Università di Trento

DIPARTIMENTO DI MATEMATICA
Doctoral Programme in Mathematics - Cycle XXXVII

Thesis for the Degree of Philosophiae Doctor

The Q-closeness technique: an application to isoperimetric inequalities in 2-d lattices and to the Faber-Krahn inequality

Candidate:
Gabriele Morselli

Supervisor:
Prof. Gian Paolo Leonardi

Academic Year 2024-2025

Contents

Introduction

Variational problems have been known since antiquity. A famous example is the legend of Queen Dido, who was challenged to enclose the largest possible area using the skin of a single ox: she cut the skin into thin strips and arranged them into a semicircular arc along the sea. Despite she effectively exploited the optimal configuration, this property, known as the isoperimetric inequality, was rigorously proved in the very general framework of finite perimeter sets in the second half of the 20^{th} century, in the celebrated works of Ennio De Giorgi [19], [18], [20]. More recently, the isoperimetric inequality was also proven in the anisotropic setting, a generalization of the classical model in which the notion of perimeter is weighted by a direction-dependent function. In this framework, the Euclidean ball is no longer the optimal shape and instead the minimizer is the Wulff shape, a modification of the Euclidean ball through the given weight function.
Another famous variational problem, related to the optimal shape enclosing a given area, involves the frequency of vibrating membranes, which was formulated by Lord Rayleigh in his work "*The Theory of Sound*" (1877). In this work, he proved that, for a given volume, the shape of a domain influences the frequency of its natural vibrations, and he conjectured that, among all drums with the same area and tension, the circular drum produces the lowest frequency. His intuition was independently proven by Faber and Krahn in the first decades of the past century in two dimensions (respectively in [23] and [35]), and later their proof was extended to higher dimensions.
Subsequent studies have focused on the stability of these results. While both the isoperimetric and Faber–Krahn inequalities identify optimal shapes, they do not quantify how far a given set deviates from optimality in terms of a geometric distance. Inequalities that provide such estimates are known as quantitative inequalities. Quantitative isoperimetric inequalities (see, for instance, [32] and [31]) were also named by Osserman ([39]) "Bonnesen-type inequalities", in honour of the Danish mathematician who studied them in dimension two in the early 20^{th} century. A cornerstone contribution in the anisotropic setting is the work of Figalli, Maggi, and Pratelli [24]: by using

the Fraenkel asymmetry, a geometric error function commonly used in the quantitative isoperimetric inequality, they were able to provide the quantitative anisotropic inequality with the sharp exponent. Similarly, quantitative Faber-Krahn inequalities were especially formulated from the early 1990s by several authors (see, for instance, [33], [38] and [26]). In particular, in [9], Brasco, De Philippis and Velichkov established a quantitative inequality with the sharp exponent, again measured in terms of the Fraenkel asymmetry.

The analysis of variational problems has historically been carried out in continuous spaces; however, the recent growing interest in material science problems brought efforts to extend these investigations to the setting of discrete configurations of particles. In fact, on discrete arrangements of points, the analysis may seem simpler and more intuitive, but many classical results no longer apply due to the lack of the richer geometric structure found in continuous spaces. Consequently, the discrete setting provides an interesting framework not only for discovering new phenomena but also for investigating whether classical theorems from the continuous setting remain valid under suitable adaptations. Among the various discrete configurations, lattices are particularly noteworthy. They frequently emerge in the study of the crystallization problem, which concerns the geometric arrangement of particles in a uniform material, arises naturally in this context and is closely tied to atomic interactions (see [6] for a review on this topic). From a physical perspective, crystallization can be understood as the study of atomic configurations at extremely low temperatures, where systems tend to settle into minimal energy states. In two dimensions, these configurations often correspond to the vertices of regular tessellations of the plane (see [43], [21], [5]), while in three dimensions, we find several distinct lattice structures (for example, see the two cases discussed in [12]).

Since classical methods and strategies are often ineffective in discrete analysis, one possible approach is to construct a "bridge" between discrete objects and their continuous counterparts, allowing known techniques from the continuous setting to be applied. The Q-closeness technique, developed by Cicalese and Leonardi in [13], is based on this idea. Their method involves associating continuous domains to discrete arrangements of point by constructing a suitable map ζ that ensures controllable approximation errors on the considered functionals. In [13], they applied the Q-closeness technique using three slightly different constructions: for the d-dimensional square lattice and the honeycomb lattice, the map ζ coincides with the union of the Voronoi cells of the given configuration, while, for the triangular lattice, ζ is the superlevel set of the sum of affine local functions centred at the points

of the given configuration. In view of extending the technique to the more challenging stability problems in dimension 3 and higher, we have investigated an alternative and more "canonical" construction of the map ζ, which works for all the three considered planar lattices. In Chapter 2, we present the results obtained by following this idea for two-dimensional lattices and we also address some issues related to extending this construction to higher dimensions, which led us to the trivial quantitative inequality on the face-centred cubic lattice briefly reported in the Appendix.
The Q-closeness technique can also be applied to other discrete variational inequalities. Among them, we aim at extending the quantitative Faber–Krahn inequality from [9] to the discrete setting. This study was further motivated by the fact that, to the best of our knowledge, only partial results had previously been obtained concerning this kind of problems in discrete configurations. An early contribution appears in [40], where it was shown that minimizers are rigid up to automorphisms. Furthermore, [42] proves that, under a volume constraint, the minimizers of the discrete first eigenvalue functional λ_N converge to the Euclidean ball. However, these results do not provide quantitative estimates of maximal fluctuations, which we are able to obtain by exploiting the Q-closeness technique. The results of this joint work are presented in Chapter 3.

Chapter 1

Preliminaries

In this chapter, we introduce the key notations, definitions, and fundamental results that will be used consistently throughout the thesis. We begin by establishing standard notations and conventions to ensure clarity and coherence in the subsequent discussion. Following this, we provide a brief review of essential topics in classic and modern Calculus of Variations, highlighting fundamental theorems that form the theoretical foundation and motivate the research presented in this work.

1.1 General Notations

We introduce some useful notations that will be used throughout all the following chapters and sections. While many of these symbols are standard in the mathematical literature, we include them here to avoid potential misunderstandings. In particular, we refer to [22], [4] and [36].

- we will denote by $e_1, \dots, e_d$ the unitary vectors of the canonical orthonormal basis of $\mathbb{R}^d$
- $\mathcal{M}(\mathbb{R}^d) = \big\{\text{measurable sets in } \mathbb{R}^d\big\}$
- given $\Omega \subset \mathbb{R}^d$, we will write
  - $\partial\Omega$ will denote the boundary of Ω
  - $\Omega_{|E|}$ to denote that $|\Omega_{|E|}| = |E|$ for a given set $E \subset \mathbb{R}^d$
  - $\Omega(x) = \{y \in \mathbb{R}^d : \ y - x \in \Omega\}$

- B_r will denote d-dimensional Euclidean ball of radius $r > 0$; moreover, ω_d we will denote the value of B_1 in dimension d:

$$\omega_d = \frac{\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2}+1)} \quad \text{with} \quad \Gamma\left(\frac{d}{2}+1\right) = \begin{cases} (\frac{d}{2})! & \text{if } d \text{ is even} \\ \pi^{\frac{1}{2}}(\frac{d}{2})(\frac{d}{2}-1)\dots\frac{1}{2} & \text{if } d \text{ is odd} \end{cases}$$

- $\overline{x,y}$ denotes the segment having $x, y \in \mathbb{R}^d$ as extremal points

- χ_E will denote the characteristic function of the set $E \subset \mathbb{R}^d$, that is

$$\chi_E(x) = \begin{cases} 1 & \text{if } x \in E \\ 0 & \text{else} \end{cases}$$

- with a commonly used abuse of notation, we will denote with $|\cdot|$ either the absolute value or the Lebesgue measure $\mathscr{L}^d(\cdot)$ of a set, depending on the context

- $\mathscr{H}^d(\cdot)$ will denote the d-dimensional Hausdorff measure

- for $p \in [1, +\infty]$, we denote with

$$L^p(\Omega) = \left\{ f\colon \Omega \to \overline{\mathbb{R}} :\ f \text{ is measurable } , \|f\|_{L^p(\Omega)} < +\infty \right\} ,$$

where

$$\|f\|_{L^p(\Omega)} = \begin{cases} \left(\int_\Omega |f|^p \,\mathrm{d}x\right)^{\frac{1}{p}} & \text{if } p < +\infty \\ \inf\left\{c > 0 :\ |f| \le c \text{ a.e. on } \Omega\right\} & \text{if } p = +\infty\,. \end{cases} \tag{1.1.1}$$

- similarly, for $p \in [1, +\infty]$,

$$W^{1,p}(\Omega) = \left\{ f\colon \Omega \to \overline{\mathbb{R}} :\ f \text{ is measurable and } f, Df \in L^p(\Omega) \right\}$$

- if $v = (v_1, \dots, v_d)$ is a vector in $\mathbb{R}^d$, then, similarly to (1.1.1), we denote its l^p norm as

$$\|v\|_p = \begin{cases} \left(\sum_{k=1}^d |v_k|^p\right)^{\frac{1}{p}} & \text{if } p < +\infty \\ \max\left\{|v_k| :\ k = 1, \dots, d\right\} & \text{if } p = +\infty\,. \end{cases}$$

1.2 Perimeter

The concept of perimeter plays a central role in many areas of mathematics, from geometric measure theory to the calculus of variations, and is deeply connected to the study of minimal surfaces and optimal shapes. Despite its intuitive meaning, a rigorous definition of perimeter was only developed in the 20th century. In modern variational analysis, the perimeter of a measurable set is defined via the theory of functions of bounded variation. Here we will briefly report some major definitions and properties; we refer to [4], [22] and [36] for further details.

Definition 1.2.1. Let $f \in L^1(\Omega)$. We say that f has **bounded variation** on Ω if

$$\sup \left\{ \int_\Omega f \cdot \mathrm{div}(\varphi)\, \mathrm{d}x : \ \varphi \in \mathcal{C}^1_C(\Omega, \mathbb{R}^d),\ \sup_{\mathbb{R}^d} |\varphi| \leq 1 \right\} < +\infty\,, \tag{1.2.1}$$

where $\mathrm{div}(\varphi)$ denotes the divergence of φ. Then, we write $BV(\Omega)$ to denote the space of L^1 functions that satisfy (1.2.1).

By observing that the boundary of a set E can be interpreted as the total variation of the characteristic function χ_E on the boundary, Definition 1.2.1 can be used to elegantly define the notion of perimeter. Hence we have:

Definition 1.2.2. Let $E \in \mathcal{M}(\mathbb{R}^d)$. We say that E has **finite perimeter** in $\Omega \subset \mathbb{R}^d$ if

$$\chi_E \in BV(\Omega)\,.$$

Remark 1.2.3. In the following, we adopt a different notation for the (finite) perimeter of a set. This notation is widely used in the mathematical literature and follows directly from Definition 1.2.2 and equation (1.2.1): indeed, we obtain that the **relative perimeter** of a given set $E \subset \mathcal{M}(\mathbb{R}^d)$ within a fixed set $\Omega \subset \mathbb{R}^d$ is

$$P(E, \Omega) := \sup \left\{ \int_E \mathrm{div}\left(\varphi(x)\right)\, \mathrm{d}x : \ \varphi \in \mathcal{C}^1_C(\Omega, \mathbb{R}^d),\ \sup_{\mathbb{R}^d} |\varphi| \leq 1 \right\}\,. \tag{1.2.2}$$

In particular, if $\Omega = \mathbb{R}^d$, then we set $P(E) := P(E, \mathbb{R}^d)$, which is also called the **perimeter** of E in $\mathbb{R}^d$. ♠

1.2.1 A brief summary of some properties of $P(E,\Omega)$

As mentioned in the second part of Maggi's book [36], the perimeter can also be characterized from a measure-theoretic point of view, by the total variation of a vector-valued Radon measure thanks to the Riesz Representation Theorem (see, for instance, [36, Theorem 4.7]):

Proposition 1.2.4. *Let $E \in \mathcal{M}(\mathbb{R}^d)$ and let $\Omega \subset \mathbb{R}^d$. Then, E is a set of locally finite perimeter if and only if there exists a $\mathbb{R}^d$-valued Radon measure μ_E on $\mathbb{R}^d$ such that*

$$\int_E \operatorname{div}(\varphi)\,\mathrm{d}x = \int_{\mathbb{R}^d} \varphi\,\mathrm{d}\mu_E \qquad \forall \varphi \in C^1_C(\mathbb{R}^d)\,.$$

Moreover, E is a set of finite perimeter if and only if $|\mu_E|(\mathbb{R}^d) < +\infty$, where

$$|\mu_E|(F) = \sup\left\{ \sum_{h=1}^{+\infty} \big|\mu_E(F_h)\big| \,:\, (F_h)_h \text{ are pairwise disjoint, } F = \bigcup_{h=1}^{+\infty} F_h \right\}.$$

Thus, one can prove properties of the perimeter by exploiting the properties of Radon measures. We collect some of the most important ones in the following Proposition.

Proposition 1.2.5. *Let $E \in \mathcal{M}(\mathbb{R}^d)$ and let $\Omega \subset \mathbb{R}^d$. Then, the following hold:*

(i) $E \mapsto P(E,\Omega)$ *is lower semi-continuous w.r.t. the local convergence of measure in* Ω.

(ii) $P(E,\Omega) = P(F,\Omega)$ *whenever* $F \in \mathcal{M}(\mathbb{R}^d)$ *such that* $\big|\Omega \cap (E \triangle F)\big| = 0$.

(iii) $P(E,\Omega) = P\left(\mathbb{R}^d \setminus E, \Omega\right)$.

(iv) *For any* $F \in \mathcal{M}(\mathbb{R}^d)$,

$$P(E \cap F, \Omega) + P(E \cup F, \Omega) \le P(E,\Omega) + P(F,\Omega)\,. \tag{1.2.3}$$

(v) *If E has C^1-class boundary, then* $P(E,\Omega) = \mathcal{H}^{d-1}(\partial E \cap \Omega)$.

Unfortunately, (1.2.2) is a little hard to use as an operative definition. Moreover, as stated in point (v) of Proposition 1.2.5, it provides limited information about the geometric structure of the boundary when the set lacks smoothness. To overcome these limitations, the concepts of the reduced boundary and outer unit normal were introduced. These notions play a crucial role in the proof of De Giorgi's celebrated Structure Theorem, as developed in [19], [18], and [20]. As before, we recall these results, following the arguments presented in the second part of [36].

Definition 1.2.6. Given $E \in \mathcal{M}(\mathbb{R}^d)$ of locally finite perimeter and given $|\mu_E|$, the Radon measure from Proposition 1.2.4, we call **reduced boundary** of E the set

$$\partial^* E = \left\{ x \in \partial E : \exists \lim_{r \to 0^+} \frac{\mu_E \big(B_r(x)\big)}{|\mu_E| \big(B_r(x)\big)} \text{ and belongs to } \mathbb{S}^{d-1} \right\} .$$

Then, we call the **outer unit normal** to E the function $\nu_E \colon \partial^* E \to \mathbb{S}^{d-1}$ such that

$$\nu_E(x) = \lim_{r \to 0^+} \frac{\mu_E \big(B_r(x)\big)}{|\mu_E| \big(B_r(x)\big)} .$$

Remark 1.2.7. The reduced boundary is well-posed definition and behaves well with respect to the perimeter properties of Proposition 1.2.5. Indeed, it is possible to show that, for $E \in \mathcal{M}(\mathbb{R}^d)$, the follwings hold:

(i) if E^t is the set of the point of density t, that is

$$E^t = \left\{ x \in \mathbb{R}^d : \lim_{r \to 0^+} \frac{|E \cap B_r(x)|}{\omega_d r^d} = t \right\} ,$$

then $\partial^* E \subset E^{\frac{1}{2}}$,

(ii) if E is such that $P(E) < +\infty$ and $|E \triangle F| = 0$, then $\partial^* E = \partial^* F$,

(iii) up to a measure zero set, $\overline{\partial^* E} = \partial E$; moreover, if E has C^1 boundary, then $\partial^* E = \partial E$.

♠

Now we can state De Giorgi's Structure Theorem (for more details see, for instance, [36][Theorem 15.9]).

Theorem 1.2.8. *Let $E \in \mathcal{M}(\mathbb{R}^d)$ be set of locally finite perimeter in $\mathbb{R}^d$ and let $x \in \partial^* E$. Then,*

$$\frac{E - x}{r} \xrightarrow[r \to 0^+]{} \left\{ y \in \mathbb{R}^d : \nu_E(x) \cdot (y - x) < 0 \right\} .$$

Moreover, the measure μ_E in Proposition 1.2.4 satisfies

$$\mu_E = \nu_E \mathcal{H}^{d-1} \llcorner \partial^* E$$

and it holds true that

$$P(E) = |\mu_E|(\mathbb{R}^d) = \mathcal{H}^{d-1}(\partial^* E)\,.$$

Remark 1.2.9. Operatively, from Theorem 1.2.8 we obtain the following formula for the generalized Gauss-Green formula:

$$\int_E \nabla\varphi(x)\,\mathrm{d}x \int_{\partial^* E} \varphi(x)\cdot\nu_E(x)\;\mathrm{d}\mathcal{H}^{d-1}(x) \qquad \forall\varphi\in C^1_C(\mathbb{R}^d)\,.$$

♣

1.2.2 The Isoperimetric Inequality

The isoperimetric inequality states that, among all sets in $\mathbb{R}^d$ having fixed volume, the set with the least perimeter is the d-dimensional ball. Although this property has been known since antiquity, the first mathematically rigorous proof was made in the past century. The proof, in the full generality of finite perimeter sets, is due to Ennio De Giorgi, in his classical paper [20] and can be formulated as follows:

Theorem 1.2.10 (Isoperimetric Inequality)**.** *Let $E \in \mathcal{M}(\mathbb{R}^d)$ be a set with $|E| < +\infty$. Then, it holds that*

$$d\omega_d^{\frac{1}{d}}|E|^{\frac{d-1}{d}} \leq P(E) \tag{1.2.4}$$

Moreover, the equality holds if and only if $\left|E \triangle B_{|E|}(x)\right| = 0$ for some $x \in \mathbb{R}^d$.

There are several different proofs of Theorem 1.2.10. The classical one, also presented in [36], is based on the non-increasing property of the perimeter under Steiner symmetrization (i.e., the symmetrization of a given set with respect to a hyperplane) and the invariance of the resulting set under reflections on hyperplanes passing through the origin. However, (1.2.4) can also be proved using alternative strategies: for instance, via the Brunn–Minkowski inequality (we refer to [28]), via the Alexandroff–Bakelman–Pucci technique (as shown in [10]) or through mass transportation involving maps such as the Knothe or Brenier map, as discussed in [24].

1.2.3 The Quantitative Isoperimetric Inequality

In order to refine the result of Theorem 1.2.10, we introduce two functions. The first one measures the deviation of the perimeter from the minimum one:

Definition 1.2.11. Let $E \in \mathcal{M}(\mathbb{R}^d)$ be such that $0 < |E| < +\infty$. We call the **isoperimetric deficit** of E

$$\delta(E) = \frac{P(E) - P(B_{|E|})}{P(B_{|E|})}\,. \tag{1.2.5}$$

Remark 1.2.12. It is direct consequence of Theorem 1.2.10 that $\delta(E) \geq 0$ and that the equality holds if and only if $|E \triangle B_{|E|}(x)| = 0$ for some $x \in \mathbb{R}^d$. ♠

We introduce a second function that captures some geometric property of the set E to compare with $\delta(E)$. In [25], Fuglede used the Hausdorff distance between sets in his proof of a quantitative inequality for convex sets, but this quantity could not be controlled by the isoperimetric deficit a priori. Among other possible choices, the Fraenkel asymmetry is probably the most commonly used in the literature and also one of the most general quantities; it was first considered by Hall, Hayman, and Weitsmann in [32].

Definition 1.2.13. Let $E \in \mathcal{M}(\mathbb{R}^d)$ be such that $0 < |E| < +\infty$. We call the **Fraenkel asymmetry** of E

$$\alpha(E) = \inf_{x \in \mathbb{R}^d} \left\{ \frac{|E \triangle B_{|E|}(x)|}{|E|} \right\}.$$

Remark 1.2.14. By using the isoperimetric deficit and the Fraenkel asymmetry, Hall proved in [31] that there exists a purely dimensional constant C_d such that

$$\alpha(E) \leq C_d \sqrt[4]{\delta(E)}\,.$$

However, even if the estimates in [31] were sharp, Hall conjectured that the exponent $\frac{1}{4}$ wasn't optimal and that it should be $\frac{1}{2}$. ♠

The quantitative isoperimetric inequality with a sharp exponent was lately proved by Fusco, Maggi and Pratelli in [27] using symmetrization techniques:

Theorem 1.2.15. *Let* $d \geq 2$*. There exists a constant* $C_d = C(d) > 0$ *such that, for every set* $E \subset \mathbb{R}^d$ *with* $0 < |E| < +\infty$*, it holds*

$$\alpha(E) \leq C_d \sqrt{\delta(E)}\,.$$

1.2.4 The Anisotropic framework

While classical perimeter theory assumes isotropy, many variational problems connected to problem modelling arise in anisotropic settings, in which different directions are privileged by a "weight" function $\psi\colon \mathbb{R}^d \to \mathbb{R}$. This function encodes the geometry of the underlying space and this motivates the introduction of the anisotropic perimeter, along with the associated optimal shapes W_ψ, called Wulff shapes, first introduced by the German scientist Georg Wulff in [44]. These objects provide a natural generalization of the classical perimeter functional and of the classical isoperimetric theory to anisotropic contexts, yielding corresponding analogues of the isoperimetric and quantitative isoperimetric inequalities.

Definition 1.2.16. We say that a function $\psi\colon \mathbb{R}^d \to \mathbb{R}$ is a **gauge** if it is non-negative, positively homogeneous of degree one and convex.

Then, fixed a gauge ψ as in Definition 1.2.16, we can define the Wulff shape associated with ψ, the anisotropic perimeter and the corresponding anisotropic isoperimetric inequalities.

Definition 1.2.17. Given a gauge ψ, then we call **Wulff shape** associated to ψ the set

$$W_\psi = \left\{ x \in \mathbb{R}^d : \ x \cdot \nu < \psi(\nu) \text{ for all } \nu \in \mathbb{S}^{d-1} \right\}. \tag{1.2.6}$$

Remark 1.2.18. By construction, W_ψ is an open, bounded and convex set that contains the origin. It is also possible to prove the converse: indeed, given a set having the same properties of W_ψ, it is possible to define a gauge ψ that satisfies the hypothesis given in Definition 1.2.17.
Moreover, we can consider the Euclidean framework as a particular case of the anisotropic one: indeed, it is sufficient to choose $\psi\colon \mathbb{R}^d \to [0, +\infty[$ such that

$$\psi(x) = \|x\|_{L^2(\mathbb{R}^d)} \qquad \forall x \in \mathbb{R}^d\,.$$

and from (1.2.6) it also follows that$W_\psi = B_1$. ♠

For sake of simplicity, in the following we will only write W and we will omit the subscript when the context does not lead to incomprehensions.
Hence, given the gauge ψ (or, equivalently, a Wulff shape W), we can also define the anisotropic perimeter and the anisotropic isoperimetric inequality, analogously to what we did in Definition 1.2.2 and Theorem 1.2.10 in the Euclidean case:

Definition 1.2.19. Given $E \in \mathcal{M}(\mathbb{R}^d)$, we define the **anisotropic perimeter** as

$$P_W(E) = \int_{\partial^* E} \psi\left(\nu_E(x)\right) \mathrm{d}\mathcal{H}^{d-1}(x) \tag{1.2.7}$$

where we recall that $\partial^* E$ denotes the reduced boundary of E and ν_E denotes the outer unit normal.

Theorem 1.2.20. *Let $d \geq 2$ and let $W \subset \mathbb{R}^d$ be a Wulff shape. Then, for every set $E \subset \mathbb{R}^d$ with $0 < |E| < +\infty$ and finite perimeter, it holds*

$$d|W|^{\frac{1}{d}}|E|^{\frac{d-1}{d}} \leq P_W(E)\,. \tag{1.2.8}$$

Remark 1.2.21. Given a Wullf shape W, we can extend both Definition 1.2.11 and Definition 1.2.13, since they depend uniquely on the Euclidean counterparts of the quantities in (1.2.6) and Definition 1.2.19. Given $E \subset \mathbb{R}^d$ with $0 < |E| < +\infty$, we can define:

- the anisotropic isoperimetric deficit of E as

$$\delta_W(E) = \frac{P_W(E) - P_W(W_{|E|})}{P_W(W_{|E|})}\,,$$

- the anisotropic asymmetry of E as

$$\alpha_W(E) = \inf_{x \in \mathbb{R}^d} \left\{ \frac{|E \triangle W_{|E|}(x)|}{|E|} \right\}\,.$$

♠

In the end, it is also possible to state and prove a quantitative anisotropic isoperimetric inequality, as shown by Figalli, Maggi and Pratelli in their celebrated article [24]. Their proof relies on the quantitative study of the

Brenier transportation map between the given set and the reference Wulff shape, but here we do not go deeper into the proof and we refer to the original paper for further details.

Theorem 1.2.22. *Let $d \geq 2$ and let $W \subset \mathbb{R}^d$ be a Wulff shape. Then, there exists a constant $C_d = C(d) > 0$ such that, for every set $E \subset \mathbb{R}^d$ with $0 < |E| < +\infty$ and finite perimeter, it holds*

$$\alpha_W(E) \leq C_d \sqrt{\delta_W(E)} \, .$$

1.3 Lattices

Lattices arise naturally in a variety of mathematical contexts, including calculus of variations, geometry and algebraic group theory. From an analytical point of view, their introduction is motivated by the study of some energy functional associated to atomic models coming from physics or material science problems. This research topic has become of great interest during the last decades and brought to many results: for instance, we cite [43], [5], [37], [11] [12].
In this Section, we provide a short introduction to lattices that present some periodicities and regularities, rather than treating general ones. In particular, we are interested in lattices which are (partially) ordered infinite set of points embedded in the Euclidean d-dimensional space, where each element is obtained by the coordinate-wise addition or subtraction of two other points of the set. Namely, we refer to lattices $\mathscr{L} \subset \mathbb{R}^d$ for which there exists a periodicity cell $T_{\mathscr{L}} \in \mathbb{R}^d$ such that

$$\mathscr{L} + T_{\mathscr{L}} = \mathscr{L} \, .$$

As in the previous cited articles, this is motivated by the choice of the Heitmann-Radin potential on $\mathscr{L}$ (we refer to the original paper [34] for more details), which implies that all the elements of the lattice are isolated and separated by a minimum distance from the other ones.
In particular, with some abuse of terminology, in the following we will refer to Bravais lattices, named after the French physicist who studied crystallography in the 19^{th} century.

Definition 1.3.1. We say that a d-dimensional lattice $\mathscr{L}$ is a **Bravais lattice** if there exists d non-null linearly independent vectors $v_1, \ldots, v_d$ such that $\|v_i\|_2 = \|v_j\|_2$ for any $i, j \in \{1, \ldots, d\}$ and

$$\mathcal{L} = span_{\mathbb{Z}} \{v_1, \ldots, v_d\} .$$

Moreover, we say that a d-dimensional lattice $\mathcal{L}$ is a superposition of Bravais lattices if there exists a non-null vector $\tau \in \mathbb{R}^d$ such that

$$\mathcal{L} = span_{\mathbb{Z}} \{v_1, \ldots, v_d\} + \big(\tau + span_{\mathbb{Z}} \{v_1, \ldots, v_d\}\big) .$$

Given a lattice $\mathcal{L}$ as in the previous definition and $p \in \mathcal{L}$, we can define the set of lattice points that are neighbours of p via the Voronoi cell of p (see also [15]):

Definition 1.3.2. Given a lattice $\mathcal{L} \subset \mathbb{R}^d$, the **Voronoi cell** of $p \in \mathcal{L}$ is defined as

$$V(p) = \Big\{ y \in \mathbb{R}^d : \ |p - y| \leq |q - y| \ \forall q \in \mathcal{L} \setminus \{p\} \Big\} .$$

Definition 1.3.3. Given a lattice $\mathcal{L}$ as in Definition 1.3.1 and a point $p \in \mathcal{L}$, we say that

- $q \in \mathcal{L} \setminus \{p\}$ is a **first-neighbour** of p if

  $$\mathcal{H}^{d-1} \big(V(p) \cap V(q)\big) > 0$$

  and we denote the set of first-neighbouring points of p as

  $$\mathcal{N}(p) = \{q \in \mathcal{L} : \ q \text{ is a first-neighbour to } p\} .$$

- $z \in \mathcal{L} \setminus \{p\}$ is a **second-neighbour** of p if $z \notin \mathcal{N}(p)$ and

  $$\exists q \in \mathcal{L} \setminus \{p, z\} : \ q \in \mathcal{N}(p) \ \text{ and } \ q \in \mathcal{N}(z) .$$

Remark 1.3.4. For a generic lattice $\mathcal{L}$ and $p \in \mathcal{L}$, we can not expect the distance between p and $q \in \mathcal{N}(p)$ to be constant: for instance, in dimension 2, we may consider the Bravais lattice

$$\mathcal{L} = span_{\mathbb{Z}} \left\{ (1, 0), \left(\frac{\sqrt{3}}{2}, \frac{1}{2} \right) \right\}$$

or the superposition of Bravais lattices given by

$$\mathcal{L} = span_{\mathbb{Z}} \left\{(1,0),(0,1)\right\} + \left(\left(0, \frac{1}{2}\right) + span_{\mathbb{Z}} \left\{(1,0),(0,1)\right\}\right) .$$

♣

Remark 1.3.4 motivates the following definition:

Definition 1.3.5. Given a lattice $\mathcal{L}$ as in Definition 1.3.1, we say that $\mathcal{L}$ has **uniform lattice spacing** if there exists $c > 0$ such that

$$\mathcal{H}^1(\overline{p,q}) = c \qquad \forall p \in \mathcal{L} \quad \forall q \in \mathcal{N}(p) .$$

Remark 1.3.6. If a lattice $\mathcal{L}$ as in Definition 1.3.1 has uniform lattice spacing, then the set of first-neighbouring points of p coincides with

$$\mathcal{N}(p) = \left\{q \in \mathcal{L} : \mathcal{H}^1(\overline{p,q}) \leq \mathcal{H}^1(\overline{p,z}) \quad \forall z \in \mathcal{L} \setminus \{p,q\}\right\} .$$

♣

Remark 1.3.7. If we consider a lattice $\mathcal{L} \subset \mathbb{R}^d$ as in Definition 1.3.1, then it is easy to verify that each element $p \in \mathcal{L}$ has the same amount of neighbouring points: namely

$$\#\mathcal{N}(p) = k(\mathcal{L}) > 0 \qquad \forall p \in \mathcal{L} .$$

In mathematical literature, this value is also called the kissing number of the lattice. It is known that the highest possible kissing number is 6 in dimension 2 (achieved in the triangular lattice) and 12 in dimension 3 (achieved either in the face-centered cubic lattice or in the HCP lattice). However, determining the maximal kissing number in higher dimensions remains an open problem.

♣

Given a lattice $\mathcal{L} \subset \mathbb{R}^d$ as in Definition 1.3.1, we can associate to it an interaction potential that depends only on the geometric displacement of the elements of $\mathcal{L}$: we choose $V : [0,+\infty[\to \overline{\mathbb{R}}$ such that

$$V(r) := V\left(|p-q|\right) \qquad \forall p,q \in \mathcal{L} .$$

Fixed $\mathscr{L}$ and its potential V, if we set

$$\mathcal{X}_N := \{Y \subset \mathscr{L} : \#Y = N\}$$

(for sake of simplicity, we do not explicit the dependence of $\mathcal{X}_N$ on $\mathscr{L}$, since this will be always clear from the context) and we consider $X \in \mathcal{X}_N$, then we can associate an energy function to X based on the potential V:

$$E_N(X) = \frac{1}{2} \sum_{\substack{p,q \in X \\ p \neq q}} V\left(|p-q|\right) .$$

In general, studying the behaviour of E_N with respect to the cardinality N or other competitors $Y \in \mathcal{X}_N$ is a very hard problem and most of the available results involve specific functions V called Lennard-Jones potentials. In particular, we focus on the Heitmann-Radin potential V_{HR} (see also [34]), that, in some sense, can be seen as the limit case of the Lennard-Jones potential. Hence, from now on, we consider $V_{HR} \colon [0, +\infty[\to \overline{\mathbb{R}}$ such that

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

Remark 1.3.8. Since the Heitmann-Radin potential takes into account only the behaviour among nearest neighbouring particles, it simplifies, in some sense, the structure of the configuration: the particles are treated as rigid balls that cannot overlap and whose interaction is minimum only when they are tangent to each other. Thus, minimizing the energy corresponds to maximizing the number of tangent "Heitmann–Radin d-dimensional spheres", that corresponds to $\#\mathcal{N}(p)$ in our case. Then, if $\mathscr{L}$ is a lattice as in Definition 1.3.1 and $X \in \mathcal{X}_N$, the energy configuration $E_N(X)$ is

$$E_N(X) = -\frac{1}{2} \sum_{p \in X} \#\left(\mathcal{N}(p) \cap X\right) . \tag{1.3.1}$$

♠

In general, one may consider potentials with weighted interaction or which consider energies between non-neighbouring points, but we are not interested in those mathematical models and we focus only on nearest-neighbours interactions.

1.3.1 The discrete perimeter

If we have a periodic lattice that is either a Bravais lattice or a superposition of Bravais lattices, then Remark 1.3.8 provides a simple formula for computing the energy of $X \in \mathcal{X}_N$. However, since X contains only a finite number of elements, some of its point must have neighbours in $\mathcal{L} \setminus X$. This motivates the extension of the notion of perimeter to the discrete framework of lattices. In order to ease the notations throughout the forthcoming Sections and chapters, we set

$$\mathcal{N} = \left\{ \{p, q\} \in \mathcal{L} \times \mathcal{L} : \; q \in \mathcal{N}(p) \right\} .$$

Remark 1.3.9. Given $X \in \mathcal{X}_N$ and $p \in X$, we can use the notation "$\mathcal{N}$" to describe the points that are, respectively, first and second neighbours of p within X. Indeed, according to Definition 1.3.3, we can say that:

- $q \in X$ is a first-neighbour of p in X if $\{p, q\} \in \mathcal{N}$.
- $z \in X$ is a second-neighbour of p in X if

$$\{p, z\} \notin \mathcal{N} \quad \text{and} \quad \exists q \in X : \; \{p, q\}, \{q, z\} \in \mathcal{N} . \tag{1.3.2}$$

♠

Definition 1.3.10. Given a lattice $\mathcal{L} \subset \mathbb{R}^d$ and a set $X \subset \mathcal{L}$ not empty, we define the **valence** of $p \in X$ as

$$\mathrm{val}(p) = \# \left\{ q \in \mathcal{L} \setminus X : \; \{p, q\} \in \mathcal{N} \right\} .$$

Remark 1.3.11. If the lattice is periodic and Bravais (or superposition of Bravais lattices), then the kissing number $k(\mathcal{L})$ of $\mathcal{L}$ is constant and we can infer that $\mathrm{val}(p) \in [0, k(\mathcal{L})]$ and

$$\mathrm{val}(p) = k(\mathcal{L}) - \# \left(\mathcal{N}(p) \cap X \right) = \# \left(\mathcal{N}(p) \setminus X \right) .$$

Morevoer, by Definition 1.3.10, we can classify the points of $X \subset \mathcal{L}$: we can say that $p \in X$ is

- an **interior point** of X if $\mathrm{val}(p) = 0$,
- a **boundary point** of X if $\mathrm{val}(p) > 0$ (in particular, p is an **isolated point** if $\mathrm{val}(p)$ is maximum).

♠

The valence of the points of X can be also used to define a functional that represents the boundary energy of a given configuration X. Indeed, we can add to (1.3.1) a bulk term made by the interactions among all the internal points and then we obtain a quantity that takes into account only the boundary points and their missing bonds: we get

$$\sum_{p\in X} \#\{q:\ \{p,q\}\in \mathcal{N}\} + E_N(X) = \sum_{p\in X} \mathrm{val}(p)\,. \tag{1.3.3}$$

From this, the definition of discrete perimeter naturally follows:

Definition 1.3.12. Given $X \subset \mathcal{L}$ such that X is non-empty, we define the **discrete perimeter** of X as $P(X) = \sum_{p\in X} \mathrm{val}(p)$.

Remark 1.3.13. With a slight abuse of notation, we choose to use the symbol $P(X)$ also in Definition 1.3.12 by analogy with the continuous case introduced earlier. This choice is made despite the fact that, in the following sections, we will often evaluate the relationship between the discrete and continuous perimeter. However, since we will be in the context of anisotropies, we will avoid confusion by using the notation introduced in Definition 1.2.19. ♠

1.3.2 Anisotropy and Wulff shapes of periodic lattices

Analogously to the continuous case, it is possible define the anisotropic energy of periodic lattices; to do that, we need to compute the anisotropic norm or the Wulff shape and, *a priori*, this can be difficult. There exists an asymptotic cell formula to compute the norm (for instance, see [2]), but thanks to [11, Proposition 2.6] we only need to do the computations on the periodicity cell of the lattice. For sake of completeness, we report here the result and some details.

Given a periodic lattice $\mathcal{L}$ with periodicity cell $T_{\mathcal{L}}$, we define the energy for a function $u\colon \mathcal{L} \to \mathbb{R}$ on $\Omega \subset \mathbb{R}^d$ as

$$E(u,\Omega) = \frac{1}{2} \sum_{i\in\mathcal{L}\cap\Omega} \sum_{j\in\mathcal{L}} c_{i,j} \left|u(i) - u(j)\right| ,$$

where the coefficients $c_{i,j} \geq 0$ satisfies

$$c_{i,j} = c_{i+T_{\mathcal{L}},j+T_{\mathcal{L}}} \qquad \forall i,j \in \mathcal{L} \tag{1.3.4}$$

and

$$\exists R > 1 : \ c_{i,j} = 0 \quad \forall i,j \in \mathcal{L} \text{ such that } |i-j| \geq R \tag{1.3.5}$$

Theorem 1.3.14. *Let* $c_{i,j} \colon \mathcal{L} \times \mathcal{L} \to [0,+\infty[$ *be such that* (1.3.4) *and* (1.3.5) *hold. Then, the anisotropic norm with respect to* $\mathcal{L}$ *is equal to*

$$\|\nu\|_{\mathcal{L}} = \frac{1}{|T_{\mathcal{L}}|} \inf \left\{ E(u, T_{\mathcal{L}}) : \ u(\cdot) - \langle \nu, \cdot \rangle \text{ is } T_{\mathcal{L}} \text{ periodic} \right\} . \tag{1.3.6}$$

Then, we can infer the Wulff shape associated to $\mathcal{L}$ from (1.3.6): like in Definition 1.2.19, we have

$$W_{\mathcal{L}} = \left\{ x \in \mathbb{R}^d : \ x \cdot \nu < \|\nu\|_{\mathcal{L}} \ \text{ for all } \nu \in \mathbb{S}^{d-1} \right\} .$$

In the following, for sake of clarity, we will simply write W_A instead of $W_{\mathcal{L}_A}$ whenever the context does not have ambiguities.

Remark 1.3.15. In the following we will usually refer to lattices whose interaction are only between neighbouring points, therefore the coefficients $c_{i,j}$ are such that

$$c_{i,j} = \begin{cases} 1 & \text{if } \{i,j\} \in \mathcal{n}, \\ 0 & \text{otherwise} . \end{cases}$$

In particular, if $\mathcal{L}$ is a periodic Bravais lattice whose neighbouring directions are $\{\xi_1, \dots, \xi_n\}$, then the energy function in formula (1.3.6) becomes

$$E(u, T_{\mathcal{L}}) = \frac{1}{2} \sum_{i \in \mathcal{L} \cap T_{\mathcal{L}}} \sum_{\xi \in \{\xi_1, \dots, \xi_n\}} \left| \langle \xi, \nu \rangle \right| .$$

♠

1.4 Γ-convergence

Γ-convergence was introduced by Ennio De Giorgi in the early 1970s to study the asymptotic behaviour of families of functionals $(F_\varepsilon)_\varepsilon$ and the convergence

of their minimizers. The key feature of this theory is its flexibility: indeed, Γ-convergence does not require a prescribed setting or assumptions on the form of the minimizers, making it particularly well-suited to capturing variational limits in problems involving homogenization, phase transitions or perturbations, including those arising in computer vision problems or in the passage from discrete to continuum systems.
There are various possible approaches to presenting this widely-used theory, depending also on the given framework. Here, we briefly provide only some fundamental definitions and properties and we refer, for further details and more general statements, to [7], [8], and [16].

Definition 1.4.1. Given a metric space (X, d) and a sequence of functionals

$$(F_\varepsilon)_\varepsilon \colon X \to [-\infty, +\infty]\,,$$

we say that F_ε **Γ-converges** to $F\colon X \to [-\infty, +\infty]$ at $x \in X$ if the two following hold:

(i) for every sequence $(x_\varepsilon)_\varepsilon \subset X$ converging to x

$$F(x) \leq \liminf_{\varepsilon\to 0} F_\varepsilon(x_\varepsilon)$$

(ii) there exists a sequence $(\overline{x}_\varepsilon)_\varepsilon \subset X$ converging to x such that

$$F(x) \geq \limsup_{\varepsilon\to 0} F_\varepsilon(\overline{x}_\varepsilon)\,.$$

We call $F(x)$ the **Γ-limit** of F_ε at x and we denote it as

$$F(x) = \Gamma - \lim_{\varepsilon\to 0} F_\varepsilon(x_\varepsilon)\,. \tag{1.4.1}$$

In particular, if (1.4.1) holds for all $x \in X$, then we say that F_ε **Γ-converges** to F and we denote it as $F = \Gamma - \lim_{\varepsilon\to 0} F_\varepsilon$.

Definition 1.4.2. Given a metric space (X, d) and a sequence of functionals $(F_\varepsilon)_\varepsilon$ such that $F_\varepsilon\colon X \to [-\infty, +\infty]$, then we say that $(F_\varepsilon)_\varepsilon$ is **equi-coercive** if

$$\forall t \in \mathbb{R}\,, \exists K_t \subset X \text{ compact set : } \big\{x \in X : \; F_e(x) \leq t\big\} \subset K_t\,.$$

The lower-semicontinuity and coercivity of a functional F are sufficient conditions to prove the existence of minimizers of F, thanks to the direct method of the calculus of variations. Similarly, Definitions 1.4.1 and 1.4.2 provide sufficient conditions to ensure the convergence of the minima of a sequence of functionals, as stated in the following theorem:

Theorem 1.4.3 (Fundamental Theorem of Γ-convergence)**.** *Let* (X, d) *be a metric space and let* $(F_\varepsilon)_\varepsilon$ *be a equi-coercive sequence of functional on* X *such that* $F = \Gamma - \lim_{\varepsilon\to 0} F_\varepsilon$*. Then, there exists* $\min_{y\in X} F(y)$ *and it holds that*

$$\min_{y\in X} F(y) = \lim_{\varepsilon\to 0} \inf_{y\in X} F_\varepsilon(y)\,.$$

Moreover, if $(x_\varepsilon)_\varepsilon$ *is a converging sequence in* X *such that*

$$\lim_{\varepsilon\to 0} F_\varepsilon(x_\varepsilon) = \lim_{\varepsilon\to 0} \inf_{y\in X} F_\varepsilon(y)\,,$$

then its limit is a minimum point for F*.*

1.4.1 Γ-convergence on lattices

As we mentioned before, Γ-convergence can be used to study passages from discrete setting into continuum systems and one of the most useful result on this setting is the convergence theorem given in [2], which also provides L^p-growth estimates for the limit functional.

Given the lattice $\mathcal{L}_\varepsilon = \varepsilon\mathbb{Z}^d$ for $\varepsilon > 0$ and a function $u\colon \mathcal{L}_\varepsilon \longrightarrow \mathbb{R}$, then we can represent an energy-interaction functional on the lattice as

$$F_\varepsilon(u) = \frac{1}{2}\sum_{i\in\mathcal{L}_\varepsilon}\sum_{j\in\mathcal{L}_\varepsilon} \varepsilon^d g^\varepsilon\left(i, j, u(i) - u(j)\right)$$

and we can investigate its behaviour as $\varepsilon \to 0$. In particular, if we consider only nearest-neighbours interactions and if F_ε is invariant under translations with homogeneous interactions, then we obtain that

$$F_\varepsilon(u) = \frac{1}{2}\sum_{i\in\mathcal{L}_\varepsilon}\sum_{\substack{j\in\mathcal{L}_\varepsilon\\ |i-j|=\varepsilon}} \varepsilon^d f^\varepsilon\left(\frac{u(i) - u(j)}{\varepsilon}\right) \tag{1.4.2}$$

and we want to infer a Γ-convergence result to some $F\colon \mathbb{R}^d \to [-\infty, +\infty]$ such that

$$F(u) = \int_{\mathbb{R}^d} f\left(Du(x)\right)\,\mathrm{d}x\,.$$

Theorem 1.4.4. *Let $(F_\varepsilon)_\varepsilon$ be a sequence of energy defined on $\Omega \cap \mathcal{L}_\varepsilon$ as in 1.4.2 and assume that there exists $c_1^\varepsilon, c_2^\varepsilon > 0$ such that*

$$c_1^\varepsilon \left(|z|^p - 1\right) \leq f^\varepsilon(z) \leq c_2^\varepsilon \left(|z|^p + 1\right)$$

holds for all $z \in \mathbb{R}$. Then, for every sequence $(\varepsilon_k)_k$ converging to 0, there exists a subsequence $(\varepsilon_{k_j})_j$ and a Carathéodory function $f\colon \Omega \times \mathbb{R}^d \longrightarrow \mathbb{R}$ that satisfies

$$c_1(|z|^p - 1) \leq f(z) \leq c_2(|z|^p + 1)$$

such that $(F_{\varepsilon_{k_j}})_j$ Γ-converges w.r.t. the $L^p(\Omega)$-topology to

$$F(u) = \int_\Omega f(Du)\,\mathrm{d}x \qquad \text{if } u \in W^{1,p}(\Omega)\,.$$

Remark 1.4.5. Moreover, if $f^\varepsilon(z)$ is a positive homogeneous quadratic form on $\mathbb{R}^d$, then also f is a positive homogeneous quadratic form on $\mathbb{R}^d$, as pointed out in Remark 3.2 and Remark 5.2 of [2]. ♠

1.5 Q-closeness

The Q-closeness technique introduced in [13] offers a rigorous framework for quantitatively analyzing the deviations of discrete lattice configurations from optimal geometric shapes in the context of functional problems. Specifically, this technique is designed to measure the deviations of periodic lattice configurations from their optimal counterparts in the continuous setting, with respect to a given functional. We report here the crucial steps of the Q-closeness technique, since in the following chapters we will make a large use of it for the anisotropic quantitative inequality and for a discrete quantitative Faber-Krahn inequality.

Fixed a lattice $\mathcal{L} \subset \mathbb{R}^d$, we consider a discrete energy functional $\mathcal{E}_N\colon \mathcal{L} \to [0, +\infty]$ such that

$$\mathcal{E}_N(X) < +\infty \quad \iff \quad X \in \mathcal{X}_N\,. \tag{1.5.1}$$

We also consider a functional $\mathcal{E}\colon \mathcal{M}(\mathbb{R}^d) \longrightarrow [0, +\infty]$ that admits, up to translations and measure-zero sets, a unique minimizing set W_v such that

$|W_v| = v$ for any $v > 0$, i.e.

$$\mathcal{E}(W_v) = \min\left\{\mathcal{E}(\Omega) : \ \Omega \in \mathcal{M}(\mathbb{R}^d)\,, |\Omega| = v\right\} \tag{1.5.2}$$

Definition 1.5.1. We say that a functional $\mathcal{E} \colon \mathcal{M}(\mathbb{R}^d) \longrightarrow [0, +\infty]$ **satisfies a φ-quantitative inequality** if, for any $\Omega \in \mathcal{M}(\mathbb{R}^d)$ such that $|\Omega| = v$, it holds that

$$\inf_{x\in\mathbb{R}^d} \frac{|\Omega \triangle (x + W_v)|}{|\Omega|} \leq \varphi\left(\frac{\mathcal{E}(\Omega) - \mathcal{E}(W_v)}{\mathcal{E}(W_v)}\right) \tag{1.5.3}$$

where $\varphi \colon [0, +\infty[\longrightarrow [0, +\infty[$ is a modulus of continuity (i.e., φ is a continuous, strictly increasing function such that $\varphi(0) = 0$).

Definition 1.5.2. Let $(\mathcal{E}_N)_N$ be a sequence of functionals as in (1.5.1) and let $\mathcal{E} \colon \mathcal{M}(\mathbb{R}^d) \to [0, +\infty]$ be a functional that satisfies (1.5.3) and (1.5.2). We say that the sequence $(\mathcal{E}_N)_N$ is **Q-close** (or quantitatively close) to $\mathcal{E}$ with respect to a map $\zeta \colon \mathcal{L} \to \mathcal{M}(\mathbb{R}^d)$ and to the non-negative parameters α_N, β_N, γ_N if, for every $X \in \mathcal{X}_N$ such that

$$\mathcal{E}_N(X) \leq \inf_{Y\in\mathcal{X}_N} \mathcal{E}_N(Y) + \alpha_N \tag{1.5.4}$$

the following two hold:

$$\mathcal{E}\left(\zeta(X)\right) \leq \mathcal{E}_N(X) + \beta_N\,, \tag{1.5.5}$$

$$\inf_{Y\in\mathcal{X}_N} \mathcal{E}_N(Y) \leq \inf_{\Omega\in\mathcal{M}(\mathbb{R}^d)\,:\,|\Omega|=|\zeta(X)|} \mathcal{E}(\Omega) + \gamma_N\,. \tag{1.5.6}$$

Under these conditions, one can immediately prove Proposition 1 in [13], that we report here for sake of completeness:

Proposition 1.5.3. *Let $(\mathcal{E}_N)_N$ be a sequence of functionals Q-close to a functional $\mathcal{E}$ that satisfies* (1.5.2) *and* (1.5.3)*. Then, the following holds*

$$\inf_{x\in\mathbb{R}^d} \frac{|\zeta(X) \triangle (x + W_v)|}{|\zeta(X)|} \leq \varphi\left(\frac{\alpha_N + \beta_N + \gamma_N}{\mathcal{E}(W_v)}\right) \tag{1.5.7}$$

where $v = |\zeta(X)|$.

Proof. Since $\mathcal{E}$ satisfies (1.5.3), by the monotonicity of φ, we have

$$\begin{aligned}
\inf_{x\in\mathbb{R}^d} \frac{|\zeta(X)\triangle(x+W_v)|}{|\zeta(X)|} &\leq \varphi\left(\frac{\mathcal{E}(\zeta(X)) - \mathcal{E}(W_v)}{\mathcal{E}(W_v)}\right) \\
&\leq \varphi\left(\frac{\mathcal{E}_N(X) + \beta_N - \inf_{Y\in\mathcal{X}_N}\mathcal{E}_N(Y) + \gamma_N}{\mathcal{E}(W_v)}\right) \\
&\leq \varphi\left(\frac{\alpha_N + \beta_N + \gamma_N}{\mathcal{E}(W_v)}\right)
\end{aligned}$$

□

Chapter 2

Quantitative estimates for the Anisotropic Isoperimetric Inequality on lattices

In this chapter, we explore a different approach to quantitatively estimate fluctuations in the anisotropic perimeter studied in the three cases from [13]. The core problem of the Q-closeness technique is to identify a suitable map ζ that characterizes, in some sense, the correct measure and perimeter of the set with respect to the given anisotropy. For example, if we consider two adjacent points p, q in a lattice $\mathscr{L}$, a very natural geometric object that represents this pair is the tubular neighbourhood of the segment $\overline{p, q}$ generated with respect to the anisotropy. By following this intuition, we define a map ζ that depends only on the given lattice and we recover the results of [13].

In Section 2.1, we will first properly define the map ζ on a suitable neighbourhood of the points of the lattice $\mathscr{L}$. In the subsequent sections, we will use ζ to compute a quantitative anisotropic isoperimetric inequality. More precisely, in Sections 2.2, 2.3, and 2.4, we will carry out the computations for the d-dimensional square lattice, the honeycomb lattice, and the triangular lattice, respectively. In the final section of this chapter, we briefly discuss some intrinsic issues that arise when attempting to extend this approach to higher-dimensional frameworks.

Before starting, we fix and recall a couple of very useful notations which will be used throughout the following chapter. Given $\mathscr{L} \subset \mathbb{R}^d$ as in Definition 1.3.1,

- we denote by $\mathscr{X}_N$ the set $\{Y \subset \mathscr{L} : \#Y = N\}$,

- we denote by $\{p,q\} \in \mathcal{N}$ an unordered couple of first-neighbouring points in $\mathcal{L}$ or $X \in \mathcal{X}_N$, depending on the context
- we denote by $\overline{p,q}$ the segment connecting $p,q \in \mathcal{L}$.

2.1 The discrete-to-continuum map ζ

The construction of the map ζ, based on an appropriate tubular neighbourhood, respects the anisotropic nature of the given setting. Hence, we need to define a geometric object that takes into account both the Wulff shape associated with the lattice and the connections between neighbouring points. To do that, we introduce the Minkowski sum:

Definition 2.1.1. Given two sets $A, B \subset \mathbb{R}^d$, the **Minkowski sum** of A and B is the subset of $\mathbb{R}^d$ defined as

$$A \oplus B = \{a + b : \ a \in A\,, b \in B\}\ .$$

In order to take into account the role of the adjacencies in the given lattice $\mathcal{L}$, we define the following subset of $\mathbb{R}^d$:

Definition 2.1.2. Let $\mathcal{L} \subset \mathbb{R}^d$ be as in Definition 1.3.1:

$$\mathcal{L} = \mathrm{span}_{\mathbb{Z}}\{v_1, \ldots, v_d\} \cup \big(\tau + \mathrm{span}_{\mathbb{Z}}\{v_1, \ldots, v_d\}\big)$$

for some $v_1, \ldots, v_d \in \mathbb{R}^d$ and for some $\tau \in \mathbb{R}^d$ and let $X \in \mathcal{X}_N$. Then, we define the **1-dimensional skeleton** of X as

$$\begin{aligned}\Xi(X) = X &\cup \big\{\overline{p,q} : \ p,q \in X \text{ and } \{p,q\} \in \mathcal{N}\big\} \\ &\cup \left\{ \overline{p,q} : \ \begin{array}{l} \diamond \ \ p,q \in X \\ \diamond \ \ p,q \text{ satisfy (1.3.2)} \\ \diamond \ \ \mathcal{H}^1(\overline{p,q}) = \|v_1\|_2 \end{array} \right\} . \end{aligned} \tag{2.1.1}$$

In particular, if $\mathcal{L}$ is a Bravais lattice, then $\mathcal{L} = \mathrm{span}_{\mathbb{Z}}\{v_1, \ldots, v_d\}$ and

$$\Xi(X) = X \cup \big\{\overline{p,q} : \ p,q \in X \text{ and } \{p,q\} \in \mathcal{N}\big\}\ .$$

The set $\Xi(X)$ is designed to include all the points of the configuration X, including isolated points, all the segments representing first-neighbour interactions and those reflecting the intrinsic geometric structure of the underlying lattice. The definition has been given in a form as general as possible to include all lattice cases discussed in this chapter and in the Appendix.

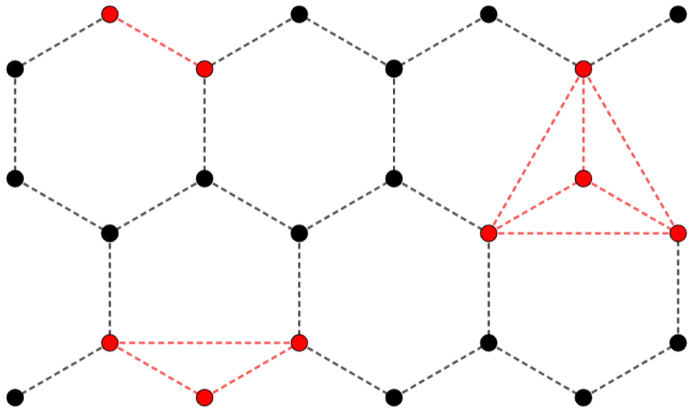

Figure 2.1: A representation of $\Xi(X)$ on the honeycomb lattice (see Section 2.3 for its definition). The set X is depicted by red dots, while $\Xi(X)$ is the union of X with the red dashed segments. In the honeycomb lattice, the segments connecting first- and second-neighbouring points in X coincide with the segments defined in (2.1.1).

Using these two definitions, we define the map ζ accordingly, in order to provide a suitable continuous representation of the discrete configuration X, by constructing a tubular neighbourhood of $\Xi(X)$ via the Minkowski sum:

Definition 2.1.3. Given a lattice $\mathscr{L} \subset \mathbb{R}^d$, given $X \in \mathcal{X}_N$ and given the Wulff shape $W_{\mathscr{L}}$ associated to $\mathscr{L}$, we define $\zeta \colon \mathscr{L} \longrightarrow \mathcal{M}(\mathbb{R}^d)$ as

$$\zeta(X) = cW_{\mathscr{L}} \oplus \Xi(X)\,, \tag{2.1.2}$$

where $\Xi(X)$ is the set in (2.1.1) and c is the biggest positive real number such that

$$\left|(p + cW_{\mathscr{L}}) \cap (q + cW_{\mathscr{L}})\right| = 0 \quad \text{for any} \quad \{p, q\} \in \mathcal{N}\,. \tag{2.1.3}$$

2.1.1 The Minkowski neighbourhood of a lattice

To apply Proposition 1.5.3, we firstly need to control the geometric behaviour of the map in (2.1.2), since we want to compute the measure and the

anisotropic perimeter of ζ with a local-to-global procedure. Thus, we have to choose firstly a suitable neighbourhood of the points of $\mathcal{L}$ in which we can localize the computations. The most natural choice for periodic lattices seems to be the Voronoi cells of the points of $\mathcal{L}$ (see Definition 1.3.2), since they define a tessellation of the whole $\mathbb{R}^d$ and, by construction, for any $p \in \mathcal{L}$ it holds that $p + cW_{\mathcal{L}} \subset V(p)$.
However, there exists lattices where, for any couple of points $p, q \in \mathcal{L}$ such that $\{p, q\} \in \mathcal{N}$, it holds that

$$cW_{\mathcal{L}} \oplus \overline{p,q} \not\subset V(p) \cup V(q)$$

and therefore $\zeta(X) \not\subset \bigcup_{p\in X} V(p)$ for any $X \in \mathcal{X}_N$. This happens even in well-known cases: for instance, this containment fails in the 2-dimensional triangular lattice $\mathcal{L}_T$ (for the precise definition and further details about $\mathcal{L}_T$, see Section 2.4) as well as for the 3-dimensional FCC lattice, as briefly explained in the Appendix.

In the following, we define a neighbourhood $U(p)$ for the points of the given lattice $\mathcal{L}$ such that

$$\zeta(X) \subset \bigcup_{p\in X} U(p) \quad \text{for any } X \in \mathcal{X}_N\,.$$

In this way, we can apply the local-to-global approach without neglecting any relevant contributions from either the measure or the perimeter of ζ.
First, we introduce the following notation: given a lattice $\mathcal{L} \subset \mathbb{R}^d$ as in Definition 1.3.1 and its associated rescaled Wulff shape $cW_{\mathcal{L}}$ as in Definition 2.1.3, we set

$$cW_{\mathcal{L}} \oplus \frac{\overline{p,q}}{2} := \bigcup_{\lambda\in\left[0,\frac{1}{2}\right[} (cW_{\mathcal{L}} \oplus \overline{p,q}) \cap \Pi_{\overline{p,q},\lambda}\,,$$

where $\Pi_{\overline{p,q},\lambda}$ denotes the hyperplane orthogonal to $\overline{p,q}$ and passing through the point $\lambda p + (1-\lambda)q$.

Remark 2.1.4. Roughly speaking, $cW_{\mathcal{L}} \oplus \frac{\overline{p,q}}{2}$ denotes the tubular neighbourhood (w.r.t. the Wulff shape and the segment $\overline{p,q}$) truncated orthogonally at the middle point of $\overline{p,q}$. ♠

Definition 2.1.5. Given a lattice $\mathcal{L} \subset \mathbb{R}^d$ and $p \in \mathcal{L}$, we define the

Minkowski neighbourhood in $p \in \mathcal{L}$ as:

$$U(p) = \begin{cases} V(p) & \text{if } \left(cW_{\mathcal{L}} \oplus \frac{\overline{p,q}}{2} \subset V(p)\right) \text{ holds } \forall q \colon \{p,q\} \in \mathcal{n}\,, \\ \bigcup_{\substack{q \in \mathcal{L} \\ \{p,q\} \in \mathcal{n}}} \left(cW_{\mathcal{L}} \oplus \frac{\overline{p,q}}{2}\right) & \text{otherwise}\,. \end{cases} \tag{2.1.4}$$

Remark 2.1.6. By the previous definition, we can infer that

$$|\zeta(X)| \leq \left| \bigcup_{p \in X} U(p) \right| .$$

In particular, when summing the local measure contributions of the internal points, each such point contributes exactly $|U(p)|$ to the measure of ζ. However, if $U(p)$ is not the Voronoi cell of the lattice, then there may be overlaps between neighbouring Minkowski neighbourhoods, which we must take care not to double-count, or there may be portions of $\mathbb{R}^d$ near p that are not covered by ζ.
In particular, if we have that $V(p) \subset U(p)$, then we can avoid computing the measure of these overlaps and simply infer that each internal point contributes $|V(p)|$ to the measure of ζ; in this case, we obtain that

$$\big|\zeta(X)\big| \leq \sum_{\substack{p \in X \\ \mathrm{val}(p)=0}} |V(p)| + \left| \bigcup_{p \in X} U(p) \setminus \bigcup_{\substack{p \in X \\ \mathrm{val}(p)=0}} V(p) \right| .$$

♠

In the following lemma, we show that the measure of the boundary of $\zeta(X)$, for a given $X \in \mathcal{X}_N$, can be computed as the sum of the local boundary measures within the Minkowski neighbourhoods of the points in X.

Lemma 2.1.7. *Given $\mathcal{L} \subset \mathbb{R}^d$, let ζ be the map in* (2.1.2) *and let $U(p)$ be the Minkowski neighbourhood of Definition 2.1.5. Let us assume that*

$$\mathcal{H}^{d-1}\big(\partial\zeta(X) \cap U(p) \cap U(q)\big) = 0 \qquad \forall p, q \in X\,. \tag{2.1.5}$$

Then, for any $X \in \mathcal{X}_N$ it holds that

$$\mathcal{H}^{d-1}\big(\partial\zeta(X)\big) = \sum_{p \in X} \mathcal{H}^{d-1}\big(\partial\zeta(X) \cap U(p)\big)\ . \tag{2.1.6}$$

In particular, it holds that

$$P_{W_{\mathcal{L}}}\left(\zeta(X)\right) = \sum_{p\in X} P_{W_{\mathcal{L}}}\left(\zeta(X)\cap U(p)\right) . \tag{2.1.7}$$

Proof. From (2.1.5) we can infer the additivity of the $(d-1)$-dimensional Hausdorff measure on the sets $\left(\partial\zeta(X)\cap U(p)\right)_{p\in X}$:

$$\begin{aligned}\mathcal{H}^{d-1}\Big(\partial\zeta(X)\cap\big(U(p)\cup U(q)\big)\Big) &= \mathcal{H}^{d-1}\Big(\big(\partial\zeta(X)\cap U(p)\big)\cup\big(\partial\zeta(X)\cap U(q)\big)\Big)\\ &\qquad - \mathcal{H}^{d-1}\left(\partial\zeta(X)\cap U(p)\cap U(q)\right)\\ &= \mathcal{H}^{d-1}\left(\partial\zeta(X)\cap U(p)\right) + \mathcal{H}^{d-1}\left(\partial\zeta(X)\cap U(q)\right) .\end{aligned}$$

Hence, we get the thesis:

$$\begin{aligned}\mathcal{H}^{d-1}\left(\partial\zeta(X)\right) &= \mathcal{H}^{d-1}\left(\partial\zeta(X)\cap\bigcup_{p\in X}U(p)\right) = \mathcal{H}^{d-1}\left(\bigcup_{p\in X}\left(\partial\zeta(X)\cap U(p)\right)\right)\\ &= \sum_{p\in X}\mathcal{H}^{d-1}\left(\partial\zeta(X)\cap U(p)\right) .\end{aligned}$$

(2.1.7) is a direct consequence of (2.1.6) and (1.2.7), since, by construction, $\partial\zeta(X)$ is made by $(d-1)$-dimensional polyhedra on which the anisotropic weight is constant.

□

We remark that, if $U(p)$ coincides with the Voronoi cell of $\mathcal{L}$, then (2.1.6) trivially holds, since Voronoi cells form a tessellation of $\mathbb{R}^d$. This is the case for the lattices considered in Section 2.2 and Section 2.3. By contrast, in Section 2.4, the Minkowski neighbourhood does not coincide with the Voronoi cell, but condition (2.1.5) still holds; therefore, by the previous Lemma, we can compute exactly the anisotropic perimeter of ζ via a local-to-global procedure.

2.2 The d-dimensional square lattice

In the study of periodic structures, the d-dimensional square lattice is probably the simplest and most fundamental configuration, where each point of the grid is spaced evenly by the vectors of the canonical orthonormal basis

$e_1, \ldots, e_d$ of $\mathbb{R}^d$; formally, we can describe the lattice as

$$\mathscr{L}_Q = \mathbb{Z}^d = span_{\mathbb{Z}} \{e_1, \ldots, e_d\} \ .$$

This description reflects the translational invariance and the scaling invari-

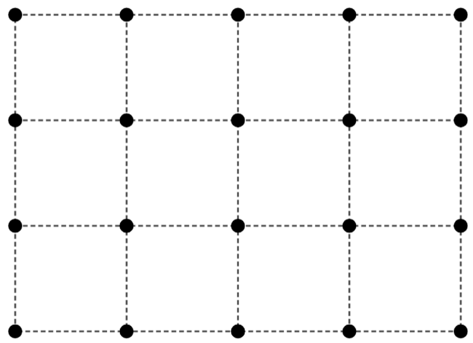

Figure 2.2: The lattice $\mathscr{L}_Q$ in two dimension.

ance of $\mathscr{L}_Q$; moreover, it is easy to see that the periodicity cell of the lattice is the unitary d-dimensional cube. Thus, for sake of simplicity, for any $p \in \mathscr{L}_Q$ we set

$$Q(p) = p + \left] -\frac{1}{2}, \frac{1}{2} \right[^d \ .$$

From Theorem 1.3.14, we know that we can compute the anisotropic norm with the periodicity cell formula (1.3.6). We get

$$\|\nu\|_Q = \sum_{k=1}^{d} \frac{1}{2} |\langle \nu, e_k \rangle| + \frac{1}{2} |\langle \nu, -e_k \rangle| = \sum_{k=1}^{d} |\langle \nu, e_k \rangle| = \|\nu\|_1 \ . \tag{2.2.1}$$

Then, the Wulff shape associated to $\mathscr{L}_Q$ is determined by the sublevel set of the dual function of the anisotropic norm:

$$W_Q = \left\{ x \in \mathbb{R}^d : \ x \cdot \nu < \|\nu\|_1 \text{ for all } \nu \in \mathbb{S}^{d-1} \right\} =]-1, 1[^d \ . \tag{2.2.2}$$

Moreover, by (1.2.7) and (1.2.8) we get

$$P_Q(E) = \int_{\partial^* E} \|\nu_E\|_Q \, \mathrm{d}\mathscr{H}^{d-1} \geq P_Q(W_{Q,|E|}) \, , \tag{2.2.3}$$

where we recall that $\left| W_{Q,|E|} \right| = |E|$.

2.2.1 Geometric properties of ζ in $\mathcal{L}_Q$

The first step in order to apply the Q-closeness is the computation of the measure and the perimeter of the map ζ defined in (2.1.2) on $\mathcal{L}_Q$. Since the Wulff shape W_Q coincides with the Voronoi cell in each point p of the lattice, we can localize the computations inside the Voronoi cells of the points of $X \in \mathcal{X}_N$. Moreover, by construction, we also get that the rescaling factor needed for (2.1.2) is $\frac{1}{2}$: hence

$$cW_Q \oplus \overline{p,q} = Q(p) \cup Q(q) \qquad \forall \{p,q\} \in \mathcal{N}\,.$$

Therefore, for the lattice $\mathbb{Z}^d$, the discrete-to-continuum map $\zeta \colon \mathcal{L}_Q \to \mathcal{M}(\mathbb{R}^2)$ defined in (2.1.2) is equivalent to

$$\zeta(X) = \bigcup_{p\in X} Q(p) \tag{2.2.4}$$

and then we can infer the following properties:

Lemma 2.2.1. *Let $X \in \mathcal{X}_N$ and let $\zeta \colon \mathcal{L}_Q \to \mathcal{M}(\mathbb{R}^d)$ be the function defined in* (2.2.4)*. Then,*

(i) $|\zeta(X)| = N$,

(ii) $P_Q\left(\zeta(X)\right) = P(X)$.

Proof of (i). This is a direct consequence of (2.2.4): indeed for any $p \in X$ we have $|Q(p)| = 1$ and hence

$$|\zeta(X)| = \left|\bigcup_{p\in X} Q(p)\right| = \sum_{p\in X} |Q(p)| = \#X\,.$$

Proof of (ii). By $\|\nu_\Omega\|_Q = \|\nu_\Omega\|_1$ and (2.2.4) we have $\left\|\nu_{\zeta(X)}\right\|_Q \equiv 1$ for a.e. point in $\partial^*\zeta(X)$; thus, (2.2.3), we get

$$P_Q\left(\zeta(X)\right) = \int_{\partial^*\zeta(X)} \left\|\nu_{\zeta(X)}(x)\right\|_Q \,\mathrm{d}\mathcal{H}^{d-1}(x) = \mathcal{H}^{d-1}\left(\partial^*\zeta(X)\right)\,.$$

The thesis follows by

$$\mathcal{H}^{d-1}\left(\partial^*\zeta(X)\right) = \sum_{p\in X} \mathcal{H}^{d-1}\left(\partial\zeta(X) \cap \partial Q(p)\right) = \sum_{p\in X} \mathrm{val}(p)\,.$$

□

Remark 2.2.2. We point out that, through our definition (2.1.2) of ζ, we obtain the same set used by Cicalese and Leonardi in their paper [13] for the lattice $\mathscr{L}_Q$. ♠

2.2.2 Q-closeness for ζ in $\mathscr{L}_Q$

In order to apply the Q-closeness, we set the discrete functional as

$$\mathcal{E}_N \colon \mathscr{L} \to [0, +\infty] \quad \text{such that} \quad \mathcal{E}_N(X) = P(X) \quad \forall X \in \mathcal{X}_N\,, \tag{2.2.5}$$

and the continuous functional as

$$\mathcal{E} \colon \mathcal{M}(\mathbb{R}^d) \to [0, +\infty] \quad \text{such that} \quad \mathcal{E}(\Omega) = P_Q(\Omega) \quad \forall \Omega \in \mathcal{M}(\mathbb{R}^d)\,. \tag{2.2.6}$$

Analogously to Remark 2.2.2, we can infer that the map (2.2.4) produces the same estimates for the parameters β_N, γ_N as the ones obtained in [13]. Therefore, we briefly report here only the results without computations and we refer to the original article for further details.
We get that the estimate (1.5.5) holds with $\beta_N = 0$ since

$$\begin{aligned}\mathcal{E}\left(\zeta(X)\right) = \mathcal{H}^{d-1}\left(\partial^*\zeta(X)\right) &= \sum_{p\in X} \mathcal{H}^{d-1}\left(\partial^*\zeta(X) \cap Q(p)\right) \\ &= \sum_{p\in X} \mathrm{val}(p) = \mathcal{E}_N(X)\,,\end{aligned}$$

while (1.5.6) holds with

$$\gamma_N \leq C_d N^{1-\frac{2}{d}}\,,$$

which is obtained by the removing-points algorithm explained in [13].
Finally, by applying Proposition 1.5.3, we get the following quantitative estimate:

Proposition 2.2.3. *Let ζ be the map defined in* (2.2.4) *with respect to the rescaled Wulff shape Q. Let $\mathcal{E}_N$, $\mathcal{E}$ be the functionals defined respectively in* (2.2.5), (2.2.6) *and let $X \in \mathcal{X}_N$ such that*

$$\mathcal{E}_N(X) \leq \inf_{Y\in\mathcal{X}_N} \mathcal{E}_N(Y) + \alpha_N\,. \tag{2.2.7}$$

Then, there exists a dimensional constant $C_d = C(d) > 0$ such that

$$\inf_{x\in\mathbb{R}^d} \left|\zeta(X) \triangle (x + W_{Q,|\zeta(X)|})\right| \leq C_d \left(\alpha_N N^{\frac{d+1}{d}} + N^{2-\frac{1}{d}}\right)^{\frac{1}{2}}$$

For sake of completeness, we report the proof from [13]:

Proof. By Proposition 1.5.3, we have

$$\inf_{x\in\mathbb{R}^d} \left|\zeta(X)\triangle(x+W_{Q,|\zeta(X)|})\right| \le C_d \left(\frac{\alpha_N+\beta_N+\gamma_N}{d}\right)^{\frac{1}{2}} |\zeta(X)|^{\frac{d+1}{2d}}$$

We know that $\beta_N = 0$ and that $\gamma_N \le C_d N^{1-\frac{1}{2d}}$; thus,

$$\begin{aligned}\inf_{x\in\mathbb{R}^d} \left|\zeta(X)\triangle(x+W_{Q,|\zeta(X)|})\right| &\le C_d \left(\frac{\alpha_N+C_dN^{1-\frac{2}{d}}}{d}\right)^{\frac{1}{2}} N^{\frac{d+1}{2d}} \\ &\le C_d \left(\alpha_N N^{\frac{d+1}{d}} + N^{2-\frac{1}{d}}\right)^{\frac{1}{2}}\end{aligned}$$

□

Remark 2.2.4. Proposition 2.2.3 gives a sharp exponent for the quantitative estimate in dimension $d = 2$, the so-called $N^{\frac{3}{4}}$-law, that was proven to be optimal in [41] and [17]:

$$\inf_{x\in\mathbb{R}^2} \left|\zeta(X)\triangle(x+W_{Q,|\zeta(X)|})\right| \le C_2 \left(\alpha_N N^{\frac{3}{2}} + N^{2-\frac{1}{2}}\right)^{\frac{1}{2}} = \widetilde{C_2} N^{\frac{3}{4}}.$$

However, the Q-closeness technique only gives a sub-optimal exponent in greater dimension: indeed, in [37] it is shown that the $N^{\frac{3}{4}}$-law still holds in three dimensions. ♠

2.3 The honeycomb lattice

The honeycomb lattice is a 2-dimensional periodic lattice, where each point has three nearest neighbors, arranged in a hexagonal pattern by the superposition of two Bravais lattices:

$$\begin{aligned}\mathcal{L}_H =& span_{\mathbb{Z}}\left\{\sqrt{3}e_1, \frac{-\sqrt{3}e_1+3e_2}{2}\right\} \cup \\ & \left(e_2 + span_{\mathbb{Z}}\left\{\sqrt{3}e_1, \frac{-\sqrt{3}e_1+3e_2}{2}\right\}\right), \end{aligned} \tag{2.3.1}$$

where we recall that e_i denotes the i^{th} vector of the standard orthonormal basis of $\mathbb{R}^d$.
By construction, the lattice has unitary uniform spacing, as in the d dimensional square lattice case, and the periodicity cell T_H of the lattice is the rhombus spanned by the two basis vectors of the Bravais lattice centred in $(0, \frac{1}{2})$, while the Voronoi cell of $p \in \mathcal{L}_H$ is an equilateral triangle of side length equal to $\sqrt{3}$ centred in p.

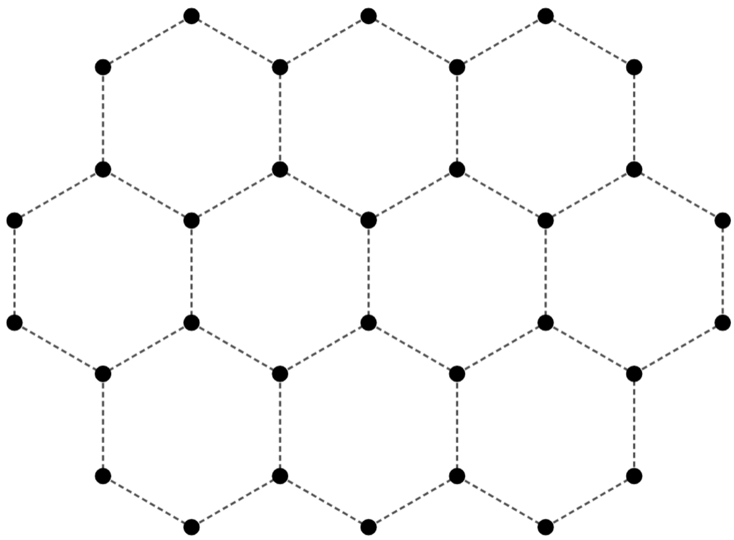

Figure 2.3: The honeycomb lattice

Analogously to the previous case of the d-dimensional square lattice, we can use Theorem 1.3.14 to compute the anisotropic norm associated to $\mathcal{L}_H$: we get

$$\|\nu\|_H = \frac{1}{3} \min \Big\{ |\nu_1 + \sqrt{3}\nu_2| + |\nu_1 - \sqrt{3}\nu_2|,\, |\nu_1 + \sqrt{3}\nu_2| + 2|\nu_1|, \\ |\nu_1 - \sqrt{3}\nu_2| + 2|\nu_1| \Big\}. \tag{2.3.2}$$

Consequently, the Wulff shape associated to $\mathcal{L}_H$ is

$$W_H = \left\{ x \in \mathbb{R}^2 :\ x \cdot \nu \leq \|\nu\|_H \ \text{ for all } \nu \in \mathbb{S}^1 \right\} ,$$

that is the regular hexagon with vertices $\left(\frac{2}{3}, 0\right)$, $\left(\frac{1}{3}, \frac{\sqrt{3}}{3}\right)$, $\left(-\frac{1}{3}, \frac{\sqrt{3}}{3}\right)$, $\left(-\frac{2}{3}, 0\right)$,

$\left(-\frac{1}{3}, -\frac{\sqrt{3}}{3}\right)$, $\left(\frac{1}{3}, -\frac{\sqrt{3}}{3}\right)$.
Moreover, again by (1.2.7) and (1.2.8), we have that

$$P_H(E) = \int_{\partial^* E} \left\|\nu_E(x)\right\|_H \, \mathrm{d}\mathscr{H}^1(x) \geq P_H(W_{H,|E|}) \,,$$

where $\left|W_{H,|E|}\right| = |E|$.

Remark 2.3.1. The anisotropic norm can be obtained as follows. Since $|T_H| = \frac{3\sqrt{3}}{2}$, from (1.3.6) we get

$$\|\nu\|_H = \frac{2}{3\sqrt{3}} \inf \left\{ \sum_{p \in T_H} \sum_{\substack{q \in \mathscr{L}_H \\ \{p,q\} \in \mathcal{N}}} \frac{1}{2} |u(p) - u(q)| \,:\, u(\cdot) - \langle \nu, \cdot \rangle \quad T_H\text{-periodic} \right\} .$$

Since, up to translations, the periodicity cell contains the points $(0,0), (0,1)$ and since $u(\cdot) - \langle \nu, \cdot \rangle$ is T_H-periodic, we can infer that

$$|u(p) - u(q)| = |\langle p - q, \nu \rangle - t| \qquad \text{for some } t \in \mathbb{R} \,,$$

where $p \in span_{\mathbb{Z}} \left\{ \sqrt{3} e_1, \frac{-\sqrt{3}e_1 + 3e_2}{2} \right\}$ and $q \in \left(e_2 + span_{\mathbb{Z}} \left\{ \sqrt{3} e_1, \frac{-\sqrt{3}e_1 + 3e_2}{2} \right\} \right)$.
Hence, we get that

$$\|\nu\|_H = \frac{2}{3\sqrt{3}} \inf_t \left\{ |t + \nu_2| + \left| t + \frac{\sqrt{3}}{2}\nu_1 - \frac{1}{2}\nu_2 \right| + \left| t - \frac{\sqrt{3}}{2}\nu_1 - \frac{1}{2}\nu_2 \right| \right\} .$$

and this yields (2.3.2). For sake of conciseness, we omit all the explicit computations here, but for further details on the computation of a similar anisotropic norm, we refer to Proposition 2.5 of [12]. ♠

Remark 2.3.2. Before applying Definition 2.1.3, we need to find a scaling value $c > 0$ such that two rescaled Wulff shapes are tangent whenever $\{p,q\} \in \mathcal{N}$. Since each direction $\overline{p,q}$ intersect orthogonally the boundary of the Wulff shape, a straightforward computation shows that the right scaling value is $c = \frac{\sqrt{3}}{2}$. For sake of simplicity, from now on we denote the rescaled Wulff shape as

$$H := \frac{\sqrt{3}}{2} W_H \quad \text{and} \quad H(p) = p + H \quad \forall p \in \mathscr{L}_H \,. \tag{2.3.3}$$

Moreover, since we will need to compute the anisotropic perimeter of (2.1.2), we also remark that, by (2.3.2), $\forall p \in \mathcal{L}_H$ we get

$$\|\nu(x)\|_H = \begin{cases} \frac{\sqrt{3}}{3} & \text{for } x \in \partial^{\frac{1}{2}} H(p) \\ \frac{2}{3} & \text{for } x \in \partial^{\frac{1}{3}} H(p) \end{cases} . \tag{2.3.4}$$

Recalling the notation introduced in Remark 1.2.7, the case $x \in \partial^{\frac{1}{3}} H(p)$ corresponds to the directions of the vertices of $H(p)$ and we explicit this value since these directions are the ones connecting second-neighbouring points in $\mathcal{L}_H$ and we will need to consider them in the forthcoming computations, due to Definition 2.1.3. ♠

2.3.1 Geometric properties of ζ in $\mathcal{L}_H$

As in the case of the d-dimensional square lattice, we consider a set $X \in \mathcal{X}_N$ and we have to select a proper set for evaluating the local contributions to the measure and perimeter. Since it holds that

$$H \oplus \overline{p,q} \subset V(p) \cup V(q) \qquad \forall \{p,q\} \in \mathcal{n} ,$$

by Definition 2.1.5 we can choose the Voronoi cells as the localization sets. Since the honeycomb lattice is generated by the superposition of two Bravais lattices, by Definition 2.1.2, the 1-dimensional skeleton of $X \subset \mathcal{L}_H$ is composed of isolated points, segments connecting neighbouring points and segments linking second-neighbouring points in the configuration. Then, we can write $\Xi(X)$ as

$$\Xi(X) = \bigcup_{\substack{p \in X \\ val(p)=3}} \{p\} \cup \bigcup_{\substack{p,q \in X \\ \{p,q\} \in \mathcal{n}}} \overline{p,q} \cup \bigcup_{\substack{p,z \in X \\ (1.3.2) \text{ holds}}} \overline{p,z} \tag{2.3.5}$$

while we define the discrete-to-continuum map $\zeta \colon \mathcal{L}_H \to \mathcal{M}(\mathbb{R}^2)$ as

$$\zeta(X) = H \oplus \Xi(X) \qquad \forall X \in \mathcal{X}_N . \tag{2.3.6}$$

Before estimating the measure and the anisotropic perimeter of (2.3.6) in Proposition 2.3.4, we state the following lemma to simplify the computations: given $p \in X$, we quantify the contributions of (2.3.6) within each $V(p) \setminus H(p)$ in the two cases of first-neighbouring points and second-neighbouring points (see also Figure 2.4).

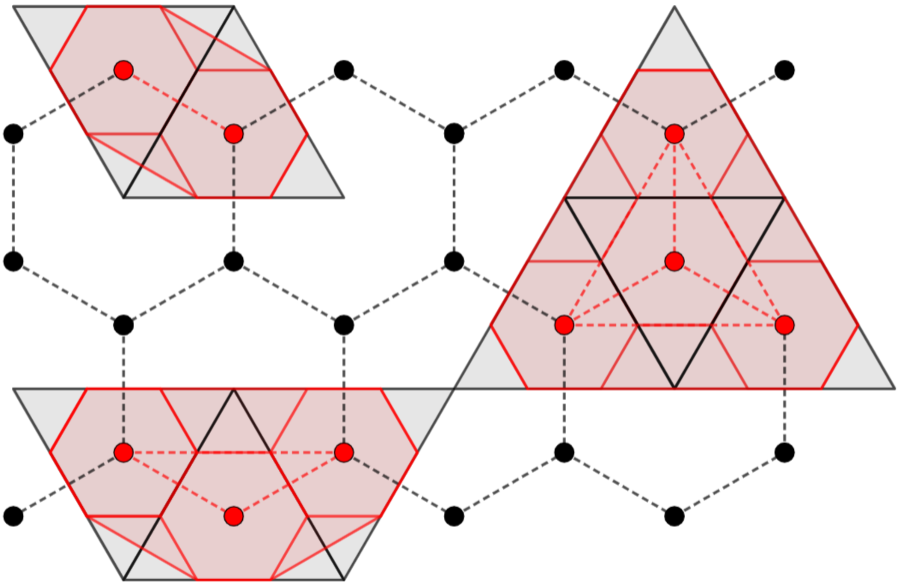

Figure 2.4: An example illustrating the behaviour of (2.3.6) on a given set $X \subset \mathcal{L}_H$ (shown as red points): the area covered by $\zeta(X)$ is depicted in red while the area of the Minkowski neighbourhoods of the points of X is in gray.

Lemma 2.3.3. *Let $X \in \mathcal{X}_N$, let $p \in X$ and let H be the set defined in* (2.3.3)*. Then, the followings hold:*

(i) if $q \in X$ is such that $\{p, q\} \in \mathcal{n}$, then

$$\left|(H \oplus \overline{p, q}) \cap \big(V(p) \setminus H(p)\big)\right| = \frac{\sqrt{3}}{12}$$
$$P_H\left(H \oplus \overline{p, q}\,,\ V(p) \setminus H(p)\right) = \frac{2}{3}\,.$$

(ii) if $z \in X$ is a second neighbour of p in X, then

$$\left|(H \oplus \overline{p, z}) \cap \big(V(p) \setminus H(p)\big)\right| = \frac{\sqrt{3}}{12}$$
$$P_H\left(H \oplus \overline{p, z}\,,\ V(p) \setminus H(p)\right) = \frac{1}{3}\,.$$

Proof of (i). If $\{p, q\} \in \mathcal{n}$, then $\left|(H \oplus \overline{p, q}) \cap V(p)\right|$ corresponds to half $|H(p)|$ plus the measure of the rectangle of basis length equal to $\mathcal{H}^1\big(\text{diam}(H(p))\big)$

and height equal to $\frac{\mathcal{H}^1(\overline{p,q})}{2}$. Thus, we have that

$$\left|(H \oplus \overline{p,q}) \cap \big(V(p) \setminus H(p)\big)\right| = \mathcal{H}^1\big(\mathrm{diam}(H(p))\big) \cdot \frac{\mathcal{H}^1(\overline{p,q})}{2} - \frac{|H(p)|}{2}\,.$$

Since, by construction, $\mathcal{H}^1\big(\mathrm{diam}(H(p))\big) = \frac{2\sqrt{3}}{3}$, $\frac{\mathcal{H}^1(\overline{p,q})}{2} = \frac{1}{2}$ and $|H(p)| = \frac{\sqrt{3}}{2}$, we get the desired value.
On the other hand, $P_H\left(H \oplus \overline{p,q}\,,\ V(p) \setminus H(p)\right)$ corresponds to the weighted 1-dimensional Hausdorff measure of the two segments of length $\frac{\mathcal{H}^1(\overline{p,q})}{2}$ parallel to $\overline{p,q}$. Since the outer unit normal $\nu(x)$ to these segments is parallel to $\nu_{H(p)}(x)$ for $x \in \partial^{\frac{1}{3}} H(p)$, by (2.3.4) we have that $\big\|\nu(x)\big\|_H$ is constantly equal to $\frac{2}{3}$. Hence, we get

$$\begin{aligned} P_H\left(H \oplus \overline{p,q}\,,\ V(p) \setminus H(p)\right) &= \int_{\partial^*(H\oplus\overline{p,q})\cap\left(V(p)\setminus H(p)\right)} \big\|\nu(x)\big\|_H \,\mathrm{d}\mathcal{H}^1(x) \\ &= \frac{2}{3} \cdot 2\frac{\mathcal{H}^1(\overline{p,q})}{2} = \frac{2}{3}\,. \end{aligned}$$

Proof of (ii). Similarly to the previous case, we can infer that $\left|(H \oplus \overline{p,q}) \cap V(p)\right|$ is equal to $|H(p)|$ plus one third of $|V(p) \setminus H(p)|$. Hence, we have

$$\left|(H \oplus \overline{p,z}) \cap \big(V(p) \setminus H(p)\big)\right| = \frac{|V(p)| - |H(p)|}{3} = \frac{\sqrt{3}}{12}\,.$$

On the other hand, $P_H\left(H \oplus \overline{p,z}\,,\ V(p) \setminus H(p)\right)$ corresponds to the weighted 1-dimensional Hausdorff measure of an edge of the equilateral triangle of side length equal to $\frac{\sqrt{3}}{3}$ (one of the congruent triangles composing $V(p) \setminus H(p)$). The outer unit normal to this edge is parallel to $\nu_{H(p)}(x)$ for $x \in \partial^{\frac{1}{2}} H(p)$ and hence it is constantly equal to $\frac{\sqrt{3}}{3}$ by (2.3.4). In the end, we get

$$P_H\left(H \oplus \overline{p,z}\,,\ V(p) \setminus H(p)\right) = \frac{\sqrt{3}}{3} \cdot \frac{\sqrt{3}}{3} = \frac{1}{3}\,.$$

□

Proposition 2.3.4. *Let* $X \in \mathcal{X}_N$ *and let* $\zeta\colon \mathcal{L}_H \to \mathcal{M}(\mathbb{R}^2)$ *be the map defined in* (2.3.6). *If we denote by* $\mathrm{Val}_k(X) = \#\{p \in X :\ \mathrm{val}(p) = k\}$, *then*

(i) $\frac{3\sqrt{3}}{4}\left(N - \frac{P(X)}{9}\right) \leq |\zeta(X)| \leq \frac{3\sqrt{3}}{4}\left(N - \frac{\mathrm{Val}_2(X)+3\mathrm{Val}_3(X)}{9}\right)$.

(ii) $P_H\big(\zeta(X)\big) = P(X) - \frac{\mathrm{Val}_2(X)+3\mathrm{Val}_3(X)}{3}$.

Proof. To compute (i) and (ii), we divide the proof in four different cases, based on the valence of the points of X. In the end, we sum up their contributions. To ease the notations, we set

$$H_M(p) := \zeta(X) \cap V(p)\,, \qquad P_H\left(H_M(p)\right) := P_H\left(\zeta(X), V(p)\right)\,.$$

We also observe that, within each $V(p)$, the map ζ affects the measure and the anisotropic perimeter by the quantities computed in Lemma 2.3.3; hence, it suffices to apply these two cases, while taking care to account for overlaps, to deduce the local contributions in the forthcoming computations.

Case 1: $\{p \in X : \operatorname{val}(p) = 3\}$.
Whenever p is an isolated point, we have $H_M(p) = H(p)$. Therefore, the local contributions of p are respectively

$$|H(p)| = \frac{\sqrt{3}}{2} \qquad \text{and} \qquad P_H\left(H(p)\right) = 2\,.$$

Case 2: $\{p \in X : \operatorname{val}(p) = 2\}$.
p has a unique first-neighbour in X, but it might have more 0, 1 or 2 second neighbours. We denote this amount by $N_2(p)$, that is

$$N_2(p) = \#\left\{z \in X : \text{(1.3.2) holds for } z\right\}\,,$$

and then we compute the three possible subcases.
For $N_2(p) = 0$, we have that the couple $\{p, q\}$ is isolated from the configuration X. Hence, we can apply directly the first point of Lemma 2.3.3: we obtain

$$\left|H_M(p)\right| = |H(p)| + \frac{\sqrt{3}}{12} = \frac{7\sqrt{3}}{12}\,,$$

while the perimeter contribution is equal to

$$\begin{aligned} P_H\left(H_M(p)\right) &= \frac{P_H\left(H(p)\right)}{2} + P_H\left(H \oplus \overline{p,q}\,,\ V(p) \setminus H(p)\right) \\ &= \frac{P_H\left(H(p)\right)}{2} + \frac{2}{3} = \frac{5}{3}\,. \end{aligned}$$

If $N_2(p) = 1$, we denote by q the first neighbouring point and by z_1 the unique second neighbour of p in X; then, the directions $\overline{p,q}$, $\overline{p,z_1}$ produce a overlap within $V(p)$ of the Minkowski sum. By Lemma 2.3.3, we have

$$\begin{aligned}|H_M(p)| = \quad & \Big|(H \oplus \overline{p,q}) \cap \big(V(p) \setminus H(p)\big)\Big| + \Big|(H \oplus \overline{p,z_1}) \cap \big(V(p) \setminus H(p)\big)\Big| \\ & + |H(p)| - \Big|(H \oplus \overline{p,q}) \cap (H \oplus \overline{p,z_1}) \cap \big(V(p) \setminus H(p)\big)\Big| \\ = \quad & \frac{\sqrt{3}}{12} + \frac{\sqrt{3}}{12} + \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{24} = \frac{15\sqrt{3}}{24}\,.\end{aligned}$$

Analogously, since half of the contribution of $P_H\left(H \oplus \overline{p,q}\,,\ V(p) \setminus H(p)\right)$ is covered by ζ in direction $\overline{p,z_1}$, we have

$$\begin{aligned}P_H\left(H_M(p)\right) &= \frac{P_H\left(H(p)\right)}{2} + \frac{P_H\left(H \oplus \overline{p,q}\,,\ V(p) \setminus H(p)\right)}{2} \\ &\qquad + P_H\left(H \oplus \overline{p,z_1}\,,\ V(p) \setminus H(p)\right) \\ &= \frac{P_H\left(H(p)\right)}{2} + \frac{1}{3} + \frac{1}{3} = \frac{5}{3}\,.\end{aligned}$$

If $N_2(p) = 2$, it is sufficient to compute the contributions in the direction of the two second neighbours z_1, z_2 of p in X: indeed, the Minkowski sum along the two $\overline{p,z_1}$ and $\overline{p,z_2}$ does not produce overlaps in $V(p) \setminus H(p)$, while it completely covers the contribution in the direction of the first neighbour q. Then, by the second point of Lemma 2.3.3, we have

$$\begin{aligned}\big|H_M(p)\big| &= |H(p)| + \sum_{k=1}^{2} \Big|(H \oplus \overline{p,z_k}) \cap \big(V(p) \setminus H(p)\big)\Big| \\ &= |H(p)| + 2\frac{\sqrt{3}}{12} = \frac{2\sqrt{3}}{3}\,.\end{aligned}$$

For the same motivation, the perimeter contribution is equal to half $P_H\left(H(p)\right)$ plus the perimeter contributions along $\overline{pz_1}$, $\overline{pz_2}$; hence, we get

$$\begin{aligned}P_H\left(H_M(p)\right) &= \frac{P_H\left(H(p)\right)}{2} + \sum_{k=1}^{2} P_H\left(H \oplus \overline{p,z_k}\,,\ V(p) \setminus H(p)\right) \\ &= \frac{P_H\left(H(p)\right)}{2} + \frac{2}{3} = \frac{5}{3}\,.\end{aligned}$$

To sum up, if $p \in X$ is such that $\operatorname{val}(p) = 2$, then

$$\frac{7\sqrt{3}}{12} \leq |H_M(p)| \leq \frac{2\sqrt{3}}{3} \qquad \text{and} \qquad P_H(H_M(p)) = \frac{5}{3}\,.$$

Case 3: $\{p \in X : \operatorname{val}(p) = 1\}$.
Similarly to Case 2, we have to consider different cases depending on $N_2(p) \in \{0, \dots, 4\}$. However, if we denote by q_1, q_2 the two first neighbours of p, then $\overline{q_1, q_2} \in \Xi(X)$, according to (2.3.5). Thus, the equilateral triangle T contained in $V(p) \setminus H(p)$ near $\overline{q_1, q_2}$ is fully covered by $\zeta(X)$, independently from the value $N_2(p)$ (see Figure 2.5). Hence, we can immediately infer that $|H_M(p)| > |H(p)| + \frac{\sqrt{3}}{12}$ and that it is sufficient to consider how many second neighbours of p in X lie outside the portion of plane delimited by the angle $\widehat{q_1 p q_2}$; we denote this quantity by $\widehat{N}_2(p)$ and, as before, $\widehat{N}_2(p) \in \{0, 1, 2\}$ gives three subcases.

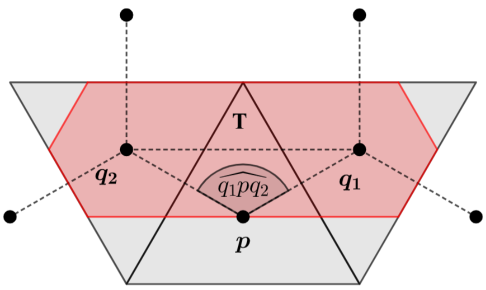

Figure 2.5: For $p, q_1, q_2 \in X$ such that $\{p, q_1\}, \{p, q_2\} \in \mathcal{n}$, we have $\overline{q_1, q_2} \in \Xi(X)$. If we denote by T the small equilateral triangle in the upper part of $V(p)$, then $T \subset H \oplus \overline{q_2, q_1} \subset \zeta(X)$. In red, the area covered by $H \oplus \overline{q_2, q_1}$.

If $\widehat{N}_2(p) = 0$, then it is enough to compute the contributions in the direction of the two first neighbours q_1, q_2 of p. Then, by Lemma 2.3.3, the measure contribution is

$$\begin{aligned} \big|H_M(p)\big| &= |H(p)| + \frac{\sqrt{3}}{12} + \sum_{k=1}^{2} \frac{\Big|(H \oplus \overline{p, q_k}) \cap \big(V(p) \setminus H(p)\big)\Big|}{2} \\ &= \frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{12} + \frac{\sqrt{3}}{12} = \frac{2\sqrt{3}}{3}, \end{aligned}$$

while the perimeter contribution is equal to $\frac{P_H(H(p))}{6}$ plus the half of the one given by the first neighbours

$$\begin{aligned} P_H\big(H_M(p)\big) &= \frac{P_H\big(H(p)\big)}{6} + \sum_{k=1}^{2} \frac{P_H\big(H \oplus \overline{p, q_k}\,,\ V(p) \setminus H(p)\big)}{2} \\ &= \frac{P_H\big(H(p)\big)}{6} + \frac{2}{3} = 1\,. \end{aligned}$$

If $\widehat{N}_2(p) = 1$, then we denote by z_1 this second neighbour of p in X and we assume, without loss of generality, that $\{p, q_1\}, \{q_1, z_1\} \in \mathcal{N}$. Therefore, we have that

$$\begin{aligned}\big|H_M(p)\big| &= |H(p)| + \frac{\sqrt{3}}{12} + \frac{\Big|(H \oplus \overline{p,q_2}) \cap \big(V(p) \setminus H(p)\big)\Big|}{2} \\ &\quad + \Big|(H \oplus \overline{p,z_1}) \cap \big(V(p) \setminus H(p)\big)\Big| \\ &= \frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{12} + \frac{\sqrt{3}}{24} + \frac{\sqrt{3}}{12} = \frac{17\sqrt{3}}{24},\end{aligned}$$

and the local perimeter is $\frac{P_H(H(p))}{6}$ plus the contributions in the directions $\overline{p,q_2}$, $\overline{p,z_1}$

$$\begin{aligned}P_H\big(H_M(p)\big) &= \frac{P_H\big(H(p)\big)}{6} + \frac{P_H\big(H \oplus \overline{p,q_2}\,,\ V(p) \setminus H(p)\big)}{2} \\ &\quad + P_H\big(H \oplus \overline{p,z_1}\,,\ V(p) \setminus H(p)\big) \\ &= \frac{P_H\big(H(p)\big)}{6} + \frac{1}{3} + \frac{1}{3} = 1\,.\end{aligned}$$

If $\widehat{N}_2(p) = 2$, then $H_M(p) = V(p)$ and $|H_M(p)| = \frac{3\sqrt{3}}{4}$. If we denote the two second neighbours of p in X by z_1, z_2, we get that the perimeter is $\frac{P_H(H(p))}{6}$ plus the contributions in the directions $\overline{p,z_1}, \overline{p,z_2}$:

$$\begin{aligned}P_H\big(H_M(p)\big) &= \frac{P_H\big(H(p)\big)}{6} + \sum_{k=1}^{2} P_H\big(H \oplus \overline{p,z_k}\,,\ V(p) \setminus H(p)\big) \\ &= \frac{P_H\big(H(p)\big)}{6} + \frac{2}{3} = 1\,.\end{aligned}$$

To sum up, if $p \in X$ is such that $\mathrm{val}(p) = 1$, then

$$\frac{2\sqrt{3}}{3} \le |H_M(p)| \le \frac{3\sqrt{3}}{4} \qquad \text{and} \qquad P_H(H_M(p)) = 1\,.$$

Case 4: $\big\{p \in X :\ \mathrm{val}(p) = 0\big\}$.
If p is an internal point of the configuration, then it immediately follows that $|H_M(p)| = |V(p)| = \frac{3\sqrt{3}}{4}$ and $P_H(H_M(p)) = 0$.

Since the Voronoi cells are a partition of $\mathbb{R}^2$, then both the measure and the anisotropic perimeter of ζ are given by the sum of the local contributions (see also Lemma 2.1.7). Since $|\zeta(X)| = \sum_{p\in X} \left|H_M(p)\right|$, by recalling that

$$N = \sum_{k=0}^{3} \mathrm{Val}_k(X) \quad \text{and} \quad P(X) = \sum_{i=1}^{N} \mathrm{val}(p_i) = \sum_{k=1}^{3} k\mathrm{Val}_k(X)\,,$$

we get conclusion (i):

$$\frac{3\sqrt{3}}{4}\left(N - \frac{P(X)}{9}\right) \le |\zeta(X)| \le \frac{3\sqrt{3}}{4}\left(N - \frac{\mathrm{Val}_2(X) + 3\mathrm{Val}_3(X)}{9}\right).$$

Similarly, conclusion (ii) is given by

$$\begin{aligned} P_H\left(\zeta(X)\right) &= \sum_{p\in X} P_H\left(H_M(p)\right) = \mathrm{Val}_1(X) + \frac{5}{3}\mathrm{Val}_2(X) + 2\mathrm{Val}_3(X) \\ &= P(X) - \frac{\mathrm{Val}_2(X) + 3\mathrm{Val}_3(X)}{3}\,. \end{aligned}$$

□

Remark 2.3.5. If we consider $X_k \subset \mathcal{L}_H$ such that $\#X_k = 6k^2$ for some $k \ge 1$, then we can construct "optimal quasi-hexagonal" configurations: it is sufficient to start from the six points that are the vertices of a regular hexagon in $\mathcal{L}_H$ of unitary side-length and then add all the neighbouring points until we enclose other $3(k-1) + 3(k-1)^2$ hexagons in our configuration (see Figure 2.6).
By construction, X_k has exactly $6k(k-1)$ internal points and $6k$ boundary points, whose valence is equal to 1; by Proposition 2.3.4, we have that

$$|\zeta(X_k)| \in \left[\frac{3\sqrt{3}}{4}\left(N - \frac{2k}{3}\right), \frac{3\sqrt{3}}{4}N\right] \quad \text{and} \quad P_H\big(\zeta(X_k)\big) = P(X_k)\,.$$

♠

Obviously, we cannot always expect to have "good" sets like those described in Remark 2.3.5. However, since in the following we are going to consider sets whose boundary energy is close to minimal one, it is reasonable to assume that configurations close to the minimal one contain few isolated points. Under this assumption, we obtain

$$P_H\left(\zeta(X)\right) \simeq P(X) - \frac{\mathrm{Val}_2(X)}{3} \quad \text{and} \quad |\zeta(X)| \le \frac{3\sqrt{3}}{4}\left(N - \frac{\mathrm{Val}_2(X)}{9}\right).$$

Improving these estimates by imposing conditions on $\mathrm{Val}_2(X)$ seems too

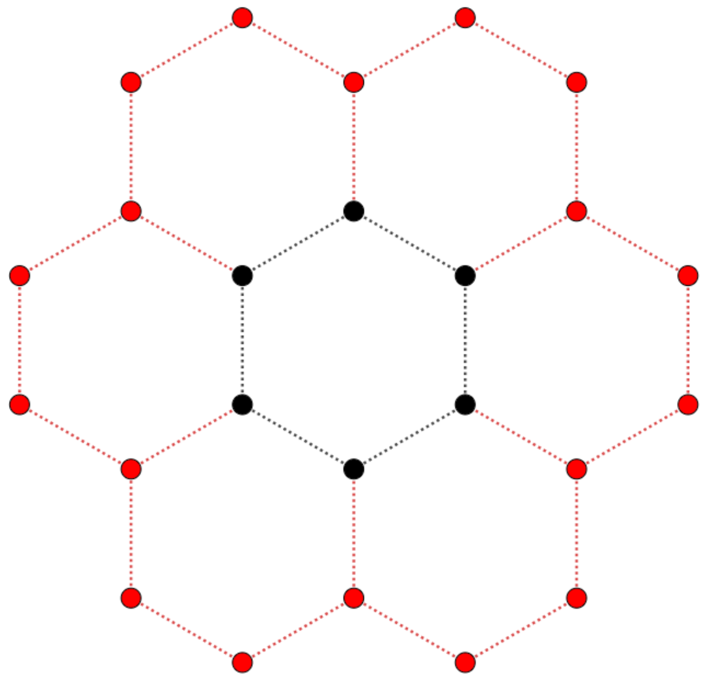

Figure 2.6: The set X_2, obtained by adding the red points to X_1 (in black).

much restrictive. Nevertheless, in the following Lemma, we show that considering sets with controlled boundary energy still allows us to avoid certain pathological configurations. For example, these sets cannot contain a large number of disconnected *dipoles*, i.e. couples of points $p, q \in X$ such that $\{p,q\} \in \mathcal{N}$ and

$$\nexists z \in X\,, z \neq p,q: \ \{p,z\} \in \mathcal{N} \text{ or } \{q,z\} \in \mathcal{N}\,. \tag{2.3.7}$$

(these configurations are the ones also considered in the first part of the second case of Proposition 2.3.4).

Lemma 2.3.6. *Let $X \in \mathcal{X}_N$ and let $\delta_1, \dots, \delta_M$ be dipoles (see (2.3.7)) for the configuration X. Let $h \geq 0$ be such that $6h^2 \leq N < 6(h+1)^2$ and assume that there exists $C > 0$ such that*

$$P(X) \leq \inf_{Y \in \mathcal{X}_{6(h+1)^2}} P(Y) + C\,. \tag{2.3.8}$$

Then, $M < 5 + \frac{C+\sqrt{3C}}{4}$.

Proof. If we denote by δ_i the couple (p_i, q_i), then it follows that

$$\mathrm{val}(\delta_i) = \mathrm{val}(p_i) + \mathrm{val}(q_i) = 4 \qquad \forall i = 1, \ldots, M\,.$$

Since the $\delta_1, \ldots, \delta_M$ are disconnected parts of the configuration, we also have

$$P(X) = \sum_{p \in X \setminus \{p_1, q_1, \ldots, p_M, q_M\}} \mathrm{val}(p) + 4M$$

If we consider $\hat{X} = X \setminus \bigcup_{i=1}^{M} \delta_i$, then there exist $k \geq 0$ such that $6k^2 \leq N - 2M \leq 6(k+1)^2$ and, by Remark 2.3.5, we can infer that

$$6k = \min_{Y \in \mathcal{X}_{N-2M}} P(Y) \leq P(\hat{X})\,.$$

Since $N - 2M < 6(k+1)^2$, we can infer also that

$$P(X) = P(\hat{X}) + 4M \geq 6k + 4M > 6\left(\sqrt{\frac{N-2M}{6}} - 1\right) + 4M$$

By (2.3.8) and by $6h^2 \leq N$, we get

$$6\left(\sqrt{\frac{N-2M}{6}} - 1\right) + 4M < 6\left(\sqrt{\frac{N}{6}} + 1\right) + C$$

and hence

$$6\left(\sqrt{\frac{N}{6}} - \sqrt{\frac{2M}{6}} - 1\right) + 4M < 6\left(\sqrt{\frac{N}{6}} + 1\right) + C\,.$$

A straightforward computation leads to $M < 5 + \frac{C + \sqrt{3C}}{4}$. □

Hence, from Lemma 2.3.6, we can infer that it is not restrictive to assume that, for a set X having anisotropic perimeter close to the minimum, the amount of dipoles is negligible as $\#X$ tends to infinity.

2.3.2 Q-closeness for ζ in $\mathcal{L}_H$

Now we want to apply Proposition 1.5.3 and we choose the discrete functionals as

$$\mathcal{E}_N \colon \mathcal{L}_H \to [0, +\infty] \quad \text{such that} \quad \mathcal{E}_N(X) = P(X) \quad \forall X \in \mathcal{X}_N\,, \tag{2.3.9}$$

and the continuous functional as

$$\mathcal{E}\colon \mathcal{M}(\mathbb{R}^2) \to [0,+\infty] \quad \text{such that} \quad \mathcal{E}(\Omega) = P_H(\Omega) \quad \forall \Omega \in \mathcal{M}(\mathbb{R}^2)\,. \tag{2.3.10}$$

The parameter β_N is null since by Proposition 2.3.4 we have

$$\mathcal{E}(\zeta(X)) = \mathcal{E}_N(X) - \frac{\mathrm{Val}_2(X) + 3\mathrm{Val}_3(X)}{3} \leq \mathcal{E}_N(X)\,,$$

while we need to be more careful with the parameter γ_N since $|\zeta(X)|$ is only estimated by Proposition 2.3.4.

Lemma 2.3.7. *Let the functionals $\mathcal{E}_N$, $\mathcal{E}$ be the ones defined respectively in* (2.3.9), (2.3.10). *Then it holds that*

$$\inf_{Y \in \mathcal{X}_N} \mathcal{E}_N(Y) \leq \inf_{\Omega \subset \mathbb{R}^2 \,:\, |\Omega| = |\zeta(X)|} \mathcal{E}(\Omega) + 8\,.$$

Proof. If $N = 6k^2$ for $k \geq 1$, then we can have a minimal quasi-hexagonal configuration X_k (the one described in Remark 2.3.5) such that

$$\inf_{Y \in \mathcal{X}_{6k^2}} P(Y) = P(X_k) = 6k\,.$$

Whenever $6k^2 \leq N < 6(k+1)^2$, we can construct an N-cardinality competitor X in the following way: starting from an optimal set X_{k+1} of $6(k+1)^2$ points, we first remove a random boundary point and then the boundary point that was a neighbour of the first one. Since it holds that

$$\sum_{q \in X_{k+1} \setminus \{p\}} \mathrm{val}(q) = \sum_{q \in X_{k+1}} \mathrm{val}(q) + 3 - 2\mathrm{val}(p)\,,$$

after removing two points p_1, p_2 we get $\sum_{q \in X_{k+1} \setminus \{p_1,p_2\}} \mathrm{val}(q) = \sum_{q \in X_{k+1}} \mathrm{val}(q)$ and then, by iterating, we can infer that $P(X) \leq P(X_{k+1}) + 1 = 6k + 7$ and

$$\inf_{Y \in \mathcal{X}_N} \mathcal{E}_N(X) \leq \mathcal{E}_N(X) \leq 6k + 7\,.$$

By Proposition 2.3.4 and the previous inequality, we have

$$\begin{aligned}
\inf_{\Omega\subset\mathbb{R}^2\,:\,|\Omega|=|\zeta(X)|}\mathcal{E}(\Omega) &= 2|W_H|^{\frac{1}{2}}|\zeta(X)|^{\frac{1}{2}} = \sqrt{\frac{8\sqrt{3}}{3}}|\zeta(X)|^{\frac{1}{2}}\\
&\geq \sqrt{6\left(N-\frac{P(X)}{9}\right)} \geq \sqrt{6\left(6k^2-\frac{6k+7}{9}\right)}\\
&\geq \sqrt{36k^2-4k-\frac{14}{3}} \geq 6k-1\,,
\end{aligned}$$

since $N \in [6k^2, 6(k+1)^2[$ for some $k \in \mathbb{N}$ such that $k > 1$. In the end, we obtain the thesis:

$$\inf_{Y\in\mathcal{X}_N}\mathcal{E}_N(Y) - \inf_{\Omega\subset\mathbb{R}^2\,:\,|\Omega|=|\zeta(X)|}\mathcal{E}(\Omega) \leq (6k+7)-(6k-1) = 8\,.$$

□

Now we can apply Proposition 1.5.3 and obtain a quantitative fluctuation estimate for the honeycomb lattice.

Proposition 2.3.8. *Let ζ be the map defined in* (2.1.2) *with respect to the rescaled Wulff shape H. Let $\mathcal{E}_N$, $\mathcal{E}$ be the functionals defined respectively in* (2.3.9), (2.3.10) *and let $X \in \mathcal{X}_N$ such that*

$$\mathcal{E}_N(X) \leq \inf_{Y\in\mathcal{X}_N}\mathcal{E}_N(Y) + \alpha_N\,, \tag{2.3.11}$$

then there exists a constant C such that

$$\inf_{x\in\mathbb{R}^2}\left|\zeta(X)\triangle(x+W_{H,|\zeta(X)|})\right| \leq C\,(\alpha_N+8)^{\frac{1}{2}}\,N^{\frac{3}{4}}$$

Proof. By Proposition 1.5.3, we have

$$\begin{aligned}
\inf_{x\in\mathbb{R}^2}\left|\zeta(X)\triangle\left(x+W_{H,|\zeta(X)|}\right)\right| &\leq C\left(\frac{\alpha_N+\beta_N+\gamma_N}{\mathcal{E}\left(W_{H,|\zeta(X)|}\right)}\right)^{\frac{1}{2}}|\zeta(X)|^{\frac{3}{4}}\\
&= C\left(\frac{\sqrt{3}}{4}(\alpha_N+\beta_N+\gamma_N)\right)^{\frac{1}{2}}|\zeta(X)|^{\frac{3}{4}}
\end{aligned}$$

The parameter β_N is null since $\mathcal{E}(\zeta(X)) \leq \mathcal{E}_N(X)$, while by Lemma 2.3.7 we get that $\gamma_N \leq 8$ and hence

$$\inf_{x\in\mathbb{R}^2} \left|\zeta(X)\triangle\left(x+W_{H,|\zeta(X)|}\right)\right| \leq C\left(\frac{\sqrt{3}}{4}(\alpha_N+8)\right)^{\frac{1}{2}} |\zeta(X)|^{\frac{3}{4}}$$

Then, by Proposition 2.3.4, we can conclude as follows:

$$\begin{aligned}\inf_{x\in\mathbb{R}^2} \left|\zeta(X)\triangle(x+W_{H,|\zeta(X)|}\right| &\leq C\left(\frac{\sqrt{3}}{4}(\alpha_N+8)\right)^{\frac{1}{2}}\left(\frac{3\sqrt{3}}{4}N\right)^{\frac{3}{4}}\\ &\leq \widetilde{C}\,(\alpha_N+8)^{\frac{1}{2}}\,N^{\frac{3}{4}}\,,\end{aligned}$$

where we set $\mathrm{Val}_k(X) = \#\{p\in X:\ \mathrm{val}(p)=k\}$. □

2.4 The triangular lattice

The triangular lattice is a 2-dimensional lattice having uniform spacing, whose points are arranged in periodic grid made by congruent equilateral triangles; a remarkable property is that the kissing number of this lattice is 6, that is the highest possible value in dimension 2 (see also Remark 1.3.7), and defines a hexagonal symmetry. Analogously to the d-dimensional square lattice, this is a Bravais lattice and, assuming that the lattice spacing is unitary, we can describe it as follows:

$$\mathcal{L}_T = span_{\mathbb{Z}}\left\{e_1, \frac{e_1+\sqrt{3}e_2}{2}\right\} \tag{2.4.1}$$

The periodicity cell of $\mathcal{L}_T$ is the rhombus generated by the two basis vectors of (2.4.1), while the Voronoi cell $V(p)$ of $p\in\mathcal{L}_T$ is a regular hexagon of side length equal to $\frac{\sqrt{3}}{3}$ and centred in p. By Theorem 1.3.14, we can compute the anisotropic norm associated to $\mathcal{L}_T$: since we have

$$\begin{aligned}\|\nu\|_T = \frac{2}{\sqrt{3}}\Bigg[\frac{1}{2}\Bigg(&|\langle\nu,e_1\rangle| + \left|\langle\nu,\frac{e_1+\sqrt{3}e_2}{2}\rangle\right| + \left|\langle\nu,\frac{e_1-\sqrt{3}e_2}{2}\rangle\right| +\\ &+|\langle\nu,-e_1\rangle| + \left|\langle\nu,\frac{-e_1-\sqrt{3}e_2}{2}\rangle\right| + \left|\langle\nu,\frac{-e_1+\sqrt{3}e_2}{2}\rangle\right|\Bigg)\Bigg]\,,\end{aligned}$$

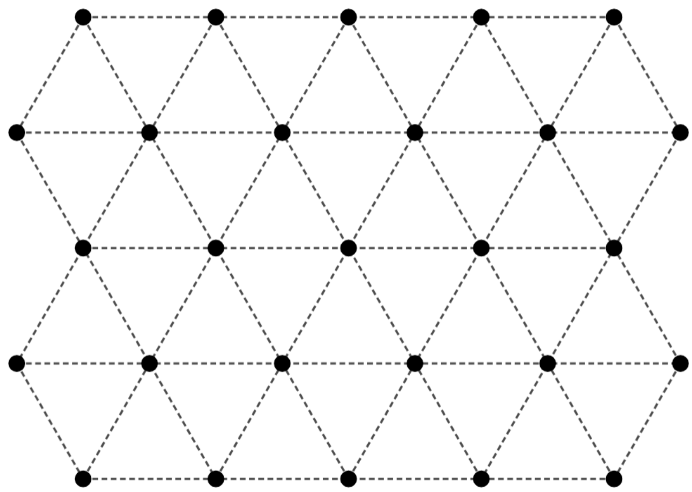

Figure 2.7: The triangular lattice $\mathcal{L}_T$

we immediately get that

$$\|\nu\|_T = \frac{2}{\sqrt{3}}\left(|\nu_1| + \left|\frac{\nu_1}{2} + \frac{\sqrt{3}}{2}\nu_2\right| + \left|\frac{\nu_1}{2} - \frac{\sqrt{3}}{2}\nu_2\right|\right) . \tag{2.4.2}$$

Thus, the Wulff shape associated to $\mathcal{L}_T$ is

$$W_T = \left\{x \in \mathbb{R}^2 : \; x \cdot \nu \leq \|\nu\|_T \text{ for all } \nu \in \mathbb{S}^1\right\} , \tag{2.4.3}$$

that, similarly to honeycomb lattice case, is the regular hexagon with vertices $\left(\frac{4}{\sqrt{3}}, 0\right)$, $\left(\frac{2}{\sqrt{3}}, 2\right)$, $\left(-\frac{2}{\sqrt{3}}, 2\right)$, $\left(-\frac{4}{\sqrt{3}}, 0\right)$, $\left(-\frac{2}{\sqrt{3}}, -2\right)$, $\left(\frac{2}{\sqrt{3}}, -2\right)$.
As before, by (1.2.7) and (1.2.8), we also have

$$P_T(E) = \int_{\partial^* E} \left\|\nu_E(x)\right\|_T \, \mathrm{d}\mathcal{H}^1(x) \geq P_T(W_{T,|E|}) ,$$

where $|W_{T,|E|}| = |E|$.

Remark 2.4.1. Similarly to the case of the honeycomb lattice discussed in Remark 2.3.2, the Wulff shape in (2.4.3) must be rescaled before using Definition 2.1.3. A simple computation shows that the right scaling value for (2.1.3) to be true is $\frac{\sqrt{3}}{8}$; thus, we set

$$T := \frac{\sqrt{3}}{8} W_T \quad \text{and} \quad T(p) = p + T \quad \forall p \in \mathcal{L}_H . \tag{2.4.4}$$

Moreover, from (2.4.2) we can also infer that $\forall p \in \mathscr{L}_T$

$$\big\|\nu(x)\big\|_T = 2 \qquad \forall x \in \partial^* T(p)\,. \tag{2.4.5}$$

♣

2.4.1 Geometric properties of ζ in $\mathscr{L}_T$

Differently from the lattices in Section 2.2 and Section 2.3, here we can not localize the computations within the Voronoi cells: indeed, for any $p, q \in \mathscr{L}_T$ such that $\{p,q\} \in \mathcal{N}$ it holds that

$$T \oplus \overline{p,q} \not\subset V(p) \cup V(q)\,.$$

Hence, according to Definition 2.1.5, the Minkowski neighbourhood in $p \in \mathscr{L}_T$ is given by

$$U(p) = \bigcup_{\substack{q \in \mathscr{L} \\ \{p,q\} \in \mathcal{N}}} \left(T \oplus \frac{\overline{p,q}}{2} \right)\,. \tag{2.4.6}$$

On the other hand, by (2.4.1), the $\mathscr{L}_T$ lattice is a Bravais lattice and its 1-dimensional skeleton of $X \in \mathcal{X}_N$ is given by the union of the isolated points of X and of the segments linking first-neighbouring points of X; thus, by Definition 2.1.2, the map ζ in the $\mathscr{L}_T$ lattice is

$$\zeta(X) = T \oplus \left(\bigcup_{\substack{p \in X \\ \mathrm{val}(p) = 6}} \{p\} \cup \bigcup_{\substack{p,q \in X \\ \{p,q\} \in \mathcal{N}}} \overline{p,q} \right)\,. \tag{2.4.7}$$

Remark 2.4.2. Conversely to the case where $U(p)$ coincides with the Voronoi cell, we observe that, in this setting, the Minkowski neighbourhood $U(p)$ is a non-convex set which overlaps with neighbouring Minkowski neighbourhoods (see also Figure 2.8 and Figure 2.9). Indeed, we have

$$\big|U(p) \cap U(q)\big| > 0 \qquad \forall p, q \in \mathscr{L}_T :\ \{p,q\} \in \mathcal{N}\,.$$

Therefore, a key challenge in estimating the measure and the perimeter of (2.4.7) via a local-to-global approach will be to combinatorially count the number of overlaps within each Minkowski neighbourhood (2.4.6), which depends on the valence of the points in $X \in \mathcal{X}_N$.

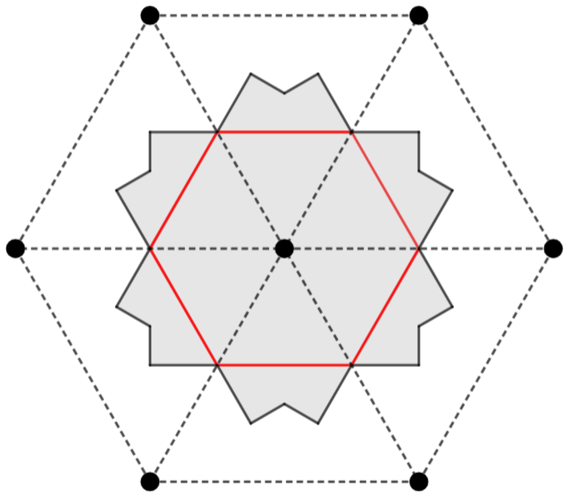

Figure 2.8: In gray, the Minkowski neighbourhood $U(p)$ of $p \in \mathcal{L}_T$. The red polygonal curve represents the boundary of the rescaled Wulff shape $T(p)$.

Moreover, we point out that formulas (2.1.6) and (2.1.7) hold by construction: indeed, for any $p, q \in X$ we have that $\mathcal{H}^1(\partial\zeta(X) \cap U(p) \cap U(q)) = 0$ and hence condition (2.1.5) is still true in the $\mathcal{L}_T$ lattice. ♠

Remark 2.4.3. Given $X \in \mathcal{X}_N$ and $p \in X$, we can also notice that the map (2.4.7) generates no overlaps within $U(p) \setminus T(p)$ whenever the first neighbours of p are not first neighbours of each other: namely, if $q_1, q_2 \in X$ such that $\{p, q_1\}, \{p, q_2\} \in \mathcal{N}$ and $\{q_1, q_2\} \notin \mathcal{N}$, we have

$$\left[\left(T \oplus \frac{\overline{p, q_1}}{2}\right) \setminus T(p)\right] \cap \left[\left(T \oplus \frac{\overline{p, q_2}}{2}\right) \setminus T(p)\right] = \emptyset\,. \tag{2.4.8}$$

The picture of $\left(T \oplus \frac{\overline{p,q}}{2}\right) \setminus T(p)$ can be seen in Figure 2.10. ♠

Analogously to the honeycomb case, before estimating the measure and the anisotropic perimeter of (2.4.7), we state a lemma to simplify the forthcoming computations.

Lemma 2.4.4. *Let $X \in \mathcal{X}_N$, let $p, q \in X$ such that $\{p, q\} \in \mathcal{N}$ and let $T(p)$*

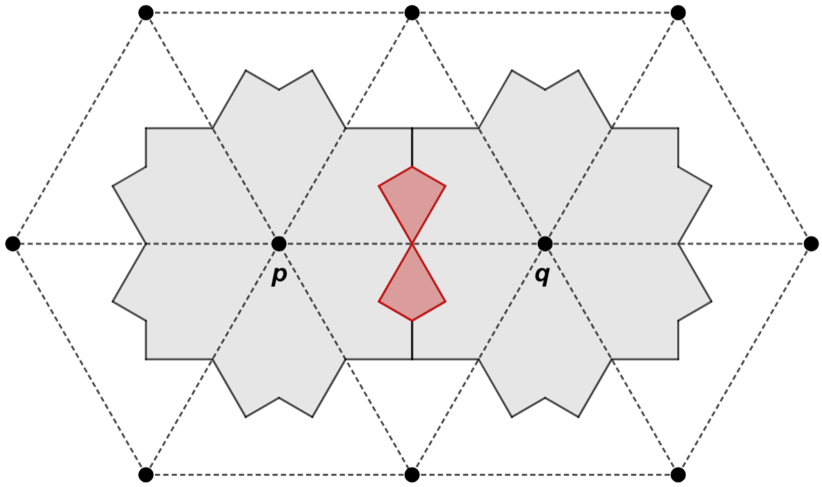

Figure 2.9: In gray, the Minkowski neighbourhoods $U(p)$, $U(q)$ of $p, q \in \mathcal{L}_T$ such that $\{p, q\} \in \mathcal{N}$. The red area represents their intersection.

be the set defined in (2.4.4)*. Then, it holds that*

$$\left| \left(T \oplus \frac{\overline{p,q}}{2} \right) \setminus T(p) \right| = \frac{\sqrt{3}}{16}$$

$$P_T \left(T \oplus \frac{\overline{p,q}}{2} \,,\; U(p) \setminus T(p) \right) = 1 \,,$$

Proof. By construction, $(T \oplus \frac{\overline{p,q}}{2}) \setminus T(p)$ consists of two congruent triangles (see Figure 2.10) whose catheti have lengths $\frac{1}{4}$ and $\frac{\sqrt{3}}{4}$. These values are a straightforward consequence of the fact that they are respectively one fourth of $\mathcal{H}^1(\overline{p,q})$ and one half of the height of the equilateral triangle of basis $\overline{p,q}$. Thus,

$$\left| \left(T \oplus \frac{\overline{p,q}}{2} \right) \setminus T(p) \right| = \frac{\sqrt{3}}{16} \,.$$

On the other hand, the perimeter contribution is equal to twice the length of the smaller cathetus, weighted by the norm of its outer unit normal, which coincides with the one in (2.4.5); therefore, we get

$$P_T \left(T \oplus \frac{\overline{p,q}}{2} \,,\; U(p) \setminus T(p) \right) = 2 \frac{\mathcal{H}^1(\overline{p,q})}{4} \cdot 2 = 1 \,.$$

□

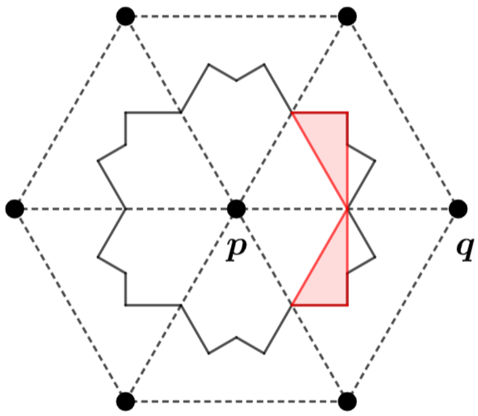

Figure 2.10: In red, the portion of $\mathbb{R}^2$ given by $\left|\left(T \oplus \frac{\overline{p,q}}{2}\right) \setminus T(p)\right|$.

Proposition 2.4.5. *Let $X \in \mathcal{X}_N$ and let $\zeta \colon \mathcal{L}_H \to \mathcal{M}(\mathbb{R}^2)$ be the map in* (2.4.7)*. Then,*

(i) $\frac{\sqrt{3}}{2}\left(N - \frac{P(X)}{24}\right) \leq |\zeta(X)| \leq \frac{\sqrt{3}}{2}\left(N + \frac{P(X)}{24}\right)$.

(ii) $P_T\left(\zeta(X)\right) = P(X)$.

Proof. Analogously to Proposition 2.3.4, we divide the proof in multiple case depending on the valence of the points of X and, in the end, we sum up the results. For sake of simplicity, we start by setting

$$T_M(p) := \zeta(X) \cap U(p) \quad \text{and} \quad P_T\left(T_M(p)\right) := P_T\left(\zeta(X), U(p)\right),$$

where $U(p)$ is the neighbourhood defined in (2.4.6).
Moreover, by Remark 2.4.3, we notice that there may be no overlaps in $\zeta(X)$ within $U(p) \setminus T(p)$ whenever $\mathrm{val}(p) \geq 4$.

Case 1: $\left\{p \in X : \, val(p) = 6\right\}$.
If p is an isolated point, then $T_M(p) = T(p)$. Hence $|T_M(p)| = \frac{3\sqrt{3}}{8}$ and

$$P_T\left(T_M(p)\right) = 2|W_T|^{\frac{1}{2}}|T(p)|^{\frac{1}{2}} = 2\sqrt{8\sqrt{3}|T(p)|} = 6\,.$$

Case 2: $\left\{p \in X : \, val(p) = 5\right\}$.

p has a unique neighbour $q \in X$. Then, by Lemma 2.4.4, we get

$$\begin{aligned} |T_M(p)| &= |T(p)| + \left| \left(T \oplus \frac{\overline{p,q}}{2} \right) \setminus T(p) \right| \\ &= |T(p)| + \frac{\sqrt{3}}{16} = \frac{7\sqrt{3}}{16}\,. \end{aligned}$$

On the other hand, by construction the perimeter contribution is equal to $\frac{2}{3}$ of the anisotropic perimeter of $T(p)$ plus $P_T\left(T \oplus \frac{\overline{p,q}}{2}\,,\ U(p) \setminus T(p)\right)$:

$$\begin{aligned} P_T\big(T_M(p)\big) &= P_T\left(T \oplus \frac{\overline{p,q}}{2}\,,\ T(p)\right) + P_T\left(T \oplus \frac{\overline{p,q}}{2}\,,\ U(p) \setminus T(p)\right) \\ &= \frac{2}{3} P_T\big(T(p)\big) + 1 = 5\,. \end{aligned}$$

Case 3: $\big\{p \in X :\ val(p) = 4\big\}$.
If we denote by $q_1, q_2 \in X$ the two first neighbours of p, then we need to consider only two subcases, depending on whether $\{q_1, q_2\} \in \mathcal{N}$ or not. Indeed, if $\{q_1, q_2\} \notin \mathcal{N}$, then by Remark 2.4.3 and (2.4.8) we get

$$|T_M(p)| = |T(p)| + \sum_{k=1}^{2} \left| \left(T \oplus \frac{\overline{p,q_k}}{2} \right) T(p) \right| = |T(p)| + \frac{\sqrt{3}}{8} = \frac{\sqrt{3}}{2}\,,$$

while the perimeter contribution is given by

$$\begin{aligned} P_T\big(T_M(p)\big) &= P_T\big(T_M(p), T(p)\big) + \sum_{k=1}^{2} P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p) \setminus T(p)\right) \\ &= \frac{P_T\big(T(p)\big)}{3} + 2 = 4\,. \end{aligned}$$

Otherwise, if $\{q_1, q_2\} \in \mathcal{N}$, then the map $\zeta(X) \cap U(p)$ covers completely, with some overlaps, the part of $U(p)$ inside the equilateral triangle $\overset{\triangle}{pq_1q_2}$ (see also Figure 2.11). Hence, it is sufficient to assign to $T_M(p) \cap \overset{\triangle}{pq_1q_2}$ a measure contribute equal to $\frac{|\overset{\triangle}{pq_1q_2}|}{3}$ and a null perimeter contribution. Outside $\overset{\triangle}{pq_1q_2}$, $T_M(p)$ coincides with $\frac{5}{6}$ of $T(p)$ united to half of $\left(T \oplus \frac{\overline{p,q_k}}{2}\right) \setminus T(p)$ for $k = 1, 2$.

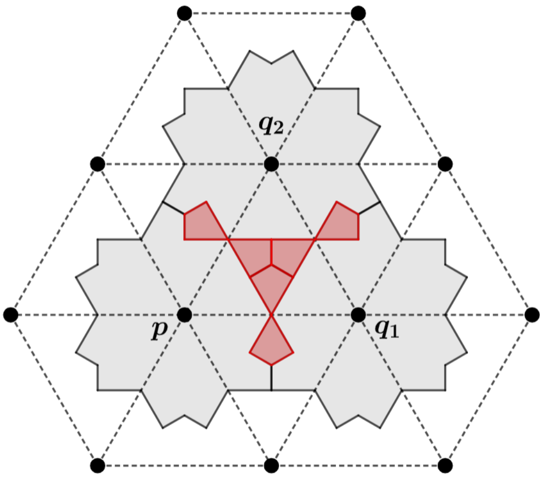

Figure 2.11: In gray, $U(p) \cup U(q_1) \cup U(q_2)$. The red areas represent their pairwise intersections. In particular, we have $\overset{\triangle}{pq_1q_2} \subset U(p) \cup U(q_1) \cup U(q_2)$.

By Lemma 2.4.4, we get

$$
\begin{aligned}
|T_M(p)| &= \frac{5}{6}|T(p)| + \sum_{k=1}^{2} \frac{\left|\left(T \oplus \frac{\overline{p,q_k}}{2}\right) \setminus T(p)\right|}{2} + \frac{|\overset{\triangle}{pq_1q_2}|}{3} \\
&= \frac{5}{6}|T(p)| + \frac{\sqrt{3}}{16} + \frac{\sqrt{3}}{12} = \frac{11\sqrt{3}}{24}\,.
\end{aligned} \tag{2.4.9}
$$

Similarly, the local perimeter is given by half of the perimeter of $T(p)$ plus half of the perimeter of both $P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p) \setminus T(p)\right)$:

$$
\begin{aligned}
P_T\left(T_M(p)\right) &= P_T\left(T_M(p), T(p)\right) + \sum_{k=1}^{2} \frac{P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p) \setminus T(p)\right)}{2} \\
&= \frac{P_T\left(T(p)\right)}{2} + 1 = 4\,.
\end{aligned} \tag{2.4.10}
$$

To sum up, if $p \in X$ is such that $\mathrm{val}(p) = 4$, then

$$
\frac{11\sqrt{3}}{24} \leq |T_M(p)| \leq \frac{\sqrt{3}}{2} \qquad \text{and} \qquad P_T\left(T_M(p)\right) = 4\,.
$$

Case 4: $\{p \in X \,:\, val(p) = 3\}$.

Again, we have to consider some subcases depending on the reciprocal positions of the three neighbours q_1, q_2, q_3 of p. We first suppose that $\{q_i, q_j\} \notin \mathcal{N}$ for each $i, j \in \{1,2,3\}$ with $i \neq j$: then, by (2.4.8) and by Lemma 2.4.4,

$$|T_M(p)| = |T(p)| + \sum_{k=1}^{3} \left| \left(T \oplus \frac{\overline{p,q_k}}{2} \right) \setminus T(p) \right| = |T(p)| + \frac{3\sqrt{3}}{16} = \frac{9\sqrt{3}}{16}$$

and the perimeter is given by three times $P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p) \setminus T(p)\right)$ (since $P_T\left(T_M(p), T(p)\right) = 0$)

$$P_T\left(T_M(p)\right) = \sum_{k=1}^{3} P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p) \setminus T(p)\right) = 3\,.$$

Now we suppose that, without loss of generality, $\{q_1, q_2\}, \{q_2, q_3\} \in \mathcal{N}$ (roughly speaking, p, q_1, q_2, q_3 are the vertices of a rhombus with $\overline{p, q_2}$ and $\overline{q_1, q_3}$ as diagonals). As in the Case 3, the map $\zeta(X)$ fully covers the regions inside the triangles $\overset{\triangle}{pq_1q_2}$, $\overset{\triangle}{pq_2q_3}$ and hence we assign to $T_M(p) \cap (\overset{\triangle}{pq_1q_2} \cup \overset{\triangle}{pq_2q_3})$ a measure contribute equal to $\frac{2|\overset{\triangle}{pq_1q_2}|}{3}$ and a null perimeter contribution; outside $\overset{\triangle}{pq_1q_2} \cup \overset{\triangle}{pq_2q_3}$, $T_M(p)$ coincides with two-third of $T(p)$ united to $\left(T \oplus \frac{\overline{p,q_k}}{2}\right) \setminus T(p)$ for $k = 1, 3$. Therefore, by Lemma 2.4.4, the measure contribution is

$$\begin{aligned} |T_M(p)| &= \frac{2}{3}|T(p)| + \sum_{k \in \{1,3\}} \frac{\left| \left(T \oplus \frac{\overline{p,q_k}}{2} \right) \setminus T(p) \right|}{2} + \frac{2|\overset{\triangle}{pq_1q_2}|}{3} \\ &= \frac{2}{3}|T(p)| + \frac{\sqrt{3}}{16} + \frac{\sqrt{3}}{6} = \frac{23\sqrt{3}}{48} \end{aligned}$$

and the perimeter contribution is

$$\begin{aligned} P_T\left(T_M(p)\right) &= P_T\left(T_M(p), T(p)\right) + \sum_{k \in \{1,3\}} \frac{P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p) \setminus T(p)\right)}{2} \\ &= \frac{1}{3} P_T\left(T(p)\right) + 1 = 3\,. \end{aligned}$$

Finally, we suppose that $\{q_1, q_2\} \in \mathcal{N}$ and $\{q_1, q_3\}, \{q_2, q_3\} \notin \mathcal{N}$. Then, p, q_1, q_2 form an equilateral triangle as in the second part of Case 3 and q_3, by (2.4.8), contributes independently of them. Hence, for this configuration, $|T_M(p)|$ can be obtained by adding $\left|\left(T \oplus \frac{\overline{p,q_3}}{2}\right) \setminus T(p)\right|$ to (2.4.9):

$$|T_M(p)| = \left|\left(T \oplus \frac{\overline{p,q_3}}{2}\right) \setminus T(p)\right| + \frac{11\sqrt{3}}{24} = \frac{25\sqrt{3}}{48}\,.$$

Similarly, the perimeter contribution can be obtained from (2.4.10) by adding $P_T\left(T \oplus \frac{\overline{p,q_3}}{2}\,,\ U(p) \setminus T(p)\right)$ and subtracting the part of $P_T\big(T(p)\big)$ covered by $\zeta(X)$ in direction $\overline{p,q_3}$: by Lemma 2.4.4,

$$\begin{aligned} P_T\big(T_M(p)\big) &= 4 + P_T\left(T \oplus \frac{\overline{p,q_3}}{2}\,,\ U(p) \setminus T(p)\right) - \frac{P_T\big(T(p)\big)}{3} \\ &= 2 + P_T\left(T \oplus \frac{\overline{p,q_3}}{2}\,,\ U(p) \setminus T(p)\right) = 3\,. \end{aligned}$$

To sum up, if $p \in X$ is such that $\mathrm{val}(p) = 3$, then

$$\frac{23\sqrt{3}}{48} \le |T_M(p)| \le \frac{9\sqrt{3}}{16} \qquad \text{and} \qquad P_T\big(T_M(p)\big) = 3\,.$$

Case 5: $\big\{p \in X :\ val(p) = 2\big\}$.
First, we assume that the two missing neighbours m_1, m_2 of p satisfy $\{m_1, m_2\} \in \mathcal{n}$ and we denote the four neighbours of p as $q_1, \ldots, q_4$ numbered counter-clockwise. Then, as in the previous two cases, $\zeta(X)$ fully covers the polygonal region with vertices $p, q_1, \ldots, q_4$. As before, we can assign to $T_M(p) \cap (p\overset{\triangle}{q_1}q_2 \cup p\overset{\triangle}{q_2}q_3 \cup p\overset{\triangle}{q_3}q_4)$ a measure contribution equal to $\frac{3|p\overset{\triangle}{q_1}q_2|}{3}$ and a null perimeter contribution. Outside this polygonal region, it is left to consider half of $T(p)$ and half of the contributions in the directions of q_1 and q_4. We get

$$\begin{aligned} |T_M(p)| &= \frac{1}{2}|T(p)| + \sum_{k \in \{1,4\}} \frac{\left|\left(T \oplus \frac{\overline{p,q_k}}{2}\right) \setminus T(p)\right|}{2} + |p\overset{\triangle}{q_1}q_2| \\ &= \frac{1}{2}|T(p)| + \frac{\sqrt{3}}{16} + \frac{\sqrt{3}}{4} = \frac{\sqrt{3}}{2}\,. \end{aligned}$$

and

$$P_T\big(T_M(p)\big) = P_T\big(T_M(p), T(p)\big) + \sum_{k\in\{1,4\}} \frac{P_T\Big(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p)\setminus T(p)\Big)}{2}$$
$$= \frac{P_T\big(T(p)\big)}{6} + 1 = 2\,.$$

If we assume that $\{m_1, m_2\} \notin \mathcal{n}$, then it is not restrictive to assume that they are symmetric with respect to p. Then, by symmetrizing, we can compute the measure contribution as twice the one in (2.4.9) minus $|T(p)|$, that is double-counted: we get

$$|T_M(p)| = 2\frac{11\sqrt{3}}{24} - |T(p)| = \frac{13\sqrt{3}}{24}\,.$$

Since $T(p)$ is fully covered by ζ, $P_T\big(T_M(p)\big)$ is given, for $k = 1, \ldots, 4$, by half of $P_T\Big(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p)\setminus T(p)\Big)$:

$$P_T\big(T_M(p)\big) = \sum_{k=1}^{4} \frac{P_T\Big(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p)\setminus T(p)\Big)}{2} = 2\,.$$

To sum up, if $p \in X$ is such that $\mathrm{val}(p) = 2$, then

$$\frac{\sqrt{3}}{2} \le |T_M(p)| \le \frac{13\sqrt{3}}{24} \qquad \text{and} \qquad P_T\big(T_M(p)\big) = 2\,.$$

Case 6: $\big\{p \in X :\ val(p) = 1\big\}$.
p has a unique missing neighbour m, then there is a unique possible configuration, up to rotations. Similarly to the previous Cases, if we denote by $q_1, \ldots, q_5$ the neighbours of p in counter-clockwise order, then, by Lemma 2.4.4, we have

$$|T_M(p)| = \frac{1}{3}|T(p)| + \sum_{k\in\{1,5\}} \frac{\Big|\Big(T \oplus \frac{\overline{p,q_k}}{2}\Big)\setminus T(p)\Big|}{2} + \frac{4|\overset{\triangle}{pq_1q_2}|}{3}$$
$$= \frac{1}{3}|T(p)| + \frac{\sqrt{3}}{16} + \frac{\sqrt{3}}{3} = \frac{25\sqrt{3}}{48}\,.$$

$P_T\big(T_M(p)\big)$ is equal to half of the perimeter contribution in the two directions

$\overline{p,q_1}$, $\overline{p,q_5}$ since $P_T\left(T_M(p), T(p)\right) = 0$:

$$P_T\left(T_M(p)\right) = \sum_{k\in\{1,5\}} \frac{P_T\left(T \oplus \frac{\overline{p,q_k}}{2}\,,\ U(p)\setminus T(p)\right)}{2} = 1\,.$$

Case 7: $\{p \in X:\ val(p) = 0\}$.
Finally, if p is an interior point, then it follows that $P_T(T_M(p)) = 0$ and $|T_M(p)| = |V(p)| = \frac{\sqrt{3}}{2}$ by Remark 2.1.6.

In the end, by $P(X) = \sum_{k=1}^{6} k\cdot\#\{p\in X:\ \mathrm{val}(p)=k\}$ and by (2.1.7), we obtain that the anisotropic perimeter of $\zeta(X)$ is

$$P_T\left(\zeta(X)\right) = \sum_{p\in X}\mathrm{val}(p) = P(X)\,.$$

By summing the measure contribution, we end up with

$$\frac{\sqrt{3}}{48}\sum_{k=0}^{6} C_k\cdot\#\left\{p\in X:\ \mathrm{val}(p)=k\right\}\ ,$$

where $C_0 = 24$, $C_1 = 25$, $C_2 \in \{24, 26\}$, $C_3 \in \{23, 25, 27\}$, $C_4 \in \{22, 24\}$, $C_5 = 21$ and $C_6 = 18$. By recalling that $N = \sum_{k=0}^{6}\#\{p\in X:\ \mathrm{val}(p)=k\}$, we get the conclusion:

$$\frac{\sqrt{3}}{2}\left(N - \frac{P(X)}{24}\right) \le |\zeta(X)| \le \frac{\sqrt{3}}{2}\left(N + \frac{P(X)}{24}\right)\,.$$

□

Remark 2.4.6. We observe that (2.4.7) generates the same figure as the one defined in [13] for $\mathcal{L}_T$. In fact, by construction, (2.4.7) completely covers the internal points of $X \in \mathcal{X}_N$ and, on each connected component of X, its boundary forms closed polygonal curves passing though the midpoints of the segments connecting the points of X with their missing neighbours. Thus, Proposition 3 of [13] can be applied to (2.4.7) and we obtain that

$$\left|\zeta(X)\right| = \sum_{p\in X}|V(p)| - \sum_{k=1}^{M}\frac{\sqrt{3}}{8}\left(1 - \#\{\text{holes of }\zeta(X_k)\}\right)\ ,$$

where $V(p)$ denotes the Voronoi cell of $\mathcal{L}_T$ centred in p and $X_1,\ldots,X_M$ denote the connected components of $X \in \mathcal{X}_N$.

Then, if we know the number of holes and connected components of the given set X, we can improve the measure estimate in Proposition 2.4.5: since $|V(p)| = \frac{\sqrt{3}}{2}$ for any $p \in X$, we can infer

$$\left|\zeta(X)\right| = \frac{\sqrt{3}}{2}N - \frac{\sqrt{3}}{8}\left(M - \#\{\text{holes of } \zeta(X)\}\right) .$$

♠

2.4.2 Q-closeness for ζ in $\mathcal{L}_T$

We choose the discrete functional as

$$\mathcal{E}_N \colon \mathcal{L}_T \to [0, +\infty] \quad \text{such that} \quad \mathcal{E}_N(X) = P(X) \quad \forall X \in \mathcal{X}_N \,, \tag{2.4.11}$$

and the continuous functional as

$$\mathcal{E} \colon \mathcal{M}(\mathbb{R}^2) \to [0, +\infty] \quad \text{such that} \quad \mathcal{E}(\Omega) = P_T(\Omega) \quad \forall \Omega \in \mathcal{M}(\mathbb{R}^2) \,. \tag{2.4.12}$$

Again, we can immediately infer that the parameter β_N in Definition 1.5.2 is null since by Proposition 2.4.5 we have

$$\mathcal{E}(\zeta(X)) = P(X) = \mathcal{E}_N(X) \,. \tag{2.4.13}$$

In the following Lemma, similarly to what we have previously done in Lemma 2.3.7 for the honeycomb lattice, we estimate the value of γ_N for $\mathcal{L}_T$:

Lemma 2.4.7. *Let the functionals $\mathcal{E}_N$, $\mathcal{E}$ be the one defined respectively in* (2.4.11)*,* (2.4.12)*. Then it holds that*

$$\inf_{Y \in \mathcal{X}_N} \mathcal{E}_N(Y) \leq \inf_{\Omega \subset \mathbb{R}^2 \,:\, |\Omega| = |\zeta(X)|} \mathcal{E}(\Omega) + 18$$

Proof. We start by noticing that, if $N = 1 + 3k + 3k^2$ for some $k \geq 0$, then we can construct a minimal hexagonal arrangement X_k with the following algorithm: starting from a point $p \in \mathcal{L}_T$, we iteratively add all the points in $\mathcal{L}_T$ that are first neighbours of the current configuration. By construction, the boundary energy of X_k satisfies

$$\inf_{Y \in \mathcal{X}_{1+3k+3k^2}} P(Y) = P(X_k) = 6(2k+1) \,. \tag{2.4.14}$$

Then, whenever $1 + 3k + 3k^2 \leq N < 1 + 3(k+1) + 3(k+1)^2$, we construct an optimal competitor $\hat{X} \in \mathcal{X}_N$ in the following way: starting from an optimal set X_{k+1}, we remove a boundary point p with $\mathrm{val}(p) = 3$ and then we iterate

this procedure on the new boundary points.
Since

$$\sum_{q\in X\setminus\{p\}} \mathrm{val}(q) = \sum_{q\in X} \mathrm{val}(q) + 6 - 2\mathrm{val}(p)\,, \tag{2.4.15}$$

and since in the first $6k$ steps we can always choose a point having valence equal to 3, we can infer that we do not change the boundary energy value and that

$$P(\hat{X}) = P(X_{k+1}) \quad \text{if } N \in [7+3k+3k^2, 1+3(k+1)+3(k+1)^2[\,.$$

Otherwise, if $N \in [1+3k+3k^2, 7+3k+3k^2[$, then we continue the algorithm by iteratively removing a point having maximal valence. Thus, by (2.4.15), we get that $P(\hat{X}) < P(X_{k+1})$.
Hence, by (2.4.14), we can infer that

$$\inf_{Y\in\mathcal{X}_N} P(Y) \leq P(\hat{X}) \leq P(X_{k+1}) = 6(2k+3) \tag{2.4.16}$$

for any $N \in \left[1+3k+3k^2,\, 1+3(k+1)+3(k+1)^2\right[$.
By the measure estimate in Proposition 2.4.5, we can infer that

$$\begin{aligned}\inf_{\Omega\subset\mathbb{R}^2\,:\,|\Omega|=|\zeta(\hat{X})|} \mathcal{E}(\Omega) &= 2|W_T|^{\frac{1}{2}}|\zeta(\hat{X})|^{\frac{1}{2}} = \sqrt{32\sqrt{3}}|\zeta(\hat{X})|^{\frac{1}{2}} \\ &\geq \sqrt{48\left(N - \frac{P(\hat{X})}{24}\right)} \\ &\geq \sqrt{48(1+3k+3k^2) - 2(12k+18)} \geq 12k\,,\end{aligned}$$

where the last row follows from (2.4.16). By (2.4.11), the conclusion follows:

$$\inf_{Y\in\mathcal{X}_N} \mathcal{E}_N(Y) - \inf_{\Omega\subset\mathbb{R}^2\,:\,|\Omega|=|\zeta(X)|} \mathcal{E}(\Omega) \leq 6(2k+3) - 12k = 18\,.$$

□

Now we can apply Proposition 1.5.3 to the functionals (2.4.11) and (2.4.12):

Proposition 2.4.8. *Let ζ be the map defined in* (2.4.7)*. Let $\mathcal{E}_N$, $\mathcal{E}$ be the functionals defined respectively in* (2.4.11), (2.4.12) *and let $X \in \mathcal{X}_N$ such that*

$$\mathcal{E}_N(X) \leq \inf_{Y\in\mathcal{X}_N} \mathcal{E}_N(Y) + \alpha_N\,. \tag{2.4.17}$$

Then, there exists a constant C such that

$$\inf_{x\in\mathbb{R}^2}\left|\zeta(X)\triangle\left(x+W_{T,|\zeta(X)|}\right)\right| \le C\left(\alpha_N+18\right)^{\frac{1}{2}} N^{\frac{3}{4}}\,.$$

Proof. We apply Proposition 1.5.3 with the parameters β_N, γ_N given by (2.4.13) and Lemma 2.4.7: we have

$$\inf_{x\in\mathbb{R}^2}\left|\zeta(X)\triangle\left(x+W_{T,|\zeta(X)|}\right)\right| \le C\left(\frac{\alpha_N+18}{16\sqrt{3}}\right)^{\frac{1}{2}} |\zeta(X)|^{\frac{3}{4}}\,.$$

By Proposition 2.4.5, we conclude as follows:

$$\begin{aligned}\inf_{x\in\mathbb{R}^2}\left|\zeta(X)\triangle\left(x+W_{T,|\zeta(X)|}\right)\right| &\le C\left(\frac{\alpha_N+18}{16\sqrt{3}}\right)^{\frac{1}{2}}\left[\frac{\sqrt{3}}{2}\left(N+\frac{P(X)}{24}\right)\right]^{\frac{3}{4}}\\ &\le \widetilde{C}\left(\alpha_N+18\right)^{\frac{1}{2}}\left(N+\frac{P(X)}{24}\right)^{\frac{3}{4}}\\ &\le \widehat{C}\left(\alpha_N+18\right)^{\frac{1}{2}} N^{\frac{3}{4}}\,.\end{aligned}$$

□

2.5 Final considerations on the definition of ζ

Our construction of the map ζ, as explained in Definition 2.1.3, allowed us, via a unified approach, to obtain estimates for the measure and anisotropic perimeter of two of the most relevant 2-dimensional lattices, as well as for the $\mathbb{Z}^d$ lattice. Although the resulting bounds involve suboptimal constants and exponents, the maximal fluctuation estimates derived from the Q-closeness technique depend only on the dimension; hence, we attempted to obtain analogous results for other higher-dimensional lattices. In particular, our interest was partly inspired by the results in [12], where the authors determine the Wulff shapes for the face-centred cubic (FCC) lattice $\mathcal{L}_{FCC}$ and the hexagonal close-packed (HCP) lattice $\mathcal{L}_{HCP}$, two of the most significant lattices in $\mathbb{R}^3$.

However, the map ζ failed to yield meaