicular to t_i. In the notation of (1.9) this coincides with $P_{R_{t_i} Q}$ where $Q = \{x \in \mathbb{R}^2 : \|x\|_1 \leq 1\}$ and R_{t_i} is the rotation that sends $(1,0)$ to t_i.

Then we have the following result:

Theorem 4.16 (**Γ-convergence, informal statement**). *The functionals $F(\mathscr{Q}_N)$ Γ-converge to the functional $P(\mathscr{E}_I)$ defined on polycrystals. Moreover compactness up to rearrangements of components holds for sequences with bounded energy.*

Before giving the precise statement we translate the problem into the space of SBV functions, and in particular in the space of piecewise constant functions on Caccioppoli partitions. Let

$$X := \{u \in SBV(\mathbb{R}^2, K \cup \{0\}) : |\operatorname{supp} u| = 1\},$$

and

$$\widetilde{X} := \{u \in SBV(\mathbb{R}^2, \widetilde{K} \cup \{0\}) : |\operatorname{supp} u| = 1\}.$$

For every function $u \in X$ we can define $\widetilde{u} \in \widetilde{X}$ by replacing e_2 with e_1 if it appears in the image of u. Define also

$$\widetilde{X}_N := \left\{ u \in \widetilde{X} : u = \sum_{i=1}^{N} t_i \mathbb{1}_{Q(t_i)} \right\}$$

where $t_i \in \widetilde{K}$ and $Q(t_i)$ is a square with area $\frac{1}{N}$ and with sides either parallel or perpendicular to t_i. In particular we have that $\widetilde{X}_N \subset \widetilde{X} \subset X \subset SBV(\mathbb{R}^2, K \cup \{0\})$. Observe that we can associate to any $u \in \widetilde{X}_N$ a family of squares $\mathscr{Q}_N$ in the obvious way and conversely to any family $\mathscr{Q}_N$ we can associate a function $u \in \widetilde{X}_N$. Define the functionals $F_N : \widetilde{X}_N \to [0, +\infty]$ by

$$F_N(u) := \begin{cases} P\left(\bigcup_{i=1}^{N} Q_N(t_i)\right) = F(\mathscr{Q}) & \text{if } u \in \widetilde{X}_N \text{ and } u = \sum_{i=1}^{N} t_i \mathbb{1}_{Q(t_i)} \\ +\infty & \text{otherwise} \end{cases}.$$

We observe that these functionals can be rewritten as

$$F_N(u) = \mathscr{H}^1(J_u) = \int_{J_u} |\nu_u| d\mathscr{H}^1 = \int_{J_u} \phi(u^+,u^-,\nu_u) d\mathscr{H}^1$$

where

$$\phi(i,j,p) = \begin{cases} \psi(i,p)+\psi(j,-p) & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

where $\psi(i,p) = |i|\left(|i\cdot p| + \sqrt{1-|i\cdot p|^2}\right)$ for $p \in \mathbb{S}^1$ and extended by 1-homogeneity. For every $i \in \mathbb{S}^1$ $\psi(i,p)$ coincides with the "square norm in direction p", while for $i=0$ it is constantly zero. In this way ψ is convex and 1-homogeneous in the variable p and therefore is jointly convex (recall (1.15)). We are therefore led to define the functional $F : X \to [0,+\infty]$ as

$$F(u) = \int_{J_u} \phi(u^+,u^-,\nu_u) d\mathscr{H}^1.$$

We also define

$$\widetilde{\phi}(i,j,p) = \begin{cases} \phi(i,j,p) & \text{if } \{i,j\} \neq \{e_1,e_2\} \\ 0 & \text{if } \{i,j\} = \{e_1,e_2\} \end{cases}$$

and we define the corresponding functional as $\widetilde{F} : X \to [0,\infty]$

$$\widetilde{F}(u) := \int_{J_u} \widetilde{\phi}(u^+,u^-,\nu_u) d\mathscr{H}^1.$$

We recall the following lower semicontinuity result.

Theorem 4.17 ([AFP00, Theorem 5.22]). *Let $K \subset \mathbb{R}^m$ compact and $\phi : K \times K \times \mathbb{R}^n \to [0,\infty]$ be a jointly convex function satisfying*

$$\phi(i,j,p) \geq c|p| \quad \forall i,j \in K, i \neq j, p \in \mathbb{R}^n$$

for some $c > 0$. Let $(u_h) \subset SBV(\Omega)^m$ be a sequence converging in $L^1(\Omega)^m$ to u, such that $(|\nabla u_h|)$ is equiintegrable and, for any $h \in \mathbb{N}$, $u_h(x) \in K$ for $\mathscr{L}^n$-a.e. $x \in \Omega$. Then $u \in SBV(\Omega)^m$, $u(x) \in K$ for $\mathscr{L}^n$-a.e. $x \in \Omega$ and

$$\int_{J_u} \phi(u^+,u^-,\nu_u) d\mathscr{H}^{n-1} \leq \liminf_{h\to\infty} \int_{J_{u_h}} \phi(u_h^+,u_h^-,\nu_{u_h}) d\mathscr{H}^{n-1}.$$

We now show the following result:

Theorem 4.18 (Γ-convergence). *The functionals F_N Γ-converge to the functional $\widetilde{F}$ in the space X, with respect to the L^1 convergence of the functions.*

Proof. $\Gamma-\liminf$: let $u \in X$ and $u_N \in \widetilde{X}_N$ such that $u_N \to u$ in $L^1(\mathbb{R}^2,\mathbb{R}^2)$. Then by Theorem 4.17 we obtain

$$\widetilde{F}(u) \leq F(u) = \int_{J_u} \phi(u^+,u^-,\nu_u) d\mathscr{H}^1 \leq \liminf_{N\to\infty} \int_{J_{u_N}} \phi(u_N^+,u_N^-,\nu_{u_N}) d\mathscr{H}^1 = F_N(u_N).$$

$\Gamma - \limsup$: given $u \in X$ we observe that $\widetilde{F}(u) = F(\widetilde{u})$ and therefore we can suppose $u \in \widetilde{X}$ and work with F. We suppose $F(u) < \infty$, otherwise there is nothing to prove. Since $\mathscr{H}^1(J_u) \leq F(u)$ we also have $\mathscr{H}^1(J_u) < \infty$. By the density of polygonal-wise constant functions [BCG17] we can also suppose that u is polygonal-wise constant. We are therefore left to prove the following: for each $u \in \widetilde{X}$ polygonal-wise constant and with $|\operatorname{supp} u| = 1$ there is a sequence $u_N \in \widetilde{X}_N$ such that $u_N \to u$ in $L^1(\mathbb{R}^2, \mathbb{R}^2)$ and such that $F_N(u_N) \to F(u)$.

To this aim, consider the lattice Q^ν obtained rotating $\mathbb{Z} \times \mathbb{Z}$ in direction ν, and let $\mathscr{Q}_N^\nu$ be the family of squares with side $1/\sqrt{N}$ obtainable with vertices in $\frac{1}{\sqrt{N}} Q^\nu$. If $u = \sum_{i=1}^k t_i \chi_{P_i}$ with P_i polygons then we define

$$P_i' = \bigcup \{Q : Q \in \mathscr{Q}_N^{t_i} \text{entirely contained in } P_i\}$$

and

$$v_N = \sum_{i=1}^k t_i \chi_{P_i'}.$$

Observe that in general the support of v_N has measure strictly less then 1. However it is easy to show that

$$0 \leq 1 - |\operatorname{supp} v_N| \lesssim \frac{1}{\sqrt{N}} \mathscr{H}^1(\partial P).$$

We can thus add some additional squares far away from $\bigcup P_i$ to reach the right number of squares. By the previous estimate we can put them in a big square configuration with side of order $\approx N^{-1/4}$, with arbitrary orientation, obtaining a function $u_N \in \widetilde{X}_N$. In this way

$$|F(u_N) - F(v_N)| \lesssim \frac{1}{N^{1/4}}$$

and

$$\|u_N - v_N\|_{L^1} \lesssim \frac{1}{\sqrt{N}}.$$

It can now be shown that the sequence v_N (and thus u_N) has the required properties. □

Of course the previous Γ-convergence result would be useless without a compactness result ensuring convergence in L^1 of sequences with bounded energy. Observe that this convergence could be false: even a sequence of minimizers could go to infinity exploiting the translation invariance of the problem. But even if we allow ourselves to translate the configurations, for sequences with bounded energy there could be many componenets going to infinity in different ways. We therefore state the compactness result with a confinement assumptions on the supports:

Proposition 4.19 (Compactness of bounded sequences). *Let (u_N) be a sequence such that $\sup_N F_N(u_N) < \infty$. Suppose that $\operatorname{supp} u_N \subset B(0,R)$ for some $R > 0$ and every $N \in \mathbb{N}$. Then there exists a subsequence, always denoted by u_N, and a piecewise constant function $u \in X$ such that $u_N \to u$ in L^1 as $N \to \infty$.*

In order to prove the previous proposition we recall two theorems from [AFP00]. Theorem 4.8, adapted to our case of piecewise constant functions with $|\nabla u_h| \equiv 0$ and $\theta \equiv 1$, can be stated in the following way:

Theorem 4.20 (Adaptation of [AFP00, Theorem 4.8]). *Let $\Omega \subset \mathbb{R}^2$ be a bounded open set, and let (u_h) be piecewise constant functions such that*

$$\sup_h \int_{J_{u_h}} |u_h^+ - u_h^-| d\mathscr{H}^1 < \infty$$

and such that $\sup_h \|u_h\|_\infty < \infty$. Then there exists a subsequence $(u_{h(k)})$ weakly converging in $BV(\Omega)$ to $u \in SBV(\Omega)$. In particular $u_h \to u$ in $L^1(\Omega)$.*

In our case the assumption of the theorem becomes simply

$$\sup_h \mathscr{H}^1(J_{u_h}) < \infty$$

which we know to be true for sequences with bounded energy. Theorem 4.25 instead deals directly with piecewise constant functions.

Theorem 4.21 ([AFP00, Theorem 4.25]). *Let Ω be a bounded open set with Lipschitz boundary. Let $(u_h) \subset SBV(\Omega)^m$ be a sequence of piecewise constant functions such that $(\|u_h\|_\infty + \mathscr{H}^1(S_{u_h}))$ is bounded. Then there exists a subsequence $(u_{h(k)})$ converging in measure to a piecewise constant function u.*

Proof of Proposition 4.19. From the first theorem above, there is a subsequence converging to $u \in SBV(\Omega)$ in $L^1(\Omega)$. From the second theorem above, the fact that convergence in L^1 implies convergence in measure and the uniqueness of the limit in measure, we obtain also that u is piecewise constant, as desired. □

We note that the limit function u belongs to X and not $\widetilde{X}$, that is in general it takes values in K and not $\widetilde{K}$.

We now show how the assumption on the supports, namely that $\operatorname{supp} u_N \subset B(0,R)$ for some $R > 0$, is not so restrictive.

Lemma 4.22. *Given a sequence (u_N) with bounded energy, there exist a modified sequence (v_N) that is obtained from u_N just by translating the components of the support and such that the compactness property $\operatorname{supp} v_N \subset B(0,R)$ holds for a sufficiently large $R > 0$. Moreover, for minimizers the same conclusion is true up to translation of the whole function.*

Proof. The sum of the diameters of the components is bounded by $F(u_N)$, which are equibounded. Since the perimeter is additive with respect to the different components, and we can translate each component by preserving the total perimeter, the conclusion follows. Observe also that minimizers are easily shown to be connected. □

We also observe that there is a trivial minimizer for the polycrystal perimeter.

Proposition 4.23. *The minimum of the functional F is attained by a constant function u supported on a square of area 1, where the value assumed by u is parallel to a side of the square.*

Proof. This follows from the anisotropic isoperimeteric inequality (1.10) and the subadditivity of the square root (used to deal with the case of many components). □

For this reason a more appropriate setting for studying polycrystals is the one with a constrained boundary, but we won't treat this case here.

4.4 Limit orientation for the sticky disk

The aim of this Section is to prove that we can define a notion of "limit orientation" for (suitably rescaled) low energy configurations $X_N = \{x_1, \dots x_N\}$ that interact by means of the sticky disk potential.

More precisely, consider the sticky disk potential $V : [0, \infty) \to \mathbb{R} \cup \{+\infty\}$ given by

$$V(r) = \begin{cases} +\infty & \text{if } 0 \le r < 1 \\ -1 & \text{if } r = 1 \\ 0 & \text{if } r > 1 \end{cases}$$

and consider configurations of N particles $X_N = \{x_1, \dots x_N\}$ that interact by means of V with energy

$$E(X_N) = \sum_{1 \le i < j \le N} V(|x_i - x_j|).$$

It is easy to show that there are configurations satisfying $E(X_N) \le -3N + C\sqrt{N}$ for some universal constant C. We therefore define

$$F(X_N) := \frac{E(X_N) + 3N}{\sqrt{N}}$$

and define **low energy sequences** as those sequences $(X_N)_{N \in \mathbb{N}}$ such that $\sup_{N \in \mathbb{N}} F(X_N) < \infty$.

We consider the subset $Int(X_N) \subset X_N$ given by those particles which have six neighbours at distance 1 and define $\partial X_N = X_N \setminus Int(X_N)$. Letting $\mathscr{N}(x)$ denote the set of neighbours of the particle x we can rewrite the energy as

$$E(X_N) = \frac{1}{2} \sum_{x \in X_N} -\#\mathscr{N}(x) \ge -3\#Int(X_N) - \frac{5}{2}\#\partial X_N = -3N + \frac{1}{2}\#\partial X_N$$

since every particle has at most six neighbours and each pair of neighoburs gives energy -1. We observe that in particular for every low energy sequence we have

$$\#\partial X_N \lesssim \sqrt{N}. \tag{4.13}$$

We now want to define a notion of orientation for any given low energy sequence (X_N). We associate to each particle $x \in Int(X_N)$ its closed Voronoi cell $\mathscr{V}(x)$ with respect to the whole configuration X_N, that is

$$\mathscr{V}(x) := \{y \in \mathbb{R}^2 : |y - x| \le |y - x_i| \, \forall i = 1, \dots, N\}.$$

These Voronoi cells are regular hexagons of sidelength $\frac{1}{\sqrt{3}}$. For technical reasons we also define the Voronoi cell of each particle in ∂X_N to be the empty set. To each of the nonempty hexagonal Voronoi cells we associate an orientation $t_{\mathscr{V}(x)}$ given by the unique unit vector $e^{i\theta} \in \mathbb{S}^1$ with $\theta \in [0, \frac{\pi}{3})$ that is perpendicular to one of the sides of the hexagons. We then associate to each configuration X_N the following *SBV* function that takes into account a rescaling by a factor $\frac{1}{\sqrt{N}}$:

$$u_{X_N} := \sum_{x \in X_N} t_{\mathscr{V}(x)} \mathbb{1}_{\frac{1}{\sqrt{N}} \mathscr{V}(x)}.$$

In particular by (4.13) $0 \leq 1 - \|u\|_{L^1} \lesssim \frac{1}{\sqrt{N}}$. Moreover

$$E(Int(X_N)) - E(X_N) \lesssim \# \partial X_N \lesssim \sqrt{N}.$$

Set $\mathscr{V}(X_N) := \bigcup_{x \in X_N} \mathscr{V}(x)$. Then it is easy to see that

$$E(Int(X_N)) = -\frac{1}{2}(6\# Int(X_N) - \sqrt{3}\mathscr{H}^1(\partial \mathscr{V}(X_N)))$$

and therefore

$$\sqrt{N}\mathscr{H}^1(J_{u_{X_N}}) = \mathscr{H}^1(\partial \mathscr{V}(X_N)) \leq E(X_N) + 3N + C\sqrt{N} \lesssim \sqrt{N}$$

from which it follows that

$$\sup_N \mathscr{H}^1(J_{u_{X_N}}) < \infty$$

for any low energy sequence (X_N). Recalling theorems 4.20 and 4.21 we have thus obtained the following:

Theorem 4.24 (Limit orientation for the sticky disk). *Let (X_N) be a low energy sequence. Suppose that $X_N \subset B(0, R\sqrt{N})$ for some $R > 0$ and every $N \in \mathbb{N}$. Then there exists a subsequence (not relabeled) such that the associated SBV functions u_{X_N} converge in L^1 to a piecewise constant function u defined on a Caccioppoli partition and with values in $\{e^{i\theta} : \theta \in [0, \frac{\pi}{3}]\}$.*

An analogous result, together with some estimates on the Γ-limit of the rescaled energies, has been obtained in [DLNP18].

Remark 4.25. Theorem 4.24 is a prototype for a compactness result that we would like to obtain in the case of planar perimeter-minimizing N-clusters. However in the latter case it is not completely clear how to define an orientation, and moreover the lack of rigidity makes compactness results subtler. In the case of the sticky disk we really exploited the fact that roughly speaking "the interaction between two different orientations is rigid", while in more general cases (for instance a potential V with a quadratic behaviour around the minimum point $r = 1$) we expect to witness some elastic behaviour due to interactions between particles that occur at distance sligthly different than 1.

Chapter 5

Mass distribution of periodic measures

We estimate the total perimeter of the hexagonal honeycomb $\mathscr{H}$ inside a disk of radius r centered at any point in the plane, proving that it goes as $\sqrt[4]{12}\pi r^2 + \mathscr{O}(r^{2/3})$ as $r \to \infty$. In particular the remainder term is smaller than the trivial "surface" term $\mathscr{O}(r)$. A similar estimate holds for any periodic measure and in any dimension: in $\mathbb{R}^n$ the remainder term is $\mathscr{O}\big(r^{(n-1)\frac{n}{n+1}}\big)$. For some "nice" measures whose Fourier transform is supported on lower-dimensional subspaces we can give a better estimate.

Contents

In this chapter we will estimate the perimeter of the honeycomb $\mathscr{H}$ inside a large disk of radius r, that is

$$P_{\mathscr{H}}(r) := P(\mathscr{H}, B_r) = \frac{1}{2}\sum_i P(\mathscr{H}(i), B_r)$$

where B_r is a disk of radius r centered at any point and $\mathscr{H}$ is the honeycomb made of unit-area hexagons. It is easy to see that the leading term scales like the area of the disk, that is

$$P(r) = \sqrt[4]{12}|B_r| + \Delta_{\mathscr{H}}(r) = \sqrt[4]{12}\pi r^2 + \Delta_{\mathscr{H}}(r)$$

where the remainder term is $\Delta_{\mathscr{H}}(r) = o(r^2)$. It is not difficult to show that actually $\Delta_{\mathscr{H}}(r) = \mathscr{O}(r)$. The aim of this chapter is to prove that a stronger estimate holds for the remainder term, namely that

$$\Delta_{\mathscr{H}}(r) = \mathscr{O}(r^{2/3}). \tag{5.1}$$

In a certain sense the truncations of the cells near the boundary compensate each other to produce a better estimate than the trivial "surface" term $\mathscr{O}(r)$. In fact we will prove that the same estimate for the (suitably defined) remainder term holds for any periodic measure.

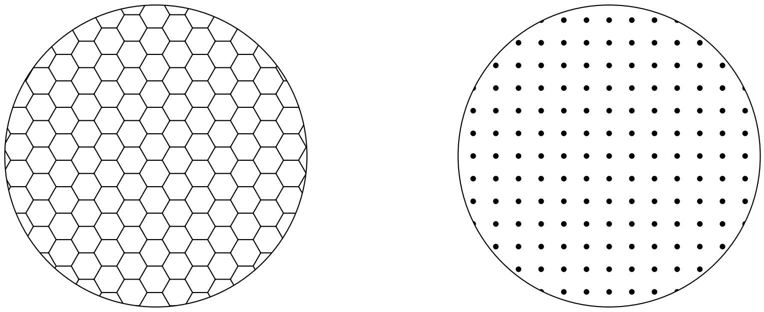


Figure 5.1: Computing the total perimeter of the honeycomb inside a disk B_r or counting the integer lattice points inside B_r can be both seen as evaluating a periodic measure on $\mathbb{1}_{B_r}$.

To understand why these compensations are at least reasonable to expect, we make a brief excursus on the famous *Gauss Circle Problem* (GCP), where the aim is counting the number of points with integer coordinates that are contained in the disk of radius r centered at the origin:

$$N(r) := \#\left\{(x,y) \in \mathbb{Z}^2 : x^2 + y^2 < r\right\}.$$

Also in this case the first term goes like the area of the disk, and the remainder term $\Delta(r) := N(r) - \pi r^2$ was known to Gauss to be bounded in modulus by $2\sqrt{2}\pi r$. This estimate was improved over the years by many authors, and it is still an active topic of research. Writing $\Delta(r) = \mathscr{O}(r^\theta)$, it has been proved by M.N. Huxley [Hux03] that we can choose $\theta = \frac{131}{208} \approx 0.6298\ldots$. On the other hand it was proved independently by Hardy [Har15] and Landau that $\Delta(r) \neq o\big(r^{\frac{1}{2}} \log(r)^{\frac{1}{4}}\big)$, thus setting a lower bound $\theta > \frac{1}{2}$. It is conjectured that $\Delta(r) = \mathscr{O}(r^{\frac{1}{2}+\varepsilon})$ for every $\varepsilon > 0$. In particular, this is much smaller than the trivial bound $\mathscr{O}(r)$.

While many papers about the GCP employ some heavy machinery to give finer and finer estimates for the exponent of r in the remainder term, we found a nice paper by C.S. Herz [Her62b] which gives the estimate $\Delta(r) = \mathscr{O}(r^{2/3})$ using only a few basic facts about the Fourier transform. It is by adapting the methods of this paper that we are able to prove the following estimate: for any measure μ in $\mathbb{R}^n$ which is periodic with respect to some lattice $\Lambda = A\mathbb{Z}^n$, where A is an invertible linear transformation, we have

$$\mu(B_r) = \frac{\mu(Q)}{|Q|}|B_r| + \mu(Q)\,\mathscr{O}\left(r^{(n-1)\frac{n}{n+1}}\right) \tag{5.2}$$

where $Q = A([0,1]^n)$ is a fundamental cell of the lattice Λ and the constants in the $\mathscr{O}$ depend on the dimension and the lattice only. In particular we obtain $\mathscr{O}(r^{2/3})$ for the honeycomb in the plane, that is for the 1-dimensional Hausdorff measure restricted to the honeycomb $\mu := \mathscr{H}^1 \llcorner \partial\mathscr{H}$, which is periodic with respect to the triangular lattice.

The result is almost certainly not optimal in the exponent of r. We actually may expect that the "continuous" nature of the support of $\mu = \mathscr{H}^1 \llcorner \partial\mathscr{H}$ (as opposed to the discrete support of the measure in the GCP) could give rise to smaller oscillations, thus making plausible a better estimate. For general periodic measures μ we may expect that the estimate for the remainder depends on the geometric properties of the support of μ. Note for instance that an easy modification of the proof of Theorem 5.4 (see Remark 5.5) shows that if instead we consider the square partition $\mathscr{Q}$ of the plane identified by $\partial\mathscr{Q} = (\mathbb{R}\times\mathbb{Z})\cup(\mathbb{Z}\times\mathbb{R})$ then we obtain

$$\Delta_{\mathscr{Q}}(r) = \mathscr{O}(r^{\frac{1}{2}}),$$

the key point being that in this case the Fourier transform of $\mu = \mathscr{H}^1 \llcorner \partial\mathscr{Q}$ (seen as a tempered distribution) is concentrated on the integer points of the two axes, instead of the whole integer lattice $\mathbb{Z}^2$ (which is the case for a generic periodic measure). We will expand on this in the last section, where we prove that indeed if the support of $\hat{\mu}$ is contained in some proper subspace then we obtain a better estimate.

The main tool in the derivation of (5.2) is a Poisson-type summation formula (Theorem 5.2) that is a generalization of the classical *Poisson summation formula* (5.3). The method of proof is taken from [Her62b].

5.1 The Fourier transform

We recall the basic definitions and results about the Fourier transform, mainly to fix the notation. We refer to [SW71] as a reference for the basics on the Fourier transform. The **Fourier transform** of a function $f \in L^1(\mathbb{R}^n)$ is defined by

$$\mathscr{F}(f)(\xi) = \hat{f}(\xi) = \int_{\mathbb{R}^n} e^{-2\pi i x\cdot\xi} f(x)dx.$$

With this convention, the **inversion formula** reads

$$f(x) = \mathscr{F}^{-1}(\hat{f})(x) = \int_{\mathbb{R}^n} e^{2\pi i x\cdot\xi} \hat{f}(\xi)d\xi$$

for every $f \in L^1(\mathbb{R}^n)$ such that $\hat{f} \in L^1(\mathbb{R}^n)$.

When we are on the torus $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n \simeq [0,1)^n$, for a given $g \in L^1(\mathbb{T}^n)$ we define its **Fourier coefficients** as

$$\hat{g}(\xi) = \int_{[0,1)^n} g(x)e^{-2\pi i x\cdot\xi}dx.$$

for $\xi \in \mathbb{Z}^n$. In this case the inversion formula on the torus, that is the Fourier series expansion of g, can be stated in the following way:

Theorem 5.1 ([SW71, Chapter VII, Corollary 1.8])**.** *Suppose $g \in L^1(\mathbb{T}^n)$ is such that $\hat{g}(\xi) \in \ell^1(\mathbb{Z}^n)$; then g is equivalent to a continuous function, and*

$$g(x) = \sum_{x\in\mathbb{Z}^n} \hat{g}(k)e^{2\pi i k\cdot t}.$$

Observe that we are using the hat $\hat{}$ to denote both the Fourier transform of a function on $\mathbb{R}^n$ and the Fourier coefficients of a function on $\mathbb{T}^n \simeq [0,1)^n$.

The **Schwartz space** $\mathscr{S}(\mathbb{R}^n)$ is given by all C^∞ functions which decay rapidly at infinity together with all their derivatives, that is

$$\mathscr{S}(\mathbb{R}^n) = \left\{ f \in C^\infty(\mathbb{R}^n) : \sup_{x\in\mathbb{R}^n} |x^\alpha \partial^\beta f(x)| < \infty \text{ for every } \alpha, \beta \text{ multi-indices} \right\}.$$

We endow this space with the topology induced by the Fréchet seminorms

$$p_{\alpha,\beta}(f) = \sup_{x\in\mathbb{R}^n} |x^\alpha \partial^\beta f(x)|.$$

The topological dual of $\mathscr{S}(\mathbb{R}^n)$ is the space of **tempered distributions** $\mathscr{S}'(\mathbb{R}^n)$.

The Fourier transform can be defined on $\mathscr{S}(\mathbb{R}^n)$, on which it is an isomorphism, and by duality also on $\mathscr{S}'(\mathbb{R}^n)$: given a tempered distribution T, its Fourier transform is the tempered distribution defined by

$$\langle \mathscr{F}(T), \phi \rangle = \langle T, \mathscr{F}(\phi) \rangle$$

for any Schwartz function ϕ. In this way we can talk about for instance the Fourier transform of any measure which grows at most polynomially at infinity.

The **Poisson summation formula** [SW71, Chapter VII, Corollary 2.6] is

$$\sum_{m\in\mathbb{Z}^n} f(m) = \sum_{k\in\mathbb{Z}^n} \hat{f}(k) \tag{5.3}$$

for every $f \in \mathscr{S}(\mathbb{R}^n)$. We can also write it in terms of tempered distributions:

$$\mathscr{F}\left(\sum_{m\in\mathbb{Z}^n} \delta_m \right) = \sum_{k\in\mathbb{Z}^n} \delta_k. \tag{5.4}$$

5.2 Poisson summation formula for periodic measures

We now want to obtain an analogue of the Poisson summation formula (5.3)/(5.4), but instead of a lattice of deltas we want to consider a generic periodic measure.

Let then μ_0 be a finite measure on $Q = [0,1)^n \subset \mathbb{R}^n$. In particular $\mu_0 \in \mathscr{M}(Q) \hookrightarrow \mathscr{M}(\mathbb{R}^n) \hookrightarrow \mathscr{S}'(\mathbb{R}^n)$. Consider the periodized measure $\mu = \sum_{m\in\mathbb{Z}^n} \tau_m \mu_0$ where τ_m is the translation by the vector m and we write $\tau_m\mu_0$ for $(\tau_m)_\# \mu_0$, the pushforward of μ_0 with respect to the translation τ_m.

Theorem 5.2 (Generalized Poisson summation formula). *Consider a function $f \in C_c(\mathbb{R}^n)$ such that $(\hat{f}(k))_{k\in\mathbb{Z}^n} \in \ell^1(\mathbb{Z}^n)$, and consider a finite measure $\mu_0 \in \mathscr{M}([0,1)^n)$. Then*

$$\sum_{m\in\mathbb{Z}^n} \langle \tau_m \mu_0, f \rangle = \sum_{k\in\mathbb{Z}^n} \hat{f}(k) \hat{\mu}_0(-k) \tag{5.5}$$

where $\hat{\mu}_0(\xi) := \langle \mu_0, e^{-2\pi i \xi \cdot t} \rangle$.

The same conclusion holds also for $f \in \mathscr{S}(\mathbb{R}^n)$, with basically the same proof. We stated the theorem in this way because it's the form in which we will use it.

Proof. Let g be the periodized function $g(t) = \sum_{m\in\mathbb{Z}^n} f(t+m)$, which is $\mathbb{Z}^n$-periodic and continuous, and let μ be the periodized measure as above. In particular we obtain

$$\langle \mu, f\rangle = \langle \sum_{m\in\mathbb{Z}^n} \tau_m \mu_0, f\rangle = \sum_{m\in\mathbb{Z}^n} \langle \mu_0, \tau_{-m} f\rangle = \langle \mu_0, g\rangle. \tag{5.6}$$

Let us relate the Fourier coefficients of g and the Fourier transform of f: given $k \in \mathbb{Z}^n$

$$\begin{aligned}\hat{g}(k) &= \int_{[0,1)^n} g(t) e^{-2\pi i k\cdot t} dt \\ &= \int_{[0,1)^n} \sum_{m\in\mathbb{Z}^n} f(t+m) e^{-2\pi i k\cdot t} dt \\ &= \int_{\mathbb{R}^n} f(t) e^{-2\pi i k\cdot t} dt \\ &= \hat{f}(k)\end{aligned}$$

where $\hat{g}$ has to be understood as a Fourier coefficient while $\hat{f}$ has to be understood as the Fourier transform of f evaluated at k.

Since g is continuous and in L^1, and by the assumption on f and the previous computation its Fourier coefficients are summable, we can apply the inversion formula of Theorem 5.1 to g, that is we can write

$$g(t) = \sum_{k\in\mathbb{Z}^n} \hat{g}(k) e^{2\pi i k\cdot t}$$

where the series is absolutely convergent. We can plug this in (5.6) obtaining

$$\langle \mu, f\rangle = \langle \mu_0, g\rangle = \langle \mu_0, \sum_{k\in\mathbb{Z}^n} \hat{g}(k) e^{2\pi i k\cdot t}\rangle = \sum_{k\in\mathbb{Z}^n} \hat{g}(k) \langle \mu_0, e^{2\pi i k\cdot t}\rangle \tag{5.7}$$

and because of the above computation we can replace $\hat{g}(k)$ with $\hat{f}(k)$ and obtain the desired conclusion. □

Remark 5.3. (i) The assumptions of the generalized Poisson summation formula can be weakened. Identity (5.5) holds for any f such that:

(a) f coincides with its Lebesgue representative, i.e.

$$f(x) = \lim_{\delta\to 0} \fint_{B_\delta(x)} f(y) dy;$$

(b) $f \in L^1(\mathbb{R}^n, \mathscr{L}^n) \cap L^1(\mathbb{R}^n, \mu)$;

(c) $\big(\hat{f}(k)\hat{\mu}_0(k)\big)_{k\in\mathbb{Z}^n} \in \ell^1(\mathbb{Z}^n)$.

To prove this, we consider a mollifier $\eta \in C_c^\infty(\mathbb{R}^n)$, $\eta \geq 0$, $\int \eta = 1$, and define $\eta_\varepsilon(x) := \frac{1}{\varepsilon^n}\eta(\frac{x}{\varepsilon})$. We prove (5.5) for $f * \eta_\varepsilon$ with the same proof above, and then pass to the limit when $\varepsilon \to 0$ using Lebesgue dominated convergence.

In particular these assumptions are satisfied for any measure μ if $f \in \mathscr{S}(\mathbb{R}^n)$.

(ii) In the following we will only use the previous formula, but let us write explicitly what is the Fourier transform of μ as a tempered distribution (observe that by the previous paragraph Theorem 5.2 holds also for $f \in \mathscr{S}(\mathbb{R}^n)$): by definition and by (5.5), for any $\phi \in \mathscr{S}(\mathbb{R}^n)$

$$\langle \hat{\mu}, \phi \rangle = \langle \mu, \hat{\phi} \rangle = \sum_{k \in \mathbb{Z}^n} \hat{\hat{\phi}}(k) \langle \mu_0, e^{2\pi i k \cdot t} \rangle.$$

By the definition of Fourier transform and the inversion formula on $\mathbb{R}^n$ we have

$$\hat{\hat{\phi}}(k) = \int_{\mathbb{R}^n} \hat{\phi}(\xi) e^{-2\pi i k \cdot \xi} d\xi = \phi(-k)$$

and therefore we obtain

$$\langle \hat{\mu}, \phi \rangle = \sum_{k \in \mathbb{Z}^n} \phi(-k) \langle \mu_0, e^{2\pi i k \cdot t} \rangle.$$

More concisely, as tempered distributions

$$\mathscr{F}\left(\sum_{m \in \mathbb{Z}^n} \tau_m \mu_0 \right) = \sum_{k \in \mathbb{Z}^n} \hat{\mu}_0(k) \delta_k. \tag{5.8}$$

We observe that in particular any periodic measure has a Fourier transform which is a measure concentrated on the integer lattice $\mathbb{Z}^n$, with uniformly bounded coefficients: indeed $|\hat{\mu}_0(k)| \le \mu_0(Q) = \|\mu_0\|$.

We obtain as a particular case the classical Poisson summation formula taking $\mu_0 = \delta_0$. Indeed

$$\hat{\delta}_0(k) = \int_{[0,1)^n} e^{-2\pi i k \cdot t} d\delta_0(t) = 1$$

which gives

$$\mathscr{F}\left(\sum_{m \in \mathbb{Z}^n} \delta_m \right) = \sum_{k \in \mathbb{Z}^n} \delta_k.$$

As another example, considering $\mu_0 = \mathscr{L}^n \llcorner [0,1)^n$ we obtain that $\hat{\mu}_0(k) = 0$ for any $k \neq 0$, while $\hat{\mu}_0(0) = 1$, therefore obtaining the basic relation

$$\mathscr{F}(1) = \delta_0.$$

(iii) An analogous result holds if the measure μ is periodic with respect to a generic **lattice** $\Lambda = A\mathbb{Z}^n$, where A is an invertible linear transformation (and therefore μ_0 is a measure on the fundamental domain AQ). In this case define the dual lattice to be $\Lambda^* = (A^{-1})^\top \Lambda = (A^{-1})^\top A\mathbb{Z}^n$. Then, setting $\mu = \sum_{\lambda \in \Lambda} \tau_\lambda \mu_0$, we have

$$\langle \mu, f \rangle = |\det(A^{-1})| \sum_{\nu \in \Lambda^*} \hat{f}(\nu) \langle \mu_0, e^{2\pi i \nu \cdot t} \rangle. \tag{5.9}$$

(iv) We refer to [Sal13, Theorem 2.4.2] for a discussion about periodic tempered distributions and their Fourier transforms. In particular there is a bijective correspondence between periodic distributions and coefficients $(a_k)_{k \in \mathbb{Z}^n}$ with polynomial growth.

5.3 Estimate of $\mu(B_r)$ for a periodic measure μ

We now come to the main result of this chapter. We first start with a heuristic argument, which is not rigorous since the involved series do not converge, but we will anyway carry on the computation to show the general method; we will see below how to modify the argument and make it rigorous.

We suppose for a moment that the generalized Poisson summation formula (5.5) holds also for $f = \mathbb{1}_{B_r}$ (which is not the case for a general measure μ; compare however with Remark 5.3(i)). We then write

$$\begin{aligned}\mu(B_r) = \langle \mu, \mathbb{1}_{B_r} \rangle &= \sum_{k\in\mathbb{Z}^n} \hat{\mathbb{1}}_{B_r}(k)\hat{\mu}_0(-k) \\ &= \|\mu_0\||B_r| + \sum_{k\in\mathbb{Z}^n\setminus\{0\}} \hat{\mathbb{1}}_{B_r}(k)\hat{\mu}_0(-k)\end{aligned}$$

since $\hat{\mathbb{1}}_{B_r}(0) = |B_r|$. Therefore we can view the last sum as the remainder term $\Delta(r)$ which we have to estimate. Unfortunately, this series is not absolutely convergent (because otherwise, by the inversion formula of Theorem 5.1, we would obtain that $\mathbb{1}_{B_r}$ is a continuous function), and this reasoning is not sound. However, recalling the general fact that the smoother a function, the quicker its Fourier transform's decay, we approximate $\mathbb{1}_{B_r}$ with a smoother function to which we can apply the Poisson summation formula and such that the above series converges. We choose in particular, as in [Her62b], the convolution with a rescaled copy of itself:

$$f(x) := \mathbb{1}_{B_r} * \left(\frac{\mathbb{1}_{B_s}}{|B_s|}\right)(x)$$

where $s \ll r$ will be suitably chosen in terms of r. The Fourier transform of $\mathbb{1}_{B_r}$ is explicitly computable in terms of Bessel functions, and the following estimate holds [Mat15, p. 34]:

$$|\hat{\mathbb{1}}_{B_r}(\xi)| \lesssim \frac{r^{\frac{n-1}{2}}}{|\xi|^{\frac{n+1}{2}}}. \tag{5.10}$$

In particular the above convolution is continuous and moreover

$$|\hat{\mathbb{1}}_{B_r}(\xi)\hat{\mathbb{1}}_{B_s}(\xi)| \lesssim \frac{r^{\frac{n-1}{2}}s^{\frac{n-1}{2}}}{|\xi|^{n+1}}$$

so that $\hat{f}$ is summable at the integer lattice, and therefore f satisfies the assumptions of the generalized Poisson formula and we can carry on rigorously the heuristic argument above. We will actually consider two slightly different versions of the function f, one to approximate $\mathbb{1}_{B_r}$ from above and one to approximate it from below.

Theorem 5.4 (**Measure in the ball**). *Given a $\mathbb{Z}^n$-periodic measure μ on $\mathbb{R}^n$, the following estimate holds:*

$$\mu(B_r(x)) = \|\mu_0\||B_r| + \|\mu_0\|\,\mathscr{O}\left(r^{(n-1)\frac{n}{n+1}}\right) \qquad \text{as } r\to\infty \tag{5.11}$$

where the implicit constant in the $\mathscr{O}$ does not depend on the center x nor on the measure μ, just on the dimension.

Notice again that the remainder term is better than the trivial "surface" term $\mathscr{O}(r^{n-1})$ in any dimension. The proof follows the lines of [Her62b, Theorem 1].

Proof. Let

$$f(x) = \mathbb{1}_{B_{r+s}} * \left(\frac{1}{|B_s|}\mathbb{1}_{B_s}\right)(x).$$

In the end we will take s proportional to $r^{-\frac{n-1}{n+1}}$, but for now we leave it as it is; we will prove in the end that the optimal choice is that one. Then we have

$$\hat{f}(\xi) = \frac{1}{|B_s|}\hat{\mathbb{1}}_{B_{r+s}}(\xi)\hat{\mathbb{1}}_{B_s}(\xi)$$

and by the considerations before the statement of the theorem we can apply the generalized Poisson formula (5.3). Observing that

$$\begin{cases} f(x) = 1 & \text{in } B_r \\ f(x) \geq 0 & \forall x \end{cases}$$

we obtain

$$\begin{aligned} \mu(B_r(x)) \leq \langle \mu, f \rangle &= \sum_{k\in\mathbb{Z}^n} \hat{f}(k)\hat{\mu}_0(-k) \\ &= \sum_{k\in\mathbb{Z}^n} \hat{\mathbb{1}}_{B_{r+s}}(k)\hat{\mathbb{1}}_{B_s}(k)\frac{1}{|B_s|}\hat{\mu}_0(-k) \\ &= \left(|B_{r+s}|\,\|\mu_0\| + {\sum_k}' \hat{\mathbb{1}}_{B_{r+s}}(k)\hat{\mathbb{1}}_{B_s}(k)\frac{1}{|B_s|}\hat{\mu}_0(-k)\right) \end{aligned}$$

where here and in the following $\sum_k'$ denotes the sum among all $k \in \mathbb{Z}^n \setminus \{0\}$. Therefore

$$\begin{aligned} \Delta_\mu(r) &:= \mu(B_r(x)) - \|\mu_0\||B_r| \\ &\leq \|\mu_0\|(|B_{r+s}| - |B_r|) + {\sum_k}' \hat{\mathbb{1}}_{B_{r+s}}(k)\hat{\mathbb{1}}_{B_s}(k)\frac{1}{|B_s|}\hat{\mu}_0(-k) \end{aligned} \tag{5.12}$$

and we estimated the error term $\Delta_\mu(r)$ from above with the last expression. With a similar reasoning we now estimate it from below with an analogous expression: consider this time

$$f(x) = \mathbb{1}_{B_{r-s}} * \left(\frac{1}{|B_s|}\mathbb{1}_{B_s}\right)(x).$$

Then

$$\begin{cases} f(x) \leq 1 & \text{in } B_r \\ f(x) = 0 & \text{in } B_r^c \end{cases}$$

and with a computation as above, using that $\mu(B_r(x)) \geq \langle \mu, f \rangle$, we obtain

$$\Delta_\mu(r) \geq -\|\mu_0\|(|B_r| - |B_{r-s}|) + {\sum_k}' \hat{\mathbb{1}}_{B_{r-s}}(k)\hat{\mathbb{1}}_{B_s}(k)\frac{1}{|B_s|}\hat{\mu}_0(-k). \tag{5.13}$$

From (5.12) and (5.13) we obtain a bound on $|\Delta(r)|$. We now estimate from above the right hand side of (5.12), the estimate from below of (5.13) being analogous.

The goal now is therefore to estimate the right hand side of (5.12) and prove that it is $\mathscr{O}(r^{(n-1)\frac{n}{n+1}})$. The first term is bounded up to a dimensional constant by $\|\mu_0\| r^{n-1}s$ because $s \ll r$. As for the sum, we pass to the absolute values and we split it in the two domains $\{k : |k| \le T\}$ and $\{k : |k| > T\}$, with T of the order $T \approx r^{\frac{n-1}{n+1}}$. Again, as with the choice for s, we will leave the parameter T in the computations and prove in the end that this is the optimal choice. For the first domain $\{k : |k| \le T\}$ we will simply estimate $|\hat{\mathbb{1}}_{B_s}(k)| \le |B_s|$ and use the estimate (5.10) for $\hat{\mathbb{1}}_{B_{r+s}}$; for the second domain $\{k : |k| > T\}$ we will really exploit the additional decay given by the convoltion term $\mathbb{1}_{B_s}$ and therefore use the estimate (5.10) for both $\hat{\mathbb{1}}_{B_{r+s}}$ and $\hat{\mathbb{1}}_{B_s}$.

- Case I: sum among $\{k : |k| \le T\}$.

$$\begin{aligned}
\left| \sum_{|k|\le T}' \hat{\mathbb{1}}_{B_{r+s}}(k)\hat{\mathbb{1}}_{B_s}(k)\frac{1}{|B_s|}\hat{\mu}_0(-k)\right| &\le \|\mu_0\| \sum_{|k|\le T}' |\hat{\mathbb{1}}_{B_{r+s}}(k)| \\
&\lesssim \|\mu_0\| \sum_{|k|\le T}' \frac{r^{\frac{n-1}{2}}}{|k|^{\frac{n+1}{2}}} \\
&\lesssim \|\mu_0\| r^{\frac{n-1}{2}} T^{\frac{n-1}{2}}
\end{aligned}$$

where we used that

$$\sum_{|k|\le T}' \frac{1}{|k|^{\frac{n+1}{2}}} \approx \int_{B_T \setminus B_1} \frac{1}{|x|^{\frac{n+1}{2}}} dx \approx \int_1^T \frac{1}{\rho^{\frac{n+1}{2}}} \rho^{n-1} d\rho \approx T^{\frac{n-1}{2}}.$$

- Case II: sum among $\{k : |k| > T\}$.

$$\begin{aligned}
\left| \sum_{|k|>T}' \hat{\mathbb{1}}_{B_{r+s}}(k)\hat{\mathbb{1}}_{B_s}(k)\frac{1}{|B_s|}\hat{\mu}_0(-k)\right| &\le \|\mu_0\| \frac{1}{|B_s|} \sum_{|k|>T}' |\hat{\mathbb{1}}_{B_{r+s}}(k)|\,|\hat{\mathbb{1}}_{B_s}(k)| \\
&\lesssim \|\mu_0\| \frac{1}{s^n} \sum_{|k|>T}' \frac{r^{\frac{n-1}{2}}}{|k|^{\frac{n+1}{2}}} \frac{s^{\frac{n-1}{2}}}{|k|^{\frac{n+1}{2}}} \\
&\lesssim \|\mu_0\| \frac{r^{\frac{n-1}{2}}}{s^{\frac{n+1}{2}}} \frac{1}{T}
\end{aligned}$$

where we used that

$$\sum_{|k|>T}' \frac{1}{|k|^{n+1}} \approx \int_{\mathbb{R}^n \setminus B_T} \frac{1}{|x|^{n+1}} dx \approx \int_T^\infty \frac{1}{\rho^{n+1}} \rho^{n-1} d\rho \approx \frac{1}{T}.$$

Putting together the previous estimates we obtain

$$\Delta_\mu(r) \lesssim \|\mu_0\| \left(r^{n-1}s + r^{\frac{n-1}{2}}T^{\frac{n-1}{2}} + \frac{r^{\frac{n-1}{2}}}{s^{\frac{n+1}{2}}T} \right).$$

Optimizing in s and T (which amounts to impose that all three terms in the brackets are of the same order) we obtain that the optimal values are

$$\begin{cases} s \approx r^{-\frac{n-1}{n+1}} \\ T \approx r^{\frac{n-1}{n+1}} \end{cases}$$

and we finally obtain

$$\Delta_\mu(r) \lesssim \|\mu_0\| r^{(n-1)\frac{n}{n+1}}.$$

$\square$

Remark 5.5. (i) There are some particularly well-behaved measures for which we can give a better estimate for the remainder term. Referring to Remark 5.3(i), if U is an open bounded subset of $\mathbb{R}^n$ the function $f = \mathbb{1}_U$ satisfies assumptions (a) and (b). If we consider the square partition $\mathscr{Q}$ of the plane given by $\partial\mathscr{Q} := (\mathbb{R}\times\mathbb{Z}) \cup (\mathbb{Z}\times\mathbb{R})$, it is easy to see that the measure $\mu = \mathscr{H}^1 \llcorner \partial\mathscr{Q}$ has a Fourier transform which is supported on the set $S := (\mathbb{Z}\times\{0\}) \cup (\{0\}\times\mathbb{Z})$, and therefore $\mathbb{1}_{B_r}$ satisfies also assumption (c), where $\mu_0 = \mu \llcorner [0,1)^2$. Therefore the generalized Poisson summation formula holds in this case and we can write

$$\begin{aligned} \mu(B_r) = \langle \mu, \mathbb{1}_{B_r} \rangle &= \sum_{k\in\mathbb{Z}^2} \hat{\mathbb{1}}_{B_r}(k)\hat{\mu}_0(-k) \\ &= \|\mu_0\||B_r| + \sum_{k\in\mathbb{Z}^2\setminus\{0\}} \hat{\mathbb{1}}_{B_r}(k)\hat{\mu}_0(-k) \end{aligned}$$

and therefore recalling (5.10) the remainder term $\Delta_{\mathscr{Q}}(r) := \mu(B_r) - \|\mu_0\||B_r|$ satisfies

$$|\Delta_{\mathscr{Q}}(r)| \lesssim r^{1/2} \sum_{k\in S\setminus\{0\}} \frac{1}{|k|^{3/2}} \lesssim r^{1/2}$$

since, unlike for the heuristic discussion preceding Theorem 5.4, this time the series is convergent.

(ii) The same estimate holds if we replace the ball $B_r = rB_1$ by rK, where K is a convex set such that

$$|\hat{\mathbb{1}}_K(\xi)| \lesssim \frac{1}{|\xi|^{\frac{n+1}{2}}}.$$

Indeed, the proof goes through with virtually no modifications. The above estimate holds for instance for any smooth convex set whose boundary has strictly positive Gaussian curvature (see [Her62b, Remark A] and [Her62a]). Even without appealing to the reference, by a change of variables it is easy to see that the estimate holds for ellipsoids. One set for which surely the estimate does not hold is the cube $Q_1(0) = [-1,1]^n$, for which the Fourier transform is a product of factors of type $\frac{\sin(\xi_k)}{\xi_k}$, with ξ_k coordinates of ξ. And in fact for, say, the GCP it is clear that using squares the remainder $\Delta(r)$ is actually of order $\approx r$ and not smaller, because $N(r)$ jumps abruptly of a quantity $\approx r$ whenever r assumes an integer value.

(iii) The estimate (5.11) actually holds in the more general form (5.2). This can be seen in two ways: on one hand, the key point in the proof was the summability of the Fourier transform in the integer lattice, and by using (5.9) the same proof goes through; on the other hand, we can use point (i) of this Remark, and in particular the fact that (5.11) holds for ellipsoids, because after a linear change of variables the measure of a ball becomes the pushforward measure of an ellipsoid.

5.4 Better estimates for better measures

Consider a measure μ_0 on $[0,1)^n$ and define the periodized μ as above. We now prove that under additional assumptions on the support of $\hat{\mu}$ we can give a better estimate for the remainder term $\Delta_\mu(r) := \mu(B_r) - \|\mu_0\||B_r|$. In particular we recover the result of [LP16] in the case when μ_0 is the Hausdorff measure $\mathscr{H}^{n-d}$ restricted to a $(n-d)$-dimensional face of the unit cube, that is when μ is the $(n-d)$-dimensional Hausdorff measure $\mathscr{H}^{n-d}$ restricted to $\mathbb{Z}^d \times \mathbb{R}^{n-d}$.

Theorem 5.6. *Suppose that $\hat{\mu}_0$ is supported on a d-dimensional subspace H (equivalently, that μ_0 is invariant under continuous translations along the directions of $H^\perp$). Then*

$$\Delta_\mu(r) \lesssim \begin{cases} r^{-\frac{n-1}{2}} & \text{if } d < \frac{n+1}{2} \\ r^{-\frac{n-1}{2}} \log r & \text{if } d = \frac{n+1}{2} \\ r^{n-\frac{2d}{2d-n+1}} & \text{if } d > \frac{n+1}{2} \end{cases}.$$

Proof. The proof is analogous to the one for Theorem 5.4. The only difference is in the estimates for the series

$$\sum_k{}' \hat{\mathbb{1}}_{B_{r+s}}(k) \frac{1}{|B_s|} \hat{\mathbb{1}}_{B_s}(k)$$

and in particular in the comparison with the integrals. The integral estimate becomes

$$\approx \int \frac{1}{\rho^{\frac{n+1}{2}}} \rho^{d-1} d\rho.$$

We again split the series between the two domains $\{k : |k| \le T\}$ and $\{k : |k| > T\}$ for some T, whose choice will depend upon r and d.

(i) Sum among $\{k : |k| \le T\}$.

$$\sum_{\substack{|k|\le T\\ k\in\mathbb{Z}^d}}{}' \frac{r^{\frac{n-1}{2}}}{|k|^{\frac{n+1}{2}}} \lesssim r^{\frac{n-1}{2}} \int_1^T \frac{1}{\rho^{\frac{n+1}{2}}} \rho^{d-1} d\rho$$
$$\lesssim \begin{cases} r^{\frac{n-1}{2}} & \text{if } d < \frac{n+1}{2} \\ r^{\frac{n-1}{2}} \log T & \text{if } d = \frac{n+1}{2} \\ r^{\frac{n-1}{2}} T^{d-\frac{n+1}{2}} & \text{if } d > \frac{n+1}{2} \end{cases}$$

(ii) Sum among $\{k : |k| > T\}$.

$$\sum_{|k|\le T}{}' \frac{r^{\frac{n-1}{2}}}{|k|^{\frac{n+1}{2}}} \frac{s^{\frac{n-1}{2}}}{|k|^{\frac{n+1}{2}}} \frac{1}{s^n} \lesssim \frac{r^{\frac{n-1}{2}}}{s^{\frac{n+1}{2}}} \int_T^\infty \frac{1}{\rho^{n+1}} \rho^{d-1} d\rho$$
$$\approx \frac{r^{\frac{n-1}{2}}}{s^{\frac{n+1}{2}}} T^{d-n-1}.$$

We thus obtain

$$\Delta_\mu(r) \lesssim \left(r^{n-1}s + \frac{r^{\frac{n-1}{2}}}{s^{\frac{n+1}{2}}} T^{d-n-1} + \begin{cases} r^{\frac{n-1}{2}} & \text{if } d < \frac{n+1}{2} \\ r^{\frac{n-1}{2}} \log T & \text{if } d = \frac{n+1}{2} \\ r^{\frac{n-1}{2}} T^{d-\frac{n+1}{2}} & \text{if } d > \frac{n+1}{2} \end{cases} \right)$$

Equating the three terms we obtain the optimal choices

$$\begin{cases} T \approx r^{\frac{n^2-1}{4(n-d+1)}} \\ s \approx r^{-\frac{n-1}{2}} \end{cases} \text{if } d \le \frac{n+1}{2} \qquad \begin{cases} T \approx r^{\frac{n-1}{2d-n+1}} \\ s \approx r^{-\frac{n-1}{2d-n+1}} \end{cases} \text{if } d > \frac{n+1}{2}$$

and thus

$$\Delta_\mu(r) \lesssim \begin{cases} r^{-\frac{n-1}{2}} & \text{if } d < \frac{n+1}{2} \\ r^{-\frac{n-1}{2}} \log r & \text{if } d = \frac{n+1}{2} \\ r^{n-\frac{2d}{2d-n+1}} & \text{if } d > \frac{n+1}{2} \end{cases}.$$

Actually in the case $d < \frac{n+1}{2}$ we don't even need all these computations: we just need to apply the generalized Poisson summation formula, which holds in this case since $\hat{f}\hat{\mu}_0 \in \ell^1(\mathbb{Z}^n)$ (see Remark 5.3(i)).

$\square$

Chapter 6

The interface problem

We consider what is the optimal way of interpolating between two regular structures with mismatching orientations, having in mind the case of perimeter-minimizing partitions (hexagonal structure expected) and of interacting particles (triangular structure expected). In order to treat both cases together (and possibly other similar energies) we consider an energy defined on graphs that favours a regular triangular pattern, and that takes into account an elastic energy due to the deformations of the triangular faces and a plastic energy due to topological defects, that is vertices with degree different from 6. Under some conditions we prove that at an interface between two triangular patterns with an angle mismatch θ some defects must appear, in proportion to the length of the interface and to the angle θ, and that the energy excess with respect to the rest state goes at least as θ. Moreover we prove that the suitably defined orientation of the graph has a *BV* limit when the microscopic lengthscale is sent to zero. We then argue why we expect an *SBV* limit, a better lower bound for the energy at an interface with angle θ, namely $\theta|\log\theta|$, and what are the difficulties in proving this result.

Contents

6.1 Introduction

In order to analyze the asymptotic behaviour of N-clusters (and N-partitions of a given open set Ω) when $N \to \infty$, we now restrict the attention to a specific subproblem which we call the *interface problem*, or also *grain boundary* problem, that can be seen as a sort of *cell problem* for a Γ-convergence result. Instead of the total number N of chambers, we consider a parameter $\varepsilon \approx \frac{1}{\sqrt{N}}$ which represents the microscopic lengthscale of chambers if we rescale the N-cluster so that the total area is fixed. The problem is essentially the following: we fix two regular hexagonal partitions on the lateral zones of a fixed square of side L, whose chambers have equal areas of order ε^2 and whose orientations differ by a small angle θ, and ask what is the optimal way to interpolate in between, that is to partition the middle portion with equal-area chambers that minimize the total perimeter (see Figure 6.2). Hales honeycomb theorem 3.1 tells us that the hexagonal honeycomb is optimal, and therefore that we expect the majority of chambers to be hexagonal, as can also be seen by numerical minimizers (Figure 6.1). Since the same interface problem could be faced for any energy in which there is a regular expected ground state (hexagonal honeycomb, triangular lattice...) we consider a more astract setting in which the admissible configurations are suitable planar graphs with triangular faces and in which the energy favours the formation of a triangular lattice. However for the rest of the introduction we fix one setting, namely the polygonal partitions in equal-area polygons of a fixed open set Ω.

Our first goal is to prove that it is never convenient to use only (distorted) hexagons to fill the middle region, and it is more effective to introduce some *defects*, that is non-hexagonal cells. Our second goal is to give an estimate of the number of defects and of the minimal energy when defects are present. We highlight these questions:

Question 5. *Do defects necessarily appear at an interface of a minimizing (or low energy) partition?*

Question 6. *If so, what is their total number in terms of the parameters L (sidelength of the square considered), θ (misorientation angle) and $\varepsilon \approx \frac{1}{\sqrt{N}}$ (microscopic lengthscale)?*

Question 7. *Can we estimate in terms of L, θ, ε the energy excess created at an interface with respect to a hexagonal ground state?*

The first step to answer these questions is to attach a notion of *orientation* to each polygonal partition, which describes the direction of the underlying hexagonal chambers, that constitute the majority of

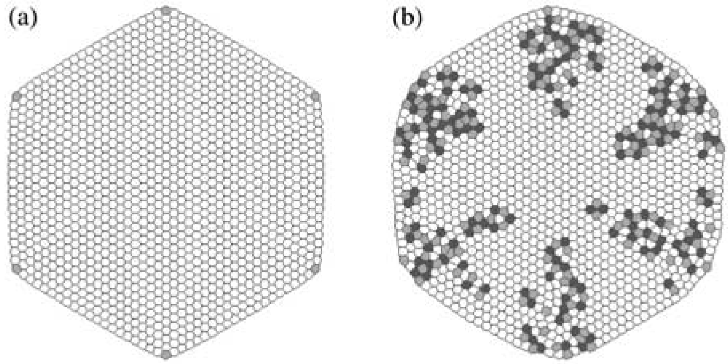


Figure 6.1: (a) A cluster with hexagonal global shape and regular honeycomb inside. (b) A cluster with a rounder global shape with some defects appearing inside, colored in light or dark grey according to the number of sides. Picture taken from [CG03].

chambers. We could naively imagine for instance a vectorfield ϕ with values in $\mathbb{S}^1$ (modulo $\frac{\pi}{3}$) that takes into account the direction of the hexagonal chambers, as we did for the case described in Chapter 4, Section 2 where we defined an orientation for clusters with hexagonal chambers. However a vectorfield does not seem to be sufficient to capture the essential features in the case of general clusters, because of the distortion that chambers could underlie. What turns out to be useful in the case of polygonal partitions is a *matrix*-field (vector field with values in the 2×2 matrices) that takes into account the elastic deformations of the chambers. We then apply the rigidity theorems by Friesecke, James and Müller [FJM02] and by Müller, Scardia and Zeppieri [MSZ14] to obtain information on how much this matrix-field is close to a rotation in terms of its associated elastic energy, and consequently how close is the partition to a hexagonal honeycomb. We will denote by β_ε the orientation matrix-field. We remark that the definition of β_ε is already a non-trivial step, since the presence of non-hexagonal chambers entails some branching problems.

In view of computing a Γ-limit of the (suitably rescaled) perimeter energy as $\varepsilon \to 0$, once we have defined a notion of orientation for polygonal partitions we want to understand what kind of compactness we expect for these orientations, in order to obtain a limit orientation that describes asymptotically the hexagonal chambers. A natural space, also in view of Chapter 4, is the space SBV. In that chapter we obtained as limit orientations piecewise constant SBV vectorfields, essentially because different orientations did not interact with each other and this created a lot of perimeter at the interface between two hexagonal zones with different orientations. This prevented the formation of a slowly varying orientation in the limit vectorfield (i.e. the absolutely continuous part of the gradient of the limit vectorfield was zero). In the setting of polygonal partitions the situation is not so rigid, and the possibility of using deformed hexagonal cells, or even non-hexagonal cells, makes the problem much more difficult. Nonetheless the result we expect is again a SBV limit matrix-field β with values in the space $SO(2)$.

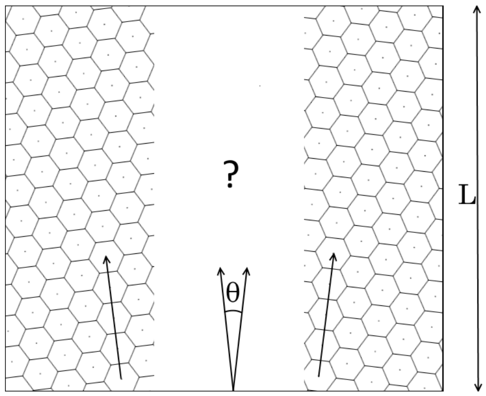


Figure 6.2: The interface problem: what is the optimal way to fill the middle region with equal-area chambers in order to minimize the perimeter? What is the behaviour of the perimeter excess in terms of the mismatch angle θ and the interface length L? Do we necessarily have to introduce some defects?

The key tool we will use in the estimates is the rigidity theorem by Friesecke, James and Müller [FJM02, Theorem 3.1] and especially the subsequent generalization [MSZ14] to incompatible (i.e. non-curl-free) vector fields, which is essential to handle the presence of defects. We here state the latter.

Theorem 6.1 (**Generalized Rigidity Estimate** [MSZ14, Theorem 3.3])**.** *Let $\Omega \subset \mathbb{R}^2$ be open, bounded, simply connected and Lipschitz. There exists a constant $C = C(\Omega) > 0$ (scaling-invariant) with the following property: for every $\beta \in L^2(\Omega;\mathbb{R}^{2\times 2})$ with $\operatorname{Curl}\beta \in \mathscr{M}_b(\Omega;\mathbb{R}^2)$ there is an associated rotation $R \in SO(2)$ such that*[1]

$$\|\beta - R\|_{L^2(\Omega;\mathbb{R}^{2\times 2})} \leq C(\|\operatorname{dist}(\beta, SO(2))\|_{L^2(\Omega)} + |\operatorname{Curl}\beta|(\Omega)). \tag{6.1}$$

6.2 The basic construction: defects, mappings on the regular lattice and the rigidity theorem

We now explain the main construction that will underlie all the following sections. We consider a polygonal partition $\mathscr{E}$ of a unit square Ω in areas $\frac{1}{N}$ that coincides on the two lateral thirds with two honeycombs with angle mismatch θ (see Figure 6.2), and seek a lower bound on the total perimeter, that is an inequality of the type

$$P(\mathscr{E}) \geq \sqrt[4]{12}\sqrt{N} + \delta(N,\theta)$$

where $\sqrt[4]{12}\sqrt{N}$ is the lower bound given by Hales inequality, and where $\delta(N,\theta)$ is a positive function that measures the increase in perimeter due to the misorientation of the lateral honeycombs and the impossibility to fill the central region with a perfect honeycomb matching both sides. $\delta(N,\theta)$ takes into

[1]The distributional curl of a matrix field β is the vector-valued distribution defined by $\operatorname{Curl}\beta = (D_1\beta_{12} - D_2\beta_{11}, D_1\beta_{22} - D_2\beta_{21})$.

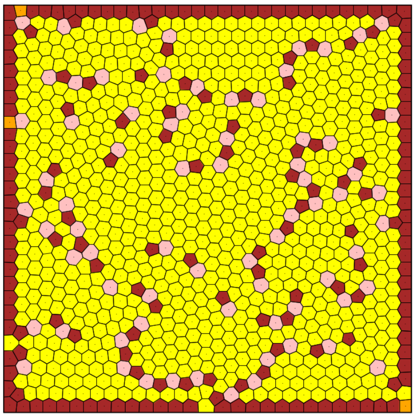


Figure 6.3: A numerical candidate for a local minimizer of an energy modeling block copolymers considered in [BPT14] and given by a perimeter-type term of each cell plus a Wasserstein transport term. Zones with hexagonal cells having almost constant orientation are separated by "lines" of defects (pentagonal and heptagonal cells). Observe that isolated pentagonal or heptagonal defects are rare and are close to some other defect.

account the misorientation θ of the two lateral honeycombs and the number N of polygonal chambers. The result we expect is the following:

$$\delta(N,\theta) \geq C|\theta \log \theta|,$$

that is a superlinear behaviour in the misorientation angle and an independence from N. We refer to the above law as the *Read-Shockley formula*. The reason behind the expected superlinear behaviour is twofold: firstly from a theoretical viewpoint, a similar law has been proved in [LL16] for the energy of a grain boundary in a semidiscrete model for dislocations; secondly from an experimental viewpoint a phenomenological consequence of the superlinear behaviour in the angle is the creation of big zones with constant-orientation regular structures, separated by lines of defects. This can be witnessed in some numerical simulations for energies similar to the perimeter (Figure 6.3) and a similar behaviour is observed in nature in many occasions, as for instance in the case of the *bubble raft* experiment by Bragg and Nye [BLN54] (see Figure 6.4).

More specifically we expect defects to appear, that is non-hexagonal chambers, because putting a stretched honeycomb (*elastic* competitor) would increase the perimeter by a big amount, much bigger than the amount due to a *plastic* competitor built extending the two honeycombs on both sides until they almost touch, and filling the middle region with equispaced deformed chambers (see Figure 6.5).

Since the emergence of defects seems to be a common feature of many different mathematical models we decide to remain in a quite abstract framework, which can then be adapted to the specific model under consideration. We therefore start from a graph that represents our model in a simplified way, defined in such a way that the expected pattern is given by equilateral triangular faces. For instance:

- for particles interacting via a Lennard-Jones type potential, with a minimum at 1, we can consider

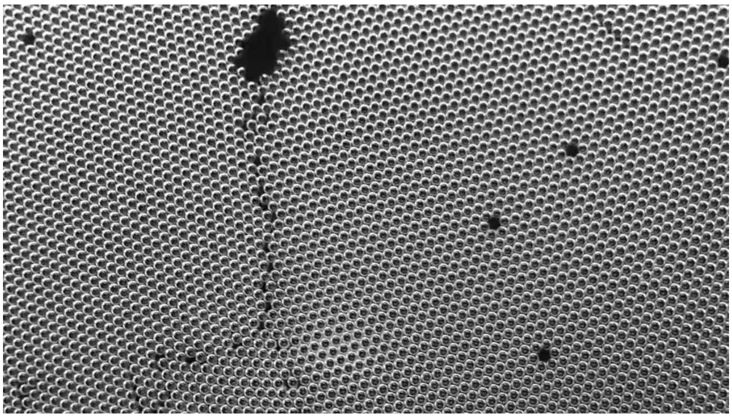
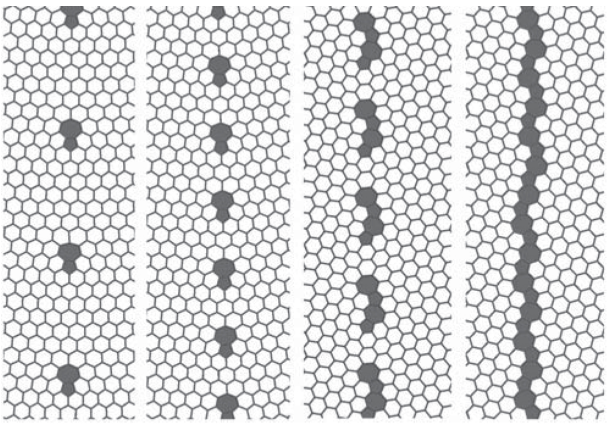


Figure 6.4: In the bubble raft experiment [BLN54] many air bubbles are created through an air compressor on the surface of a soap-water solution. This allows their size to be highly uniform. The bubbles create many regular zones forming a triangular lattice, separated by “lines” of vacancies. This model was used to describe in a simplified way the properties and the motion of dislocations in metals.



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

Figure 6.5: It is expected that between two honeycombs with different orientations some defects (non-hexagonal cells, here greyed out) will appear. Their number per unit length of the interface depends on the misorientation angle θ. Figure taken from [Ge+16].

the *bond graph* given by all pairs of particles x, x' such that $\big||x-x'|-1\big| < \alpha$ for a certain $\alpha > 0$;

- for perimeter-minimizing polygonal partitions we can consider the dual graph of the given polygonal graph, or alternatively triangulate each polygon with triangles by connecting each vertex with the barycenter of the faces it belongs to.

Starting from a graph G we will then give a notion of topological defect, that is a face/vertex that constitutes a non-removable type of singularity (e.g. a vertex with degree different from 6). We will then give a notion of orientation of the triangular faces of the graph. These notions depend essentially on the topology of the graph, and each defect will contribute with a fixed amount to the total energy. Then we will introduce an elastic energy $\mathscr{E}_\varepsilon^{el}$, depending on the microscopic parameter $\varepsilon > 0$, that really depends not just on the topology but on the metric of the graph and favours the formation of equilateral triangular faces of sidelength ε. $\mathscr{E}_\varepsilon^{el}$ takes into account the elastic energy given by the deformation of the regular faces, and is given by a common integrand in nonlinear elasticity theory, $\|\mathrm{dist}(\beta, SO(2))\|_{L^2}$, where β coincides with the gradient of a function u mapping affinely the triangular face into an equilateral triangle of side ε.

An analysis of defects on triangulated graphs arising as bond graphs of minimal configurations for the sticky-disk has been carried out in [DLF18], but it is not clear how we could use their results in our situation.

6.3 Planar graphs and related concepts

We will consider in the following only connected finite planar graphs G with straight edges and triangular faces; this means that the graph is realized by a finite union of segments in $\mathbb{R}^2$, each of which represents an edge, that intersect only at the endpoints where there is a vertex. Every time we will consider a planar graph it will have these properties, unless otherwise stated. We have to begin with many definitions. Although many of them are elementary concepts they will be necessary in the following.

Paths

Given a triangulated planar graph G in $\mathbb{R}^2$, let $V(G)$ be the set of vertices of G, $E(G)$ be the set of (directed) edges and $F(G)$ be the set of faces, that is bounded regions delimited by edges and not containing any vertex in its interior. We will consider an edge as both an ordered pair of vertices and as a closed segment in the plane, the distinction being clear from the context, and we can think of it as an arrow pointing from one vertex to another. We will respectively write $e = (v, w)$ (ordered pair) or $e = [v, w]$ (segment) to denote the edge e between vertices v and w. If $e = (v, w)$ we write $\overline{e} := (w, v)$ for the edge with opposite direction. We will assume that if $e \in E(G)$ then also $\overline{e} \in E(G)$. By the assumptions on G each edge contains exactly two vertices, its endpoints. We call **neighbours**, or **neighbouring vertices**, or **adjacent** vertices any pair of vertices joined by an edge and given any vertex v we denote by $\mathscr{N}(v)$ the set of neighbours of v. In particular the degree of a vertex v coincides with the cardinality of $\mathscr{N}(v)$.

We define the domain of a graph as the open set

$$\Omega_G := Int\left(\bigcup_{F\in F(G)} F\right)$$

where Int denotes the interior.

The set of **regular vertices** is denoted by $V_{reg}(G)$ and is the subset of $V(G)$ of all vertices v of degree 6. The set of **defects** is denoted by $V_{def}(G)$ and is given by $V(G)\setminus V_{reg}(G)$. A regular face is a trianguar face whose vertices are all regular. We associate to G the **defect measure**

$$\sigma_G := \sum_{v\in V(G)} (\deg(v)-6)\delta_v. \tag{6.2}$$

A **path** of length ℓ between two vertices v, w is a map $\gamma : \{0,\dots,\ell\}\to V(G)$ such that

- $\gamma(0) = v$;
- $\gamma(\ell) = w$;
- for every $i = 0,\dots,\ell-1$, $(\gamma(i),\gamma(i+1)) \in E(G)$, i.e. two consecutive distinct elements are joined by an edge.

Observe that by definition we require that paths do not stop at a vertex, i.e. for every $i = 0,\dots,\ell-1$ we suppose $\gamma(i)\neq\gamma(i+1)$.

A path of length ℓ is **closed** if $\gamma(0) = \gamma(\ell)$. We denote the length of a path γ by $\ell(\gamma)$. We say that a path γ is **regular** if $\gamma(i)\in V_{reg}(G)$ for every $i = 0,\dots,\ell(\gamma)$. We denote a path also by $(\gamma_0,\dots,\gamma_\ell)$. Given two paths $\gamma^1 : \{0,\dots,\ell_1\}\to V(G)$ and $\gamma^2 : \{0,\dots,\ell_2\}\to V(G)$ such that $\gamma^1(\ell_1) = \gamma^2(0)$, their **composition** is the path $\gamma^1 * \gamma^2 : \{0,\dots,\ell_1+\ell_2\}\to V(G)$ given by

$$\gamma^1 * \gamma^2(i) = \begin{cases} \gamma^1(i) & \text{if} \quad 0\le i\le \ell_1 \\ \gamma^2(i-\ell_1) & \text{if} \quad \ell_1+1\le i\le \ell_1+\ell_2 \end{cases}.$$

Given a path γ we denote by $\overline{\gamma}$ the same path walked backwards, i.e. if $\gamma = (\gamma(0),\dots,\gamma(\ell))$ then $\overline{\gamma} = (\gamma(\ell),\dots,\gamma(0))$.

We could also consider a path as a sequence of edges: $\gamma = (e_1,\dots,e_\ell)$ where $e_i = (\gamma_{i-1},\gamma_i)$ are edges connecting two consecutive vertices[2]. In this case we can write $\overline{\gamma} = (\overline{e}_\ell,\dots\overline{e}_1)$.

Given a closed path γ, its **image** $Im(\gamma)$ is the union of all its geometric edges:

$$Im(\gamma) := \bigcup_{i=1}^{\ell(\gamma)} [\gamma_{i-1},\gamma_i]$$

and its **domain** $\Omega(\gamma)$ is the complement of the unbounded connected component of $\mathbb{R}^2\setminus Im(\gamma)$.

[2]The notation is the same if we consider a path as a sequence of vertices or a sequence of edges, but the distinction will be clear from the context, and moreover edges are usually denoted by the letter e.

Displacement of a closed path: Burgers vector and rotation

We recall that the triangular lattice $\mathscr{A}_2$ is given by

$$\mathscr{A}_2 := \left\{ m\begin{pmatrix}1\\0\end{pmatrix} + n\begin{pmatrix}1/2\\ \sqrt{3}/2\end{pmatrix} : m,n \in \mathbb{Z} \right\}.$$

We view it as a graph, the vertices being its elements and the edges being each pair of points at unit distance from each other.

We now want to define two types of displacement for every closed regular path γ in G, which say how much translational and rotational displacement there is between the starting and the ending point when we reconstruct γ to a path $L\gamma$ (*lift* of γ) with values in the regular triangular lattice $\mathscr{A}_2$. A version of this displacement is usually referred to as *Burgers vector*, however we will need a more refined notion that takes into account not only translational displacement but also rotational displacement.

Given a triangulated planar graph G and one of its regular vertices x, a (orientation preserving) **local embedding** around x is an injective map $\iota : \{x\} \cup \mathscr{N}(x) \to \mathscr{A}_2$ that preserves neighbours and orientation, i.e.

- if $(x_1,x_2) \in E(G)$ then $(\iota(x_1),\iota(x_2)) \in E(\mathscr{A}_2)$;
- for every triple of distinct pairwise neighbouring vertices x_0,x_1,x_2, the unique affine map interpolating ι in the triangle $co(x_0,x_1,x_2)$ is orientation preserving.

The set $V_{reg}(G)$ of regular vertices can be divided in path-connected components. Given a connected component $\mathscr{C}$ of $V_{reg}(G)$ with at least two vertices, fix two neighbouring vertices $x_0,x_1 \in \mathscr{C}$ (**base points**). Consider the set $\mathscr{P}(x_0,x_1)$ of all regular paths γ such that $\gamma(0) = x_0$ and $\gamma(1) = x_1$. We can think of x_0 and x_1 as indicating, in addition to the starting point x_0, also the "initial velocity" of the path. Denote by $\overline{\mathscr{P}}(x_0,x_1)$ the set of all *closed* paths in $\mathscr{P}(x_0,x_1)$.

Given a path $\gamma \in \mathscr{P}(x_0,x_1)$ of length ℓ, its **lift** $L\gamma : \{0,\dots,\ell\} \to \mathscr{A}_2$ is a path of length ℓ with values in the triangular graph $\mathscr{A}_2$ such that:

- $L\gamma(0) = \binom{0}{0}$;
- $L\gamma(1) = \binom{1}{0} =: e_1$;
- For $i \geq 1$, $L\gamma(i+1)$ is inductively defined as the unique vertex of $\mathscr{A}_2$ such that $(\gamma(i-1),\gamma(i),\gamma(i+1))$ and $(L\gamma(i-1),L\gamma(i),L\gamma(i+1))$ are in correspondence through a local embedding around $\gamma(i)$.

For technical reasons, and with a slight abuse of notation, if γ is a *closed* path in $\overline{\mathscr{P}}(x_0,x_1)$ we also define $L\gamma(\ell+1)$ as $L(\gamma*\gamma)(\ell+1)$.

We are now ready to define the two types of displacement of closed paths, the translational and the rotational one.

Given a closed path $\gamma \in \overline{\mathscr{P}}(x_0,x_1)$ of length γ there is a unique affine isometry (of $\mathscr{A}_2$ or even of the whole plane) $A = A(\gamma) : \mathbb{R}^2 \to \mathbb{R}^2$ of the form $A(\gamma)(x) = R(\gamma)x + b(\gamma)$, $R(\gamma) \in SO(2), b(\gamma) \in \mathbb{R}^2$ such

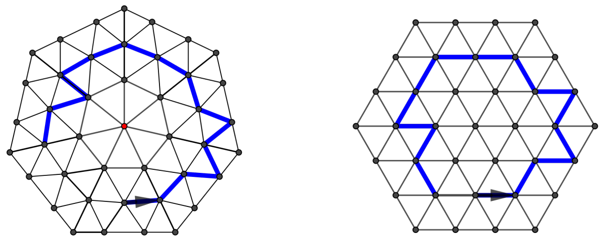


Figure 6.6: On the left a path on a graph G with one defect (middle vertex). On the right the lift of the path on the regular lattice. The two base points are marked by the vector.

that $A(0) = L\gamma(\ell)$ and $A(e_1) = L\gamma(\ell+1)$. We call $b(\gamma)$ the **translational displacement** of γ (or **Burgers vector**) and $R(\gamma)$ the **rotational displacement** (or **Burgers rotation**).

The purpose of the displacements $b(\gamma)$ and $R(\gamma)$ (or equivalently, of the associated isometry $A(\gamma)$) of a path γ is to detect singularities in the graph G, i.e. defects: as we will see for any given closed path γ if $A(\gamma)$ is not the identity then this means that in the region contained inside γ there must be some defect.

We say that a closed regular path γ identifies a **dislocation** if $R(\gamma) = Id$ and $b(\gamma) \neq 0$, while it identifies a **disclination** if $R(\gamma) \neq Id$. We should imagine disclinations as a more essential type of defect (e.g. an isolated pentagon inside a hexagonal configuration) and dislocations as a milder type of singularity, typycally a pair heptagon-pentagon (see Figure 6.11). We will often refer to polygonal partitions (instead of triangulated graphs) to explain the meaning and properties of dislocations and disclinations, but one should keep in mind that we can obtain a triangulated graph from a polygonal partition by either considering the dual graph or by triangulating each face connecting vertices to the barycenter. Referring to Figure 6.11, roughly speaking we can say that the effect of a dislocation is adding/removing a new line of hexagons, while the effect of a disclination is adding/removing a whole wedge ($\frac{\pi}{3}$-sector) of hexagons. As an example of disclination, if a defect v has regular neighbours, and we consider the counterclockwise path γ around v passing through all of its neighbours, then γ identifies a disclination if and only if $\deg(v)$ is not a multiple of 6.

The **tangent field** of a path $\gamma \in \mathscr{P}(x_0, x_1)$ is the map $\tau_\gamma : \{0, \ldots, \ell\} \to \mathscr{A}_2 \cap \mathbb{S}^1$ given by

$$\tau_\gamma(i) = L\gamma(i+1) - L\gamma(i)$$

where $L\gamma$ is the lift of γ. If the meaning is clear from the context the subscript will be omitted, writing just τ.

From the definition of $A(\gamma)$ it follows that $A(\gamma * \gamma') = A(\gamma')A(\gamma)$ where on the right the operation is just the composition of isometries. We therefore obtain the following:

Lemma 6.2. *The map*

$$A : (\overline{\mathscr{P}}(x_0, x_1), *) \to (Isom(\mathscr{A}_2), \bullet)$$

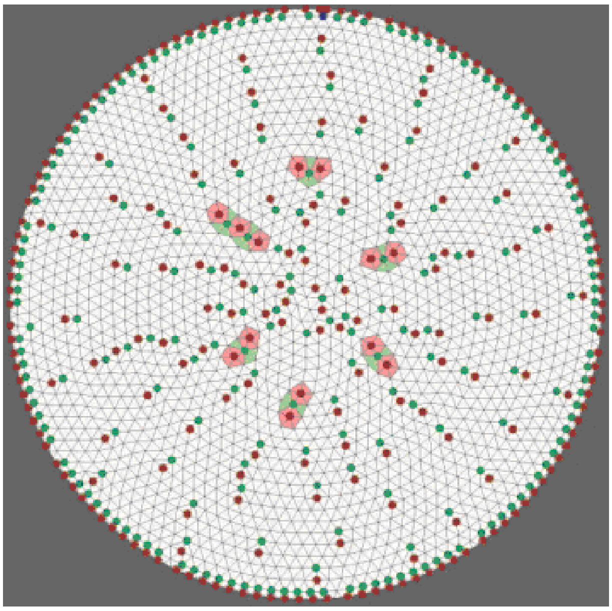


Figure 6.7: An example highlighting defects in a triangulated graph whose domain is a disk: green dots represent heptagonal defects, while red dots represent pentagonal defects. All other vertices are regular, i.e. they have degree 6. The shaded/colored areas highlight a disclination: if we take a path that walks around the boundary of the shaded area its Burgers rotation is not the identity. Picture taken from [MMZ11].

is a homomorphism where $(A \bullet A')(x) = A'(A(x))$. *As a consequence given two closed paths* $\gamma, \gamma' \in \overline{\mathscr{P}}(x_0, x_1)$ *with Burgers vectors* $b(\gamma)$ *and* $b(\gamma')$ *and Burgers rotations* $R(\gamma)$ *and* $R(\gamma')$*, their composition* $\gamma * \gamma'$ *has displacements*

$$b(\gamma * \gamma') = b(\gamma) + R(\gamma) b(\gamma') \tag{6.3}$$

$$R(\gamma * \gamma') = R(\gamma) R(\gamma'). \tag{6.4}$$

We now describe a concept of homotopy of paths. Given a regular path $\gamma = (\gamma_0, \dots, \gamma_\ell)$ we can obtain a new path γ' through one of the following procedures, called **basic deformations**:

- by inserting a regular vertex v between two adjacent vertices γ_k, γ_{k+1} whenever v is adjacent to both:
$$\gamma' = (\gamma_0, \dots, \gamma_k, v, \gamma_{k+1}, \dots, \gamma_\ell);$$
- by removing a vertex γ_k whenever γ_{k-1} and γ_{k+1} are adjacent:
$$\gamma' = (\gamma_0, \dots, \gamma_{k-1}, \gamma_{k+1}, \dots, \gamma_\ell).$$

Observe that if the paths are not closed we always keep the extremes fixed, while if they are closed we can move them. Given two paths γ, γ' with the same starting- and end- points a **homotopy** between them is a sequence of paths $\gamma^0, \dots, \gamma^m$ such that $\gamma^0 = \gamma$, $\gamma^m = \gamma'$ and each γ^j is obtained by γ^{j-1} through a basic deformation for $j = 1, \dots, m$.

Properties

From here on we just consider regular paths. We will prove some preliminary results about paths, their lifts and their Burgers vector and rotation. Many results follows directly from the definitions but we state them as separate lemmas for an easier reference.

It is easily seen that each basic deformation preserves the endpoint of the lift of a given path, and also its tangent vector at the endpoint. We thus obtain the following:

Lemma 6.3. *Given two paths* $\gamma, \gamma' \in \mathscr{P}(x_0, x_1)$ *with the same endpoint* x*, suppose that there is a homotopy between* γ *and* γ'*. Then* $L\gamma$ *and* $L\gamma'$ *have the same endpoint. If* γ, γ' *are closed their Burgers vectors and rotations coincide.*

Lemma 6.4. *Given two paths* γ *and* γ' *with the same starting- and end- points, suppose that the domain* $\Omega(\gamma * \overline{\gamma}')$ *does not contain defects. Then there exists a homotopy between* γ *and* γ'.

In particular if there are no defects we can always find a homotopy between two paths with the same starting- and end- points.

Proof. The proof is the same as Lemma 4.6 in [The06]. □

For any closed path $\gamma = (\gamma_0, \dots, \gamma_\ell = \gamma_0)$, we can choose any pair of distinct consecutive vertices γ_i, γ_{i+1} as base points x_0, x_1, construct the lift of γ as a path belonging to $\overline{\mathscr{P}}(x_0, x_1)$ and compute its Burgers rotation. From the definition of $R(\gamma)$ we have the following.

Lemma 6.5. *For any closed path $\gamma = (\gamma_0, \dots, \gamma_\ell = \gamma_0)$ its Burgers rotation $R(\gamma)$ does not depend on the choice of base points x_0, x_1.*

We can therefore define the Burgers rotation for any loop, that is any closed path without mention of the base points, and by linearity also for any linear combination of closed paths, that is for any polygonal 1-chain with integer coefficients supported on the edges of G:

$$R\left(\sum_i n_i \gamma_i\right) := \prod_i R(\gamma_i)^{n_i}$$

where we consider the sum on the left as a formal sum. Since each R is a rotation of a multiple of $\frac{\pi}{3}$ we can also consider 1-chains with coefficients in $\mathbb{Z}_6 = \mathbb{Z}/(6\mathbb{Z})$.

Given a closed regular path γ, for every point x not on the image of γ define $I(\gamma, x)$ as the **index** of γ around x. Viewing γ as a curve in the complex plane $\mathbb{C}$ composed by the union of all its directed edges, we can write the index as the complex integral

$$I(\gamma, x) = \frac{1}{2\pi i} \oint_\gamma \frac{1}{z - x} dz.$$

This counts how many times (with sign) the curve γ circles around x, with a positive sign if it is counter-clockwise. Define the **defect measure of γ** as

$$\sigma_\gamma := \sum_{v \in V_{def}(G)} I(\gamma, v)(\deg(v) - 6)\delta_v.$$

This counts the number of defects enclosed by γ, each counted with the multiplicity of how many times γ circles around it and multiplied by $\deg(v) - 6$. For every closed regular path γ define

$$\theta(\gamma) := \frac{\pi}{3} \sum_{v \in V_{def}(G)} I(\gamma, v)(\deg(v) - 6) = \frac{\pi}{3} \sigma_\gamma(V(G)). \tag{6.5}$$

Call two paths γ and γ' **cobordant** if there exists an open set Ω not containing defects such that $\partial\Omega = \gamma - \gamma'$, where we consider the oriented boundary.

Lemma 6.6. *$R(\gamma)$ coincides with a rotation of angle $\theta(\gamma)$. Moreover if two paths are cobordant then they have the same Burgers rotation.*

The proof of the previous Lemma will be given below after we introduce a different point of view, where we associate to each graph a flat manifold with point singularities. In this new setting it will be a simple consequence of the Gauss-Bonnet theorem.

We now define a way of creating some "cuts" on the graph G, which are a union of edges of G that link together different defects, so that in each component of a cut the defects are balanced, that is their sum cancel out modulo 6; equivalently, for every closed regular path avoiding the vertices in the cut its Burgers rotation is zero.

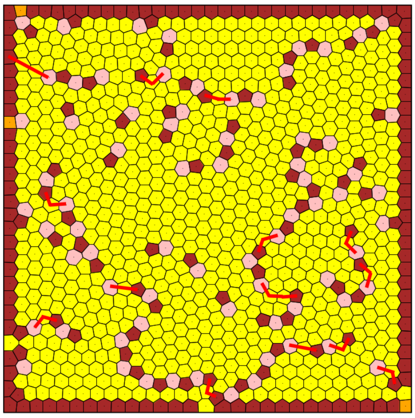


Figure 6.8: An example of cut. Consider the dual graph of the depicted partition, that is in each face put a vertex (e.g. the barycenter) and draw an edge between each pair of neighbouring polygons. Then a possible cut is shown in red (thick line). In the complement of this cut each regular closed path encloses the same amount of pentagonal and heptagonal defects, and therefore has no rotational displacement.

Definition 2. *A **cut** of a triangulated straight planar graph G is a subgraph $S \subset G$ such that the following holds: for every closed regular path γ with values in $V_{reg}(G) \setminus V(S)$, its Burgers rotation $R(\gamma)$ is the identity.*

By Lemma 6.6 this is equivalent to the following: for every connected component S_i of S

$$\sigma_G(S_i) \equiv 0 \pmod 6$$

where

$$\sigma_G := \sum_{v \in V(G)} (\deg(v) - 6)\delta_v$$

is the defect measure of G (recall (6.2)).

We can also identify a cut with a 1-current T with coefficients in $\mathbb{Z}_6 := \mathbb{Z}/(6\mathbb{Z})$ such that $\partial T = \sigma_G \pmod 6$. An example of a cut is shown in Figure 6.8.

The motivation of creating these cuts will be clear in the following: essentially in the complement of these cuts we will be able to define a curl-free orientation map β as explained in the following section. The situation is similar to the possibility of defining a branch of the complex square root when we remove a half-line from the origin.

6.4 Construction of the orientation map β

The goal of this section is to construct, given a triangulated graph G, a matrix field $\beta : \Omega_G \to \mathbb{R}^{2\times 2}$ that represents in some way the orientation, or better the distortion, of the triangular faces that constitute the graph G. The following construction follows the idea by Theil [The06], which however dealt only with the defect-free case. We will extend his construction also to the case with defects.

In the case there are no defects in the graph we obtain the orientation β in the following way. First we prove that we can identify the graph G with a subgraph of $\mathscr{A}_2$ through a map $y : V_{reg}(G) \to \mathscr{A}_2$ that is a local embedding around every point. In particuar we can define its piecewise affine extension on every triangular face to obtain a map $u : \Omega(G) \to \mathbb{R}^2$. Then we define simply $\beta := \nabla u$. The whole point in this case is to prove that such a map u exists. To this aim we fix two base points x_0, x_1 and for every regular vertex x we consider a path $\gamma \in \mathscr{P}(x_0, x_1)$ with endpoint x and define $y(x) := L\gamma(x)$ where $L\gamma$ is the lift of γ. In words, we take any path starting from two fixed points x_0, x_1 and ending at x and we reconstruct it in the triangular lattice $\mathscr{A}_2$ through its lift, and define $y(x)$ as the endpoint of the reconstructed path. If there are no defects this map is well-defined thanks to Lemma 6.3 and Lemma 6.4.

In the case there are defects, the map u could not exist. However under some circumstances the map defined locally by $\beta = \nabla u$ is still well-defined. This is the case if we remove from $\Omega(G)$ a cut as per Definition 2. Roughly speaking we can say the following: we can define u whenever for any closed path γ we have $A(\gamma) = Id$, while we can define "$\beta = \nabla u$" whenever for any closed path γ we have $R(\gamma) = Id$, which is a weaker requirement that allows for translational dispacements. In other words, the existence of paths with non-zero Burgers vectors is an obstruction to the construction of u but not necessarily of β; only the existence of paths with non-trivial Burgers rotation is an obstruction to the construction of β. We now give some more details.

Construction of β in absence of defects

We consider the case without interior defects, that is we suppose the following:

- the subgraph of regular vertices is connected;
- there exist two base points x_0, x_1 such that for any closed path $\gamma \in \overline{\mathscr{P}}(x_0, x_1)$ the associated Burgers isometry is the identity: $A(\gamma) = Id$.

Then by the first assumption for any regular vertex x we can find a path $\gamma \in \mathscr{P}(x_0, x_1)$ with endpoint x. We define the map $y : V_{reg}(G) \to \mathscr{A}_2$ by $y(x) := L\gamma(x)$. This is well-defined thanks to the second assumption. We define u as the piecewise affine interpolation of y on each face. Finally, we define $\beta := \nabla u$.

Observe that in this case we are able to define u, the *potential* of β.

Construction of β in presence of defects

The key idea is that if there are some defects we can remove a cut S to obtain a configuration in which any closed path has $R(\gamma) = Id$ (no rotational displacement). We then define again the map $\beta = \nabla u$ by constructing u locally in the complement of the cut through the lift construction. Even though the map u is not globally well-defined, the absence of rotational displacement implies that instead β is globally well-defined.

Consider then any cut S, and consider a path-connected component $\mathscr{C}$ of $V_{reg}(G)\setminus V(S)$. Fix two base points x_0, x_1, and consider any triangular face F whose vertices belong to $\mathscr{C}$, and fix one of its vertices, call it x. Let us define a map u on F with values in $\mathbb{R}^2$. Choose any path $\gamma \in \mathscr{P}(x_0, x_1)$ (of length ℓ) with endpoint $\gamma(\ell) = x$ and define the map u on the face F through the lift construction: $u(x) := L\gamma(\ell)$, and u is accordingly defined on the other two vertices by adding to the path γ the only edge that is missing to reach the vertices (and then we extend u to the whole face through the affine interpolation). Finally define $\beta := \nabla u$. Just in case, in the faces where β is not defined, and possibly in the unbounded face of G, we put $\beta = Id$.

The above definition of u depends on the chosen path γ; however the definition of β does not. Indeed if we choose another path γ' connecting x_0, x_1 to x, and define u' accordingly, then the maps u and u' differ only by a translation, thanks to the fact that on the complement of the cut every closed path has no rotational displacement. Therefore $\nabla u = \nabla u'$ and β is well-defined. Not only this, β is curl-free in distributional sense outside the cut S because we can always locally find a primitive u.

Observe that the above construciton of β depends on the choice of the cut S.

Remark 6.7. To define β we could also adopt a more abstract approach: define the class of admissible orientations $\mathscr{A}(G)$ as the family of all maps $\beta : \Omega(G) \to \mathbb{R}^{2\times 2}$ such that on every triangular face F the map β coincides with ∇u for some map $u : F \to \mathbb{R}^2$ which is affine and sends injectively the vertices $V(F)$ in the three vertices of some unit equilateral triangle of $\mathscr{A}_2$.

With this definition there is no attention paid to the creation of distributional curl of β. With this viewpoint our goal in the following will be to find a "good" admissible orientation β, that is such that $\|\mathrm{Curl}\,\beta\|$ is as low as possible, in order to obtain the most from the Rigidity Theorem 6.1. Observe that the term involving $\|\mathrm{dist}(\beta, SO(2))\|_{L^2}$ in the right hand side of (6.1) is the same for all admissible orientations, and therefore to prove estimates about the elastic energy we can choose any admissible orientation that we wish. Observe also that due to the rigidity of the class $\mathscr{A}(G)$ (piecewise affine maps) for every $\beta \in \mathscr{A}(G)$ we have that $\mu_\beta := |\mathrm{Curl}\,\beta|$ is necessarily a finite measure which is concentrated on a 1-dimensional set, namely the union of finitely many edges of the graph G. We can say even more: the measure $\mathrm{Curl}\,\beta$ is "quantized" in the following sense.

Lemma 6.8. *For any admissible β the measure $\mu_\beta := \mathrm{Curl}\,\beta$ coincides with*

$$\sum_{e\in E(G)} \tau(e) \frac{1}{\mathscr{H}^1(e)} \mathscr{H}^1 \llcorner e$$

for a suitable function $\tau : E(G) \to \mathscr{A}_2 \cap \overline{B}(0,2)$.

In other words along every edge $e = [v,w]$ of G the measure μ_β is a constant vector multiple of the length measure $\mathscr{H}^1$, and $\mu_\beta([v,w])$ is a vector of the lattice $\mathscr{A}_2$ with norm at most 2 (i.e. the difference between two unit vectors in $\mathscr{A}_2$).

Proof. It is clear that along each edge $e = [v,w]$ μ_β is a constant multiple of $\mathscr{H}^1$ since β is constant on both sides. Call β^+ and β^- the value on the two sides, and let u^+, u^- be a primitive of β on the two sides.

Let $t = \frac{w-v}{|w-v|}$ be the unit tangent vector to e and let $\gamma : [0,1] \to [v,w]$ be a constant speed parametrization of the segment $[v,w]$. Then

$$\int_e \beta^+ \cdot t \, d\mathscr{H}^1 = \int_e \nabla u^+ \cdot t \, d\mathscr{H}^1 = \int_0^1 \frac{d}{ds} u^+(\gamma(s)) ds$$
$$= u^+(\gamma(1)) - u^+(\gamma(0)) = u^+(w) - u^+(v).$$

But u^+ is a map that in every triangular face sends the vertices of the graph into the vertices of $\mathscr{A}_2$, and therefore $u^+(w) - u^+(v)$ is a unit length vector in $\mathscr{A}_2$. The same holds for u^-.

Now to compute $\mu_\beta(e)$ we compute $\mu_\beta(I_\delta(e))$ where $I_\delta(e)$ is a δ-neighbourhood of e, and then send $\delta \to 0$. We have

$$\mu_\beta(I_\delta(e)) = \oint_{\partial I_\delta(e)} \beta \cdot t \, d\mathscr{H}^1 = u^+(w) - u^+(v) + u^-(v) - u^-(w) + O(\delta)$$

and thus sending $\delta \to 0$ we obtain $\mu_\beta(e) = u^+(w) - u^+(v) + u^-(v) - u^-(w)$ which is a vector of $\mathscr{A}_2 \cap \overline{B}(0,2)$. □

6.5 Defects as singular curvature points of a locally flat surface

In this section we want to briefly explain a point of view that is useful to analyze defects, namely we see defects as points with singular Gaussian curvature inside a flat two-dimensional surface. This point of view has been used in some works on the so-called *incompatible elasticity* to describe elastic deformations of bodies whose rest configuration is not flat [KS12], [KMS15], [KM15], [KM16]. Even though we don't use the results contained in the references above, which are a bit abstract for our case, it is still useful to have this connection in mind. Besides a theoretical interest this point of view has a practical interest in the topic of creation of graphene sheets with a controlled location of its grain boundaries [WC17], which can actually improve the resistence of the graphene sheet [Son+15]. We also cite a review article about the effect of defects in graphene [Liu+15].

The starting point is the following example: the configuration in Figure 6.9 with a single pentagonal disclination fits *exactly* in a cone with an appropriate angle. More precisely, construct a cone in the following way: consider $\mathbb{R}^2$ without a $\frac{\pi}{3}$ sector starting from the origin, and identify the edges that are formed in the obvious way. Then in the conical surface that results from this construction we could insert a pentagon in the origin and *regular* hexagons outside. In other words we can realize the topological configuration of a single pentagonal defect without creating any distortion in the surrounding hexagons. We could see this "conical honeycomb" as a stress-free reference configuration for a pentagonal disclination, like the usual honeycomb is a reference configuration for a defect-free configuration. A similar construction works in the case of, say, a heptagonal defect. In this case we have instead to add a $\frac{\pi}{3}$ sector.

Similarly we can construct a reference configuration for any given distribution of defects, i.e. we can build a two-dimensional manifold that is flat everywhere except for some singular points that correspond to defects, and that fits exactly the original topological configuration with the only difference that with the given metric all hexagons become regular: we just have to impose the appropriate flat metric outside the

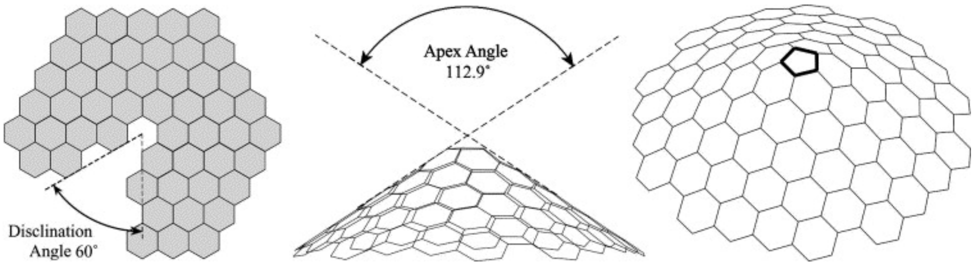


Figure 6.9: An isolated disclination surrounded by hexagons could fit exactly in a cone, without distortion of the hexagons. Picture taken from [EN06].

defects. In the case of triangulated graphs, this amounts to impose that all triangular faces are equilateral triangles of side ε.

Essentially we proceed in the following way: for any triangular face F we consider the map u that sends F into an equilateral triangle of side ε, and define $\beta = \nabla u$. Then the metric tensor on F is given by the matrix $g = \beta^\top \beta$, with respect to the usual basis (∂_x, ∂_y) of tangent vectors on F. This metric coincides with the pullback metric $u_* g_E$ where g_E is the Euclidean metric on $\mathbb{R}^2$, and therefore defines a flat metric in which by definition F is an equilateral triangle of side ε. The only problem with this definition is that in passing from one face to a neighbouring one the metric could change discontinuously, and thus this does not define a smooth metric. However this is not a fundamental issue, and we can circumvent this difficulty by defining locally the metric through charts that are a union of triangles. More precisely, consider the fundamental open sets pictured in Figure 6.10:

- an equilateral triangle;
- two adjacent equilateral triangles (including the common edge);
- six adjacent equilateral triangles (including the common edges and the middle vertex);

Then we define the metric on $\Omega(G) \setminus V_{def}(G)$ as follows: whenever there is a local embedding $\phi : U \to \Omega(G)$ that sends vertices of $\overline{U}$ to vertices of G and is affine on each face, we put on $\phi(U)$ the induced metric $\phi_*^{-1} g_E$. This is a good definition since every change of charts is a rigid motion, and therefore no matter which embedding ϕ we are using we are really defining the same metric. This defines a flat metric on the whole domain $\Omega(G)$ of the graph, except in the defects.

With this construction, to any graph G containing some defects we can associate a manifold that represents the "unstretched" reference configuration with the same topological structure. Referring to the elastic energy defined later on, we are in a certain sense removing the elastic part of the energy and keeping just the one given by defects. The elastic energy of the original graph G can then be viewed as the elastic energy required to flatten the manifold into $\mathbb{R}^2$.

Using Gauss-Bonnet theorem in the conical surface we can say that the curvature associated to a pentagon is positive and the one associated to a heptagon is negative. Indeed, consider a vertex v with degree $d = \deg(v)$ and belonging to d triangular faces. It has d edges emanating from it. Consider the

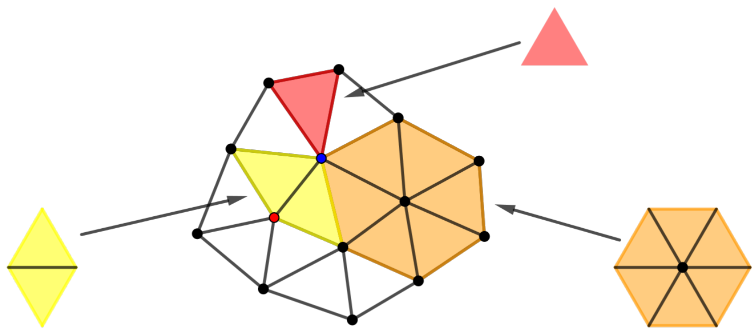


Figure 6.10: To define a metric on the domain of the graph (minus the defects) we impose the metric through the parametrizations shown above: whenever we can affinely embed one of the three reference open sets into our graph (sending vertices to vertices) we put the correspondent induced metric. If two parametrizations overlap the induced metric is the same since the change-of-chart functions are rigid motions, and thus the metric is well defined. In particular we obtain a Riemannian manifold which is flat outside the defects, and by Gauss-Bonnet we can identify vertices as singular curvature points.

polygonal path γ given by traveling counterclockwise through the outer edges of the triangular faces.We apply Gauss-Bonnet to γ, with the usual convention of counting counterclockwise angles with positive sign and clockwise angles with negative sign. The geodesic curvature of the edges is zero, because the metric is flat. The external angles at each turning point are $\frac{\pi}{3}$, by definition of the metric. Writing K for the gaussian curvature of the manifold we formally have

$$2\pi = \int_{\Omega(\gamma)} K dx + \int_{\gamma} \kappa_g + \sum_{i=1}^{d} \frac{\pi}{3} \implies \int_{\Omega(\gamma)} K dx = \frac{\pi}{3}(6-d).$$

Since the same holds for any concentric path obtained by shrinking γ through a dilation with center v, we obtain that in the neighbourhood of v

$$K = \frac{\pi}{3}(6-d)\delta_v = -\theta(\gamma)\delta_v$$

where $\theta(\gamma)$ is given by (6.5), and therefore we can view the Gaussian curvature K as an atomic measure supported on singular vertices. Considering all vertices we obtain that $-K$ coincides with the defect measure σ_G:

$$K = -\sigma_G.$$

In particular we can now prove Lemma 6.6, as previously anticipated.

Proof of Lemma 6.6. Consider a discrete path γ and call $\tilde{\gamma}$ its naturally associated continuous path obtained traveling through the edges between consecutive vertices. The rotation $R(\gamma)$ is the sum of all the turning angles of its lift $L\gamma$, which coincide with the exterior angles at each vertex of the continuous path $\tilde{\gamma}$, and therefore we conclude. □

6.6 Definition of the energy on graphs

We now introduce an energy $\mathscr{E}_\varepsilon$ defined on a triangulated graph G that depends on an elastic part (deformation of regular faces) and on a singular part (number of defects), and moreover on a microscopic parameter ε that represents the ideal length at rest of the edges. We will see how the previous construction of the orientation β together with the Rigidity Theorem 6.1 allows to find lower energy estimates for the interface problem under some natural assumptions on the energy.

In particular for a class of energies defined on G arising from different mathematical models we would like to be able to relate the two terms in the right hand side of (6.1) to the elastic part of the energy ($\|\mathrm{dist}(\beta, SO(2))\|_{L^2(\Omega)}$) and to the energy given by defects ($\|\mathrm{Curl}\,\beta\|$).

We introduce a parameter $\varepsilon > 0$ that represents the microscopic scale of the system. It can be seen as a reference length for the ground state, which is ideally a triangular lattice of step ε. We consider a triangulated graph G where each edge has length of order ε:

$$\mathscr{H}^1(e) \approx \varepsilon \tag{6.6}$$

that is $m\varepsilon \leq \mathscr{H}^1(e) \leq M\varepsilon$ for two absolute constants $0 < m \leq M < \infty$. We consider the admissible orientations $\mathscr{A}_\varepsilon(G)$ as the naturally rescaled counterpart of $\mathscr{A}(G)$: each admissible map is locally the gradient of a function u which sends $V(G)$ into $\varepsilon\mathscr{A}_2$. In particular $\beta \in \mathscr{A}_\varepsilon(G)$ is a pure rotation on every regular face which is an equilateral triangle of side ε. Moreover by Lemma 6.8 and (6.6) we have

$$|\mathrm{Curl}\,\beta| \approx \mathscr{H}^1 \llcorner \mathrm{spt}(\mathrm{Curl}\,\beta) \tag{6.7}$$

and in particular

$$|\mathrm{Curl}\,\beta| \lesssim \mathscr{H}^1 \llcorner S$$

for any cut S.

We see the energy $\mathscr{E}_\varepsilon = \mathscr{E}_\varepsilon^{el} + \mathscr{E}_\varepsilon^{def}$ as a measure on $\Omega(G)$, composed by an absolutely continuous elastic part $\mathscr{E}_\varepsilon^{el}$ and a singular part $\mathscr{E}_\varepsilon^{def}$ concentrated on defects. We actually consider the energy $\mathscr{E}_\varepsilon$ as an *energy excess* with respect to some ground state, and we explain this point with two examples.

Motivating examples

1. As a first example consider configurations of N particles $X_N = \{x_1, \dots, x_N\}$ minimizing an energy I given by

$$I(X_N) = \sum_{1 \leq i < j \leq N} V(|x_i - x_j|)$$

where $V : (0, +\infty) \to \mathbb{R} \cup \{+\infty\}$ is a small elastic perturbation of the sticky-disk potential, e.g. it satisfies

   - $V(1) = -1$ where it has a minimum;
   - $V(1+z) \geq -1 + cz^2$ for $|z| \leq \alpha$ and some constants $c > 0$ and $0 < \alpha < 1$ sufficiently small (i.e. the potential has quadratic growth around the minimum point);

- $V(r) = +\infty$ if $0 \le r < 1-\alpha$;
- $V(r)$ is identically zero for $r > 1+\alpha$.

In order to deal with bounded configurations we consider the rescaled energies

$$I_\varepsilon(X_N) := \sum_{1\le i<j\le N} V\left(\frac{|x_i-x_j|}{\varepsilon}\right)$$

where $N \approx \frac{1}{\varepsilon^2}$, which favour a triangular lattice of step ε. Then the graph $G = G(X_N)$ associated to X_N is the *bond graph* which connects with an edge a pair of particles x_i, x_j if and only if $\left|\frac{|x_i-x_j|}{\varepsilon} - 1\right| < \alpha$. A suitable sequence of competitors built as subsets of the triangular lattice gives an upper bound for the energy

$$I_\varepsilon(X_N^{min}) \le -3N + C\sqrt{N}$$

and therefore the rescaled energy $\mathscr{E}_\varepsilon$ would be in this case

$$\mathscr{E}_\varepsilon(X_N) = \frac{1}{\sqrt{N}}(I_\varepsilon(X_N) + 3N).$$

Let us show that we can relate the elastic part of the energy to $\|\mathrm{dist}(\beta, SO(2))\|_{L^2}$, where β is an admissible orientation for the configuration. We have that

$$\begin{aligned}
I_\varepsilon(X_N) &= \frac{1}{2}\sum_{x\in X_N}\sum_{x'\in\mathscr{N}(x)} V\left(\frac{|x-x'|}{\varepsilon}\right)\\
&\ge \frac{1}{2}\sum_{x\in X_N}\sum_{x'\in\mathscr{N}(x)} \left(-1 + c\left(\frac{|x-x'|}{\varepsilon} - 1\right)^2\right)\\
&\ge -3N + \frac{1}{2}\#V_{def}(G) + \frac{c}{2}\sum_{x\in X_N}\sum_{x'\in\mathscr{N}(x)} \left(\frac{|x-x'|}{\varepsilon} - 1\right)^2
\end{aligned}$$

and thus

$$\begin{aligned}
\mathscr{E}_\varepsilon(X_N) = \frac{1}{\sqrt{N}}(I_\varepsilon(X_N)+3N) &\gtrsim \frac{1}{\sqrt{N}}\#V_{def}(G) + \frac{1}{\sqrt{N}\varepsilon^2}\sum_{x\in X_N}\sum_{x'\in\mathscr{N}(x)} (|x-x'|-\varepsilon)^2\\
&= \varepsilon\#V_{def}(G) + \frac{1}{\varepsilon}\sum_{x\in X_N}\sum_{x'\in\mathscr{N}(x)} (|x-x'|-\varepsilon)^2
\end{aligned}$$

where we used $\varepsilon \approx \frac{1}{\sqrt{N}}$. Now a simple computation (see Lemma 4.2 in [The06]) tells us that the last sum is related to $\|\mathrm{dist}(\beta, SO(2))\|_{L^2}$ in the following sense: given a triplet of points x_1, x_2, x_3, let β denote the gradient of the affine function that sends x_1, x_2, x_3 injectively to the vertices of an equilateral triangle of side 1. Then

$$\mathrm{dist}(\beta, SO(2))^2 \le K \max_{i\ne j} \left||x_i - x_j| - 1\right|^2$$

for an absolute constant K. In particular for any triangular face F, that is for any triplet of neighbouring points x_1, x_2, x_3, we have

$$\begin{aligned}\sum_{1\le i<j\le 3}(|x_i-x_j|-\varepsilon)^2 &= \varepsilon^2\sum_{1\le i<j\le 3}\left(\frac{|x_i-x_j|}{\varepsilon}-1\right)^2\\ &\gtrsim \varepsilon^2\int_{\frac{1}{\varepsilon}F}\operatorname{dist}\left(\beta\left(\frac{\cdot}{\varepsilon}\right),SO(2)\right)^2\\ &= \int_F \operatorname{dist}(\beta,SO(2))^2\end{aligned}$$

and therefore

$$\mathscr{E}_\varepsilon(X_N)\gtrsim \varepsilon\#V_{def}(G)+\frac{1}{\varepsilon}\int_{\Omega(G)}\operatorname{dist}(\beta,SO(2))^2.$$

2. As a second example consider the perimeter functional for clusters with equal areas: for a (polygonal) N-cluster $\mathscr{E}$ with areas $\frac{1}{N}$ the microscopic parameter would be $\varepsilon=\frac{1}{\sqrt{N}}\sqrt[4]{\frac{4}{3}}$ (the distance between the centers of two adjacent hexagons in the honeycomb with areas $\frac{1}{N}$) and the total energy would be

$$\mathscr{E}_\varepsilon(\mathscr{E})=P(\mathscr{E})-\sqrt{N}\sqrt[4]{12}.$$

Again we are subtracing the bulk part of the energy (in this case given by Hales theorem) in order to obtain an energy that is equibounded on minimizing sequences. In this case we have at least two choices to associate a graph G to the configurations: we can triangulate each polygon and consider the graph naturally associated to the triangulation (faces are triangles; vertices and edges are triangles' vertices and edges) or we can consider the dual graph of the graph associated to the original polygonal partition.

In the case of polygons we have a strong Hales-type inequality in the following form: consider a polygon E with area 1 and k sides, with a uniform bound on the length of the sides. Then

$$P(E)\ge P(\Pi_6)-a_1(k-6)+a_2(1-\delta_{6,k})+a_3\delta_{6,k}d(E,\Pi_6)^2 \tag{6.8}$$

for some constants a_1, a_2, a_3 where:

- Π_k is the regular polygon with k sides and with area 1;
- $d(\cdot,\cdot)$ is any reasonable distance among polygons, for instance the minimum Hausdorff distance between ∂E and an isometric copy of $\partial\Pi_k$:

$$d(E,F):=\inf_{\substack{\tau\in\mathbb{R}^2\\ R\in SO(2)}}\left\{d_H(\partial E,\partial(\tau+R\Pi_6))\right\}.$$

- $\delta_{6,k}$ is the Kronecker delta, equal to 1 if $k=6$ and zero otherwise.

Equation (6.8) holds for the following reason:

- When $k = 6$ it reduces to

$$P(E) \geq P(\Pi_6) + a_3 d(E, \Pi_6)^2$$

for all polygons with 6 sides, area 1 and uniformly bounded perimeter, which is true by the results of [CM16, Proposition 2.1], see also [IN15, Corollary 1.3].

- When $k \neq 6$ it reduces to

$$P(E) \geq P(\Pi_6) - a_1(k-6) + a_2.$$

for every polygon E with $k \neq 6$ sides and area 1. This inequality follows immediately from the polygonal isoperimetric inequality $P(E) \geq P(\Pi_k)$ and from the strict convexity of the function $k \mapsto P(\Pi_k) = 2\sqrt{k \tan \frac{\pi}{k}}$.

Consider now an N-cluster $\mathscr{E}_N$ with areas 1. Summing inequality (6.8) among all the polygonal chambers of $\mathscr{E}_N$ we obtain

$$\begin{aligned} P(\mathscr{E}_N) &= \frac{1}{2}\sum_{i=0}^{N} P(\mathscr{E}_N(i)) \\ &\geq \frac{1}{2}P(\mathscr{E}_N(0)) + \frac{1}{2}\sum_{i=1}^{N}\left(P(\Pi_6) - a_1(k_i - 6) + a_2(1-\delta_{6,k_i}) + a_3\delta_{6,k_i} d(\mathscr{E}_N(i), \Pi_6)^2\right) \\ &= \frac{1}{2}P(\mathscr{E}_N(0)) + \sqrt[4]{12}N - a_1\sum_{i=1}^{N}(k_i - 6) + a_2\#\{i : k_i \neq 6\} + a_3 \sum_{i:k_i=6} d(\mathscr{E}_N(i), \Pi_6)^2. \end{aligned}$$

Now we can neglect the sum of $(k_i - 6)$ because by Euler's formula for planar graphs the contribution is positive (see Remark 6.9 below). We now rescale the cluster $\mathscr{E}_N$ by a factor $\frac{1}{\sqrt{N}}$ so to obtain a cluster $\tilde{\mathscr{E}}_N$ with areas $\frac{1}{N}$. The previous inequality becomes

$$P(\tilde{\mathscr{E}}_N) \geq \sqrt[4]{12}\sqrt{N} + \frac{1}{\sqrt{N}}\#\{i : k_i \neq 6\} + \sqrt{N}\sum_{i:k_i \neq 6} d\left(\tilde{\mathscr{E}}_N(i), \tfrac{1}{\sqrt{N}}\Pi_6\right)^2.$$

Recalling that $\varepsilon \approx \frac{1}{\sqrt{N}}$ the original energy $\mathscr{E}_\varepsilon$ therefore satisfies, for any N-cluster $\mathscr{E}$ with areas $\frac{1}{N}$

$$\mathscr{E}_\varepsilon(\mathscr{E}) := P(\mathscr{E}) - \sqrt{N}\sqrt[4]{12} \gtrsim \varepsilon \# F_{def}(\mathscr{E}) + \frac{1}{\varepsilon}\sum_{i:k_i=6} d\left(\mathscr{E}(i), \tfrac{1}{\sqrt{N}}\Pi_6\right)^2$$

where F_{def} is the family of defective faces with a number of sides different from 6. Again, as in the first example, we can relate the last quadratic sum to $\|\mathrm{dist}\beta, SO(2))\|_{L^2}$ where β is a suitable map that sends the hexagonal face to a regular hexagon of area $\frac{1}{N}$ (for instance partition the hexagonal face in 6 triangles and send affinely each triangle in a suitable equilateral triangle; we omit the details). If we consider the dual graph G of the original partition, the term $\#F_{def}(\mathscr{E})$ becomes exactly $\#V_{def}(G)$, and thus we obtain exactly the same kind of energy as in example 1.

Definition of the energy

Keeping in mind the previous examples we therefore impose the following assumptions on the energy $\mathscr{E}_\varepsilon$:

- $\mathscr{E}_\varepsilon$ admits a decomposition $\mathscr{E} = \mathscr{E}_\varepsilon^{el} + \mathscr{E}_\varepsilon^{def}$ where $\mathscr{E}_\varepsilon^{el}$ is the *elastic energy* due to deformations of the regular triangular faces while $\mathscr{E}_\varepsilon^{def}$ is the energy caused by defects:

$$\mathscr{E}_\varepsilon^{def}(G) = \sum_{v \in V(G)} \mathscr{E}_\varepsilon^{def}(v), \qquad \mathscr{E}_\varepsilon^{el} = \sum_{F \in F(G)} \mathscr{E}_\varepsilon^{el}(F);$$

- *Quadratic elastic energy.* For any admissible $\beta \in \mathscr{A}_\varepsilon$

$$\mathscr{E}_\varepsilon^{el}(F) \approx \frac{1}{\varepsilon} \int_F \operatorname{dist}(\beta, SO(2))^2. \tag{6.9}$$

  In particular $\mathscr{E}_\varepsilon^{el}(F) = 0$ whenever $\beta \in \mathscr{A}_\varepsilon(G)$ and F is an equilateral triangle of sidelength ε;

- *Quantization of defects.*

$$m \le \frac{1}{\varepsilon} \mathscr{E}_\varepsilon^{def}(v) \le M \tag{6.10}$$

  for any defect $v \in V_{def}(G)$ and for some constants m, M.

In view of the previous discussion, the energy we consider is therefore

$$\boxed{\mathscr{E}_\varepsilon(G) = \frac{1}{\varepsilon} \int_\Omega \operatorname{dist}(\beta, SO(2))^2 + \varepsilon \# V_{def}(G)}. \tag{6.11}$$

Remark 6.9. The lower bound of (6.10) is verified *on average* if we know that a Hales-type inequality holds for defects:

- *Hales-type inequality for defects.*

$$\frac{1}{\varepsilon} \mathscr{E}_\varepsilon^{def}(v) \ge a_1(6 - \deg(v)) + a_2 \delta(\deg(v)). \tag{6.12}$$

for some universal constants a_1, a_2, M, where $\delta : \mathbb{N} \to [0, \infty)$ vanishes only when $\deg(v) = 6$ and is bounded away from zero otherwise: $\delta(k) \ge 1$ for every $k \ne 6$.

This lower bound follows from Euler's formula for planar graphs. Indeed, denoting by E_{ext} the external edges we have $2E - E_{ext} = 3F$, or

$$E = \frac{3}{2} F + \frac{1}{2} E_{ext}.$$

From Euler's formula $F + V - E = 1$ we obtain

$$F + V - \left(\frac{3}{2} F + \frac{1}{2} E_{ext} \right) = 1 \implies V = \frac{1}{2} F + 1 + \frac{1}{2} E_{ext}.$$

Moreover $2E = \sum_v \deg(v)$ and thus

$$\sum_v (\deg(v) - 6) = 2E - 6V = (3F + E_{ext}) - 6\left(\frac{1}{2}F + 1 + \frac{1}{2}E_{ext}\right) = -6 - 2E_{ext}. \tag{6.13}$$

Therefore summing $\mathscr{E}_\varepsilon^{def}$ among all vertices we obtain

$$\mathscr{E}_\varepsilon^{def}(\Omega) \geq \varepsilon a_1(6 + E_{ext}) + a_2\varepsilon \sum_v \delta(\deg(v)) \geq \varepsilon a_1(6 + E_{ext}) + a_2\varepsilon \# V_{def}(G).$$

Even if we do not count the outer vertices as defects we still have

$$\mathscr{E}_\varepsilon^{def}(G) \geq a_2\varepsilon \# V_{def}(G).$$

□

Relation between $\|\operatorname{Curl}\beta\|$ and the number of defects: the balance condition

We repeat that the energy that we will consider in the following is

$$\mathscr{E}_\varepsilon(G) = \frac{1}{\varepsilon}\int_\Omega \operatorname{dist}(\beta, SO(2))^2 + \varepsilon \# V_{def}(G)$$

for any admissible orientation β. Observe that the value of $\operatorname{dist}(\beta, SO(2))$ does not depend on the specific choice of β, since any two choices differ on each face by a rotation. For this reason we could write interchangeably $\mathscr{E}_\varepsilon^{el}(G)$, $\mathscr{E}_\varepsilon^{el}(\beta)$ or $\mathscr{E}_\varepsilon^{el}(\Omega)$ with the underlying agreement that there is a graph G that gives rise to β and Ω.

The goal is now to apply Theorem 6.1 to the map β. While the elastic energy is naturally related to $\|\operatorname{dist}(\beta, SO(2))\|_{L^2}$ (and we put this in the definition of the elastic energy, see (6.9)), it is less clear what is the exact role of $\|\operatorname{Curl}\beta\|$ in terms of the defect part of the energy. Indeed we can say that for admissible orientations β, $\|\operatorname{Curl}\beta\|$ is related not really to the number of defects but rather to their flat norm, i.e. to the length of a cut that connects them.

In order to obtain the most from inequality (6.1) we need to find a map β such that $\|\operatorname{Curl}\beta\| = |\operatorname{Curl}\beta|(\Omega)$ is as low as possible. The point of having introduced the notion of *cut* in the previous section is that we can give an upper bound on $\|\operatorname{Curl}\beta\|$ in terms of the length of the cut. Indeed, by the construction of β in presence of defects we know that we can always have $\|\operatorname{Curl}\beta\| \lesssim \mathscr{H}^1(S)$ where S is a cut. Therefore we encounter the following problem: given a set of defects, find the shortest possible cut that connects them. We introduce here an assumption, called *balance* assumption: we say that defects are **balanced** if there is a cut S such that

$$\|\operatorname{Curl}\beta\| \leq C\varepsilon \# V_{def}(G) \tag{6.14}$$

for a universal constant C, not depending on ε. As we shall now prove this is the case if for instance there are only dislocations and no disclinations, or even if there are disclinations but they are balanced within a radius of order ε. This could seem a rather strong assumption, but indeed single isolated disclinations are hard to find because they create an enormous amount of elastic energy in the surrounding cells, compare with Lemma 6.20 below.

Lemma 6.10 (No disclinations imply balance). (i) *Suppose there are dislocations but no disclinations, that is for every closed path going through regular vertices the rotational displacement is zero. Then the blance condition holds, that is we can choose β such that*

$$\|\operatorname{Curl}\beta\| \lesssim \varepsilon \# V_{def}(G).$$

(ii) *The same conclusion holds if we know that there is a cut S which is contained in $\bigcup_{v\in V_{def}(G)} B(v,C\varepsilon)$ for some universal constant C.*

Proof. (i) From the assumption we obtain that we can create a cut S by considering the union of all edges starting from defects, that is

$$S := \bigcup_{v\in V_{def}(G)} \bigcup_{w\in\mathscr{N}(v)} [v,w]$$

because any path with values in $V(G)\setminus S$ is regular and therefore by assumption must have trivial Burgers rotation. Moreover we know from (6.7) and (6.6) that

$$\|\operatorname{Curl}\beta\| \lesssim \mathscr{H}^1(S) \lesssim \varepsilon \sum_{v\in V_{def}(G)} \deg(v)$$

and from (6.13) we obtain that

$$\sum_{v\in V_{def}(G)} \deg(v) \leq 6\# V_{def}(G)$$

and therefore we conclude.

(ii) The proof is analogous. There is a uniformly bounded number of edges that could be contained in the ball $B(v,C\varepsilon)$ because of the assumption of "bounded distortion" (6.6). □

6.7 The interface problem: number of defects, weak lower bound on the energy and convergence to a BV orientation

We now finally consider the interface problem in a square of side L and with angle mismatch θ. Since we are interested in small angles, we suppose $|\theta| \leq \frac{\pi}{12}$. Consider all planar graphs G that on $(-\infty,-\frac{L}{4})\times\mathbb{R}$ coincide with a translation of $\varepsilon R_\theta \mathscr{A}_2$, R_θ being the rotation of angle θ around the origin, while on $(\frac{L}{4},+\infty)\times\mathbb{R}$ coincide with a translation of $\varepsilon R_{-\theta}\mathscr{A}_2$. We suppose for simpicity that the graphs taken into consideration are periodic with period $L_1 = L + O(\varepsilon)$ in the vertical direction, and call $\mathscr{G}(\theta,L,\varepsilon)$ the class of all such graphs. We are then interested in $G\cap\Omega$ (seen as a periodic graph in the vertical direction) where $\Omega := \big([-\frac{L}{2},\frac{L}{2}]\times[-\frac{L_1}{2},\frac{L_1}{2}]\big)$.

From the construction of β in the case without defects we obtain the following:

Lemma 6.11. *If there are no defects then we can choose a curl-free orientation β, that is $\|\operatorname{Curl}\beta\| = 0$.*

In particular we can now obtain a lower bound for the energy at an interface without defects.

Theorem 6.12 (Energy lower bound at an interface without defects). *If there are no defects at an interface with angle mismatch equal to θ then the energy satisfies*

$$\mathscr{E}_\varepsilon = \mathscr{E}_\varepsilon^{el} \gtrsim \frac{1}{\varepsilon} L^2 \theta^2.$$

Proof. By the rigidity theorem 6.1 there is a rotation R such that

$$\int_\Omega |\beta - R|^2 \lesssim \int_\Omega \mathrm{dist}(\beta, SO(2))^2 \approx \varepsilon \mathscr{E}_\varepsilon^{el}(\beta)$$

and it is easy to see that the left hand side is at least $\theta^2 L^2$. □

Since by the previous estimate in absence of defects the energy blows up as $\varepsilon \to 0$, we obtain the following.

Corollary 6.13 (Defects must appear at an interface). *For fixed θ and L consider a family of graphs $G_\varepsilon \in \mathscr{G}(\theta, L, \varepsilon)$ with bounded energy, that is*

$$\limsup_{\varepsilon \to 0} \mathscr{E}_\varepsilon(G_\varepsilon) < \infty.$$

Then for sufficiently small ε defects must appear.

The previous Corollary tells us that at an interface it is always necessary to introduce some defect to avoid an energy that blows up, but does not tell us how many defects have to be introduced, and does not exclude the case of a single magical defect that makes the energies equibounded. Actually we can prove that the number of defects must go to infinity with a similar argument: we divide Ω in a finite number of congruent horizontal stripes and apply the above estimate on each stripe, obtaining that in each one there is eventually at least one defect. This argument however is just qualitative in that it gives no rate for the number of defects in terms of ε (observe that the constant $C(\Omega)$ of the rigidity theorem, although invariant under rescaling, does not behave well with respect to dilations in only one direction). Looking at a grain boundary (see Figure 6.5) and assuming equispaced defects it is natural to conjecture that in a square domain Ω of side L, angle mismatch θ and microscopic parameter ε we should have a precise estimate on the number of defects:

$$\# V_{def}(G) \gtrsim \frac{L\theta}{\varepsilon}.$$

Indeed the distance between two consecutive defects, in the depicted configuration, is approximately $\frac{\varepsilon}{\theta}$.

We are able to prove an estimate of this type under the balance assumption.

Lemma 6.14 (Number of defects and weak energy lower bound under the balance condition). *Suppose the balance condition (6.14) holds. Then*

$$\# V_{def}(G) \gtrsim \frac{L\theta}{\varepsilon}$$

and we have the weak energy lower bound

$$\mathscr{E}_\varepsilon(G) \gtrsim L\theta.$$

Proof. Observe that from the energy bound $\mathscr{E}_\varepsilon^{el} \lesssim L$ and the rigidity theorem in the form

$$\int_\Omega |\beta - R|^2 \leq C(\Omega)(\varepsilon \mathscr{E}_\varepsilon^{el} + \|\operatorname{Curl}\beta\|^2)$$

we obtain in particular that for sufficiently small ε

$$\|\operatorname{Curl}\beta\| \gtrsim L\theta$$

and therefore using the balance assumption (6.14) we conclude. □

Remark 6.15. The same conclusion of Lemma 6.12, Corollary 6.13 and Lemma 6.14 actually holds not only for the interface case, where there are two well-separated regular zones, but also in the case when the different orientations are "mixed": it is sufficient that there is oscillation, i.e. that the lower bound $\|\beta - R\|_{L^2} \gtrsim C|\theta|$ holds.

Even though the lower bound on the energy of Lemma 6.14 is not the optimal bound that we are expecting, which is $L\theta|\log\theta|$ (hence the adjective *weak*), it is a first indication towards a compactness result in the space of BV orientations. To prove this we can use the following lemma taken from [LL16].

Lemma 6.16 ([LL16, Proposition 3])**.** *Let $\Omega \subset \mathbb{R}^n$ be an open, bounded, simply connected set and consider a sequence $\beta_j \in L^2(\Omega, M^{n\times n})$ such that*

$$\lim_{j\to\infty} \|\operatorname{dist}(\beta_j, SO(n))\|_{L^2} = 0 \qquad \sup_j |\operatorname{Curl}\beta_j|(\Omega) < \infty.$$

Then up to a subsequence β_j converge strongly in L^2 to a matrix field $\beta \in BV(\Omega, SO(n))$. Moreover the set of points where β does not belong to $SO(n)$ has Hausdorff dimension at most $n-1$, and finally

$$|D\beta|(\Omega) \leq C|\operatorname{Curl}\beta|(\Omega)$$

for a dimensional constant C.

Proposition 6.17 (**The limit orientation is** BV)**.** *Assume the balance condition (6.14) holds, and consider a family of graphs G_ε whose domain is a common open set Ω. Fix an open set $\tilde\Omega \Subset \Omega$, and suppose*

$$\limsup_{\varepsilon\to 0}(\mathscr{E}_\varepsilon \llcorner \tilde\Omega)(G_\varepsilon) < \infty.$$

Then up to a subsequence the orientations β_ε (that are well-defined up to rotations of multiples of $\frac{\pi}{3}$) converge strongly in L^2 to a limit orientation $\beta \in BV(\tilde\Omega, SO(2))$.

Proof. We apply the lemma above. We observe that from the upper bound on the energy $\mathscr{E}_\varepsilon(G) \lesssim L$ we obtain

$$\int \operatorname{dist}(\beta_\varepsilon, SO(2))^2 \leq L\varepsilon$$

which implies the first assumption of the lemma. From the balance assumption $\|\operatorname{Curl}\beta\| \lesssim \varepsilon \# V_{def}(G)$ and inequality (6.10) we obtain

$$\|\operatorname{Curl}\beta_\varepsilon\| \leq \varepsilon \# V_{def}(G) \leq \frac{1}{m}\mathscr{E}_\varepsilon^{def} \leq \frac{L}{m}$$

which implies the second assumption of the lemma, and thus we conclude. □

If instead of relying on the last Lemma above we rely on the full result of [LL16], we can almost obtain a polycrystalline limit orientation (called **microrotation** in the reference above), that is a limit matrix-field β such that $D\beta = D^j\beta$. The "almost" is because we have to assume again the balance condition, and furthermore we have to assume that a *logarithmic upper bound* holds, that is

$$\mathscr{E}_\varepsilon(G_\varepsilon) \leq C\theta|\log\theta|. \tag{$UB_{\log}$}$$

This upper bound is currently not proved. Moreover the result is not about the sequence of orientations β_ε, but about a slightly modified sequence.

We briefly describe their setting and explain how their results can be used in our case. Given a fixed square $\Omega = [-L,L]^2$ and a microscopic parameter ε they consider the admissible class $\mathscr{A}_\varepsilon$ of all maps $\beta : \Omega \to M^{2\times 2}$ such that $\operatorname{Curl}\beta$ is a finite measure and such that, setting $S_\beta := \operatorname{supp}(\operatorname{Curl}\beta)$:

- $\beta \in L^1_{loc}(\Omega, M^{2\times 2}) \cap L^2(\Omega \setminus B_{\lambda\varepsilon}(S_\beta), M^{2\times 2})$ where λ is a fixed real parameter (describing the *core radius*) and where, given a set S, $B_{\lambda\varepsilon}(S)$ denotes its $\lambda\varepsilon$-neighbourhood;
- β coincides with a rotation R_θ of an angle θ on $[-L, -L+\ell] \times [-L,L]$ and a rotation $R_{-\theta}$ on $[L-\ell, L] \times [-L,L]$, for some $\ell \ll L$;
- for every closed Lipschitz curve γ contained in $\Omega \setminus B_{\lambda\varepsilon}(S_\beta)$ either

  $$\int_\gamma \beta \cdot \tau = 0$$

  or

  $$\left|\int_\gamma \beta \cdot \tau\right| \geq c\varepsilon$$

  for a constant $c > 0$. This assumption corresponds to a *quantization* of the dislocations.

The energy is then defined (up to constants) by

$$\mathscr{E}_\varepsilon(\beta) = \frac{1}{\varepsilon}\int_{\Omega \setminus B_{\lambda\varepsilon}(S_\beta)} \operatorname{dist}(\beta, SO(2))^2 + \frac{1}{\lambda\varepsilon}|B_{\lambda\varepsilon}(S_\beta)|.$$

If S_β is 1-dimensional and regular enough, as is the case for our admissible orientations defined in 6.7, then the second term of the energy is equivalent to $\mathscr{H}^1(S_\beta)$, which in turn by the balance condition is equivalent to $\varepsilon\#V_{def}(G)$, and therefore the energy reduces to our energy $\mathscr{E}_\varepsilon$. Adapted to our case, Corollary 12 in [LL16] reads as follows.

Proposition 6.18 (**The limit orientation is a microrotation**). *Assume that the balance condition* (6.14) *and the logarithmic upper bound* ($UB_{\log}$) *hold, and consider a family of graphs G_ε whose domain is a common open set Ω. Fix an open set $\tilde\Omega \Subset \Omega$, and suppose*

$$\limsup_{\varepsilon\to 0} \mathscr{E}_\varepsilon|_{\tilde\Omega}(G_\varepsilon) < \infty.$$

Then there exists another family $\tilde{\beta}_\varepsilon$ of admissible maps in $\mathscr{A}_\varepsilon$ such that $\mathscr{E}_\varepsilon(\tilde{\beta}_\varepsilon) \leq C\mathscr{E}_\varepsilon(\beta_\varepsilon)$ and such that up to a subsequence they converge strongly in L^2 to a limit orientation $\tilde{\beta}$ which is a microrotation, that is

$$D\tilde{\beta} = D^j\tilde{\beta}, \qquad \beta \in SO(2) \text{ a.e.}$$

and moreover the measures

$$\frac{1}{\varepsilon}\mathrm{dist}(\tilde{\beta}_\varepsilon, SO(2))^2 \mathscr{L}^2 \llcorner \Omega + \frac{1}{\varepsilon}\mathscr{L}^2 \llcorner B_{\lambda\varepsilon}(S_\beta)$$

converge to a measure μ such that

$$C\mu \geq |\tilde{\beta}^+ - \tilde{\beta}^-| \, |\log(|\tilde{\beta}^+ - \tilde{\beta}^-|)| \mathscr{H}^1 \llcorner S_{\tilde{\beta}}.$$

Proof. The conclusion follows from the above discussion and from [LL16, Corollary 12]. ☐

We remark however that for now we do not have a logarithmic upper bound, that is we do not have a sequence of competitors with a logarithmic energy in the angle θ, and moreover we would like to conclude that the original sequence (and not a modified one) has the properties described by the Proposition.

6.8 The ball construction

In this last Section we explain what is the result we would like to obtain, what is the path we would like to follow and what are the difficulties that for now do not allow us to conclude.

The goal is to give a better estimate from below of the energy $\mathscr{E}_\varepsilon$ in terms of L, θ and ε. In Lemma 6.14 we gave the estimate $\mathscr{E}_\varepsilon^{el} \gtrsim L\theta$. We expect that a better estimate holds:

$$\mathscr{E}_\varepsilon \gtrsim L\theta|\log\theta|, \tag{6.15}$$

and we call this estimate for short *logarithmic lower bound*. We remark that the energy due to the single defects is expected to be $\approx \theta L$, much smaller than the above estimate. The extra logarithmic factor is really coming from the elastic deformations that propagate *around* each defect and not to the defects themselves. We first look at the energy around a single group of defects.

Elastic deformation around defects

We now analyze the case of a single defect or of a group of defects inside an otherwise regular configuration, with the goal of proving that the presence of the defects creates an elastic deformation on the surrounding regular cells (see Figure 6.11). As we will see this deformation propagates even at long distances, and the elastic energy contained in a ball of radius ρ depends on whether the defect is a dislocation (the energy is logarithmic in ρ) or a disclination (the energy is quadratic in ρ). The situation presents many similarities with the Ginzburg-Landau models where analogous logarithmic estimates hold. To pass from the estimate of the energy around a single defect to an estimate for the whole configuration we would like to adapt a proof given by Sandier in the context of planar Ginzburg-Landau models [San98] (a similar result was proved at the same time by Jerrard [Jer99]).

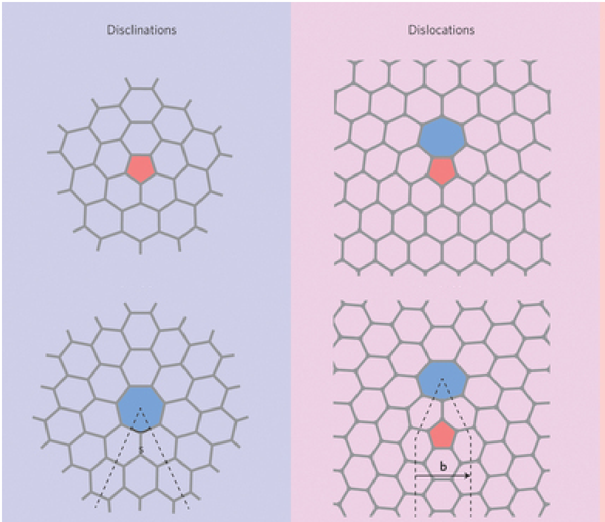


Figure 6.11: Example of disclinations and dislocations in the case of the hexagonal lattice. The deformation on the surrounding cells propagate even at long distance and depends on whether the defect is a disclination or a dislocation: in the first case all cells are stretched and the elastic energy in a certain ball is at least proportional to its area (Lemma 6.20); in the second case the defect is less severe and the elastic energy has a logarithmic behaviour: the energy in an annulus $B_\rho \setminus B_r$ goes like $\log\left(\frac{\rho}{r}\right)$ (Lemma 6.19).

Lemma 6.19 (Elastic energy around a dislocation). *Suppose $\beta : B_\rho \setminus B_r \to \mathbb{R}^{2\times 2}$ is curl-free and that*

$$\oint_{\partial B_r} \beta \cdot \tau = \varepsilon \vec{b}.$$

Then we have that

$$\int_{B_\rho \setminus B_r} \operatorname{dist}(\beta, SO(2))^2 \geq C(\rho, r) \frac{1}{2\pi} |\vec{b}|^2 \varepsilon^2 \log\left(\frac{\rho}{r}\right) \tag{6.16}$$

where $C(\rho, r)$ is the rigidity constant of the annulus $B_\rho \setminus B_r$, which is uniformly bounded whenever $\frac{\rho}{r} \geq 1 + \delta$ for some positive δ.

Proof. We remove a cut and a hole from B_ρ, obtaining the set

$$B_{\rho,r} := B_\rho \setminus (B_r \cup \ell)$$

with ℓ a half line starting from the origin. Then in this domain β admits a primitive, that is $\beta = \nabla u$ for a map $u \in W^{1,2}(B_{\rho,r}, \mathbb{R}^2)$, and we can apply the Rigidity estimate with a cut and a hole from [SZ12]:

$$\int_{B_\rho \setminus B_r} \operatorname{dist}(\beta, SO(2))^2 \geq C(\rho, r) \int_{B_\rho \setminus B_r} |\beta - R|^2$$

for some rotation R. Moreover

$$\begin{aligned}\int_{B_\rho\setminus B_r}|\beta-R|^2 &= \int_r^\rho dt\int_{\partial B_t}|\beta-R|^2 ds\\ &\geq \int_r^\rho dt\frac{1}{2\pi t}\left|\int_{\partial B_t}(\beta-R)\cdot\tau dt\right|^2\\ &= \frac{|\vec{b}|^2}{2\pi}\varepsilon^2\log\left(\frac{\rho}{r}\right)\end{aligned}$$

and the result follows. $\square$

Lemma 6.20 (Elastic energy around a disclination). *Suppose $\beta : B_\rho\setminus B_r \to \mathbb{R}^{2\times 2}$ is an admissible map associated to a graph without defects in $B_\rho\setminus B_r$ and suppose the rotational defect of a path around ∂B_r is non-zero. Then we have that*

$$\int_{B_\rho\setminus B_r}\operatorname{dist}(\beta,SO(2))^2 \gtrsim C(\rho,r)|B_\rho\setminus B_r|.$$

Proof. Set for simplicity $\Omega := B_\rho\setminus B_r$. We remove again a cut to obtain the set $\Omega_1 := \Omega\setminus\ell$, where ℓ is, say, the vertical half-line $\{(x_1,x_2)\in\mathbb{R}^2 : x_1 = 0, x_2\geq 0\}$. In this domain there exists an orientation β_1 such that $\beta_1 = \nabla u_1$ for a map $u_1\in W^{1,2}(\Omega_1,\mathbb{R}^2)$, and we can again apply the Rigidity estimate with a cut and a hole from [SZ12]:

$$\int_{\Omega_1}\operatorname{dist}(\beta_1,SO(2))^2 \geq C(\rho,r)\int_{\Omega_1}|\beta_1-R_1|^2$$

for some rotation R_1. Now we consider another cut domain, namely the one where the cut is opposite to ℓ: we define $\Omega_2 := \Omega\setminus(-\ell)$. We consider the orientation β_2 defined on Ω_2 which coincides with β_1 in $\Omega_+ := \Omega\cap\{x_1>0\}$ and which is continued without creating curl, and as above we apply the rigidity to obtain a rotation R_2 such that

$$\int_{\Omega_2}\operatorname{dist}(\beta_2,SO(2))^2 \geq C(\rho,r)\int_{\Omega_2}|\beta_2-R_2|^2.$$

Since B_r contains rotational defect, on the domain $\Omega_- := \Omega\cap\{x_1<0\}$ the new map β_2 differ from β_1 by a constant non-trivial rotation by a multiple of $\frac{\pi}{3}$, that is $\beta_2 = R_0\beta_1$ on Ω_-, with $R_0 = R^k_{\pi/3}$ for some $k\not\equiv 0 \pmod 6$. Then we obtain

$$\begin{aligned}\int_{\Omega_1}|\beta_1-R_1|^2+\int_{\Omega_2}|\beta_2-R_2|^2 &= \int_{\Omega_+}(|\beta_1-R_1|^2+|\beta_1-R_2|^2)+\int_{\Omega_-}(|\beta_1-R_1|^2+|\beta_1-R_0^{-1}R_2|^2)\\ &\geq \frac{1}{2}\int_{\Omega_+}|R_1-R_2|^2+\frac{1}{2}\int_{\Omega_-}|R_1-R_0^{-1}R_2|^2\\ &= \frac{1}{4}|\Omega_+||R_2-R_0^{-1}R_2|^2 = \frac{1}{8}|\Omega|\,|Id-R_0|^2\end{aligned}$$

where we used twice that $(a^2+b^2)\geq\frac{1}{2}(a+b)^2$ and the triangle inequality. The last term is clearly bounded away from zero by a universal constant times $|\Omega|$. $\square$

Remark 6.21. In particular, as could be intuitively clear, the energy around a single disclination contained in some ball B_r is much bigger than the energy around a single dislocation contained in the same ball: indeed for any fixed constant C we have

$$\rho^2 \geq Cr^2 \log\left(\frac{\rho}{r}\right)$$

as soon as $\rho \geq c(C)r$ for some constant $c(C)$ big enough (i.e. such that $x^2 \geq C \log x$ for every $x \geq c(C)$).

Remark 6.22 (Logarithmic lower bound under the equidistance assumption on defects). In view of Lemma 6.19 we can prove the logarithmic lower bound (6.15) if for instance we suppose a priori that the disposition of defects at an interface is similar to the one depicted in Figure 6.5 (a), that is a pair of pentagonal-heptagonal defects appears at regular intervals of length $d \approx \frac{\varepsilon}{\theta}$. Indeed, for every pair of defects we can consider a ball of radius $\approx \frac{\varepsilon}{2\theta}$ and apply the logarithmic estimate of Lemma 6.19. We obtain

$$\mathscr{E}_\varepsilon = \frac{1}{\varepsilon}\int \mathrm{dist}(\beta, SO(2))^2 \gtrsim \varepsilon \# V_{def} \log\left(\frac{d}{\varepsilon}\right) \approx L\theta \log\left(\frac{1}{\theta}\right)$$

which is exactly what we wanted.

The two main difficulties in extending this result to general configurations are the following:

- Taking into account also disclinations, or equivalently prove that the balance condition (6.14) holds. A hint that this condition should be verified is given by Lemma 6.20: the energy around a disclination is much bigger than the energy around a dislocation, and this suggests that even if some disclinations exist they are close to other defects and, within some radius of order ε, they balance with some other disclination. The main difficulty in making this rigorous is that the estimate of Lemma 6.20 holds in the ideal situation where there are no defects in a certain annulus $B_\rho \setminus B_r$, but in general this could be false and there could be many defects grouped together. That is, the situation could not be so clean with a disclination at the center and then an annulus without any defect. To solve this problem a way could be proving some rigidity theorems inside domains with many holes and cuts, in the spirit of [SZ12], the key being a uniform estimate for the rigidity constants on these domains.

- The second difficulty is that, even if we assume a priori the balance condition (6.14), we still do not know that the dislocations are evenly spaced. As a consequence if we try to apply as above Lemma 6.19 to some annuli surrounding dislocations, we could obtain a very poor lower bound because if two dislocations are close to one another then the ratio between the outer and inner radii of their annuli is close to 1. This means not only that the logarithmic factor will be close to zero, but also that the constant $C(\rho, r)$ of the rigidity theorem are not controlled, because they blow up on thin annuli. Actually the second problem is the most fundamental one: as we explain below, a *ball construction* in the spirit of the one given by Sandier ad Jerrard for Ginzburg-Landau models could be used to circumvent the first problem. In particular, if the rigidity constant didn't blow up on thin annuli, we could really obtain the logarithmic factor.

A similar issue, with the rigidity constants blowing up on thin annuli, has been already faced in [DLGP12]. They considered a core-radius approach to dislocations, and used the linearized energy

$$\mathscr{E}(\mu,\beta) = \int_{\Omega_\varepsilon} |\beta^{sym}|^2 dx + |\mu|(\Omega),$$

where the measure $\mu = \sum_{i=1}^N b_i \delta_{x_i}$ represents dislocations, $\Omega_\varepsilon = \Omega \setminus \bigcup_{i=1}^N B(x_i,\varepsilon)$ is the domain without the core-radius of each dislocation, and where the admissible maps are given by all curl-free matrix-fields $\beta : \Omega_\varepsilon \to M^{2\times 2}$ such that

$$\fint_{\partial B(x_i,\varepsilon)} \beta \cdot \tau = b_i$$

and finally $\beta^{sym} = \frac{1}{2}(\beta + \beta^\top)$ is the symmetric part of β. They circumvent the blowing up of the constants by means of a *discrete ball construction*, where the annuli have a fixed ratio bigger than 1 between outer and inner radius. This construction, however, seems capable of handling at most $|\log \varepsilon|$ dislocations, while we know by Lemma 6.14 that in our case we have $\approx \frac{1}{\varepsilon}$ of them.

The original ball construction

We now explain the *ball construction* taken from Sandier [San98] and Jerrard [Jer99] which was originally used to give lower bounds for the Ginzburg-Landau energy of a map $u : \Omega \to \mathbb{S}^1$ in terms of its degree $\deg(u, \partial\Omega)$ at the boundary.

We briefly explain the original setting. It is an easy computation [San98, Lemma 1.1] to show that given $u \in C^1(B_R \setminus \overline{B}_r, \mathbb{S}^1)$ with $d = \deg(u, \partial B_R)$ we have the following lower bound for the Dirichlet energy:

$$E(B_R \setminus B_r, u) := \frac{1}{2}\int_{B_R \setminus B_r} |\nabla u|^2 \geq \pi d^2 \log\left(\frac{R}{r}\right).$$

Indeed we can rewrite the integral in polar coordinates (s,Θ) to obtain

$$\int_{B_R\setminus B_r} |\nabla u|^2 = \int_r^R ds \int_{\partial B_s} |\nabla u|^2 \geq \int_r^R \int_0^{2\pi} \frac{1}{s^2}|u_\Theta|^2 s ds d\Theta$$

where u_Θ is the derivative of u with respect to the angle Θ. Now we have that

$$\int_0^{2\pi} |u_\Theta| \geq 2\pi d$$

and by Cauchy-Schwartz we conclude

$$E(B_R \setminus B_r, u) \geq \frac{1}{2}\int_r^R \frac{1}{s} ds 2\pi d^2 = \pi d^2 \log\left(\frac{R}{r}\right).$$

Consider now a function $u : \Omega \setminus \omega \to \mathbb{S}^1$ where $\omega \subset \Omega$ is a compact set, and suppose to look for a lower bound for

$$E(\Omega \setminus \omega, u) = \frac{1}{2}\int_{\Omega\setminus\omega} |\nabla u|^2$$

among all u with fixed degree at the boundary $\partial\Omega$. Typically ω is made of a finite number of small balls. The ball construction allows to start from the above estimate on annuli and extend the validity of a similar logarithmic estimate to the whole $\Omega\setminus\omega$ in the following sense: define the **radius** $|\omega|$ as the infimum of $r_1+\ldots+r_m$ over all finite families of balls with radius $r_1,\ldots,r_m$ that cover ω, and suppose ω is at distance at least 2ρ from $\partial\Omega$. Then

$$\frac{1}{2}\int_{\Omega\setminus\omega}|\nabla u|^2 \geq \pi|d|\log\left(\frac{\rho}{|\omega|}\right)$$

where now $d := \deg(u,\partial\Omega)$. The argument starts considering some disjoint balls that cover ω. Then we modify these balls through two phases that alternate: *expansion* and *merging*. We start by letting each ball expand at a specified rate. When two of them touch we perform merging and replace them with a new single ball that contains both; if this new ball touches some other ball we replace these with still another ball that contains both, and we keep going in this way. When we obtain disjoint balls we restart the expansion phase, and so on. At each instant, to each ball we apply the estimate on annuli proved above. The details can be found in [San98].

The ball construction adapted to our case

We now explain how we could prove a similar estimate in our situation. The opportunity of adapting this ball construction to our situation comes directly from the similar logarithmic behaviour of our elastic energy on annuli around dislocations, where the degree d is replaced by the Burgers vector b. In fact one can see the Dirichlet energy (of the symmetrized gradient) as a suitable linearization near the identity of the non-linear energy $\int \mathrm{dist}(I+\nabla u, SO(2))^2$.

We therefore consider an interface with angle mismatch θ and sidelength L, and we suppose that the energy satisfies

$$\mathscr{E}^{el}_{\varepsilon}(B_\rho\setminus B_r) \gtrsim |\vec{b}|^2\varepsilon\log\left(\frac{\rho}{r}\right)$$

whenever there are no defects in $B_\rho\setminus B_r$ and $\rho\geq r\geq\varepsilon$, and where

$$|\vec{b}| = |b(\partial B_r)| = \left|\int_{\partial B_r}\beta\cdot\tau\right| = |\mathrm{Curl}\,\beta(B_r)|\,.$$

The implicit assumption is that the constants involved in the inequality above do not depend on ρ and r. This is false in the case of the rigidity theorem; however we go on and show how, assuming the uniformity on the constants, we could obtain the wanted logarithmic lower bound (6.15). Notice that the vector b depends on the base points which we choose to compute it, but not its modulus $|b|$ which is independent of the choice.

We start by covering the set of defects $V_{def}(G)$ with (closed) balls of radius ε. If two balls of radius r_1, r_2 overlap we can replace them with a single ball of radius at most r_1+r_2 that covers both, and we keep going until the set of balls we end up with is disjoint. The final set is our compact ω.

Then we apply [San98, Proposition, p.385] replacing the degree d with the Burgers vector b, and with the following key observation: if there are no disclinations then the Burgers vector $b(\gamma)$ is additive

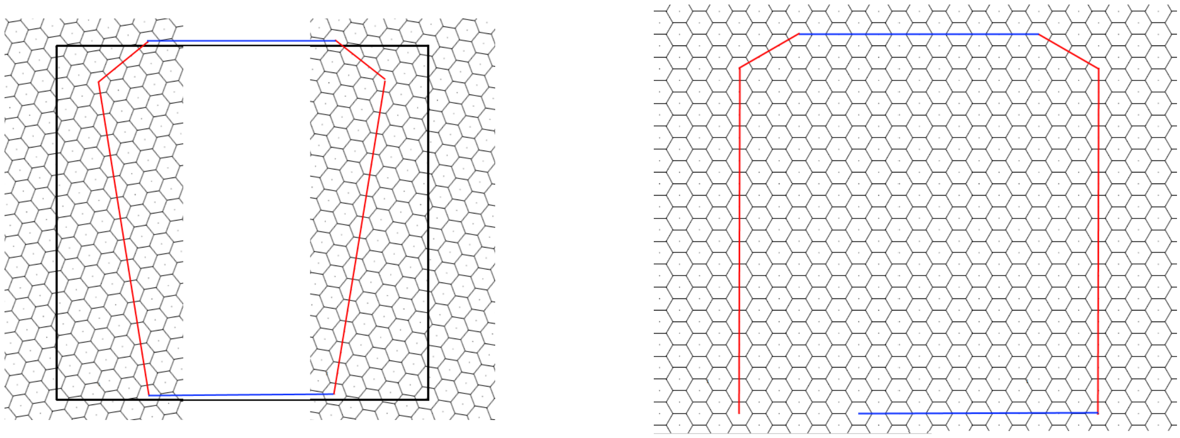


Figure 6.12: The closed path to compute $b(\partial\Omega)$ (on the left) and its lift on the regular lattice (on the right). Instead of triangles here we consider hexagons, but the idea is the same. The two lateral paths, when lifted, will "diverge" in opposite direction. On the other hand the blue paths, being periodic images of each other, when lifted will result in the same path. The net result is a non zero Burgers vector given by the discrepancy shown on the right between the two endpoints of the coloured path. This discrepancy is of order $L\theta$.

with respect to path composition. This is the only property of the degree that is used in [San98]. Observe also that since we are considering a vertical periodicity for the graph and for the set Ω, and since all defects are concentrated on the central stripe by assumption, the distance of ω from $\partial\Omega$ is of order L. In particular we conclude the following:

$$\mathscr{E}_\varepsilon^{el}(\Omega) \geq |b(\partial\Omega)| \log\left(\frac{L}{|\omega|}\right).$$

It is now left to relate the terms $|b(\partial\Omega)|$ and $|\omega|$ to our parameters L, θ, ε.

Let us first compute $b(\partial\Omega)$. We refer to figure 6.12. We compute it in this way: fix a "horizontal" path η that starts from a vertex v_l in the leftmost regular zone and ends at a vertex v_r in the rightmost regular zone. Choose then a "vertical" regular path γ that connects v_r to its periodic copy, and consider the symmetrically defined path γ' that connects the copy of v_l to v_l. Then we compute the Burgers vector $b(\partial\Omega) = b(\eta * \gamma * \overline{\eta} * \gamma')$ where we recall that $\overline{\eta}$ is the path η travelled in opposite direction. No matter what is the lift $L\eta$, we will have the situation pictured in Figure 6.12: the lifts $L\gamma$ and $L\gamma'$ will "diverge" due to the symmetry of the initial configuration, while the lifts $L\eta$ and $L\overline{\eta}$ will be translated copies one of the other. The Burgers vector is therefore at least of order

$$|b(\partial\Omega)| \approx L \tan\theta \approx L\theta.$$

Regarding ω, by definition we have $|\omega| \leq \varepsilon \# V_{def}(G)$. Suppose for a moment to know that the following upper bound on the energy holds:

$$\mathscr{E}_\varepsilon \lesssim L\theta^\alpha \tag{UB_α}$$

for some $\alpha > 0$. Then we trivially have

$$|\omega| \leq \varepsilon \# V_{def}(G) \lesssim \mathscr{E}_\varepsilon^{def} \leq \mathscr{E}_\varepsilon \lesssim L\theta^\alpha$$

and therefore

$$\log\left(\frac{L}{|\omega|}\right) \gtrsim \log\left(\frac{1}{\theta^\alpha}\right) \approx \log\left(\frac{1}{\theta}\right)$$

and we conclude that

$$\mathscr{E}_\varepsilon^{el}(\Omega) \gtrsim L\theta|\log\theta|$$

as we wanted. We now want to show that we can obtain the same conclusion even without the assumption (UB_α). Let us state this as a Lemma:

Lemma 6.23. *Consider the setting above and suppose that the estimate*

$$\mathscr{E}_\varepsilon^{el} \geq cL\theta\log\left(\frac{L}{|\omega|}\right)$$

holds for a certain constant $0 < c < 1$ *and* θ *sufficiently small. Then*

$$\mathscr{E}_\varepsilon^{el} \geq \frac{c}{2}L\theta|\log\theta|$$

for θ *sufficiently small.*

Proof. Suppose this is not the case. Then

$$|\omega| \leq \varepsilon \# V_{def}(G) \lesssim \mathscr{E}_\varepsilon^{def} \leq \mathscr{E}_\varepsilon \leq \frac{c}{2}L\theta|\log\theta|$$

and therefore

$$\mathscr{E}_\varepsilon^{el} \geq cL\theta\log\left(\frac{1}{\frac{c}{2}\theta|\log\theta|}\right) \geq cL\theta\log\left(\frac{1}{\theta^{1/2}}\right) = \frac{c}{2}L\theta|\log\theta|$$

for sufficiently small θ, and we conclude. □

We have thus obtained:

Theorem 6.24 (Conditional energy lower bound). *Suppose the balance condition* (6.14) *holds at an interface inside a domain of side L, angle mismatch* θ *and parameter* ε*, with vertical periodicity. Suppose that a logarithmic estimate* (6.16) *holds around any dislocation with constants* $C(\rho, r)$ *uniformly bounded. Then*

$$\mathscr{E}_{el} \gtrsim L\theta|\log\theta|.$$

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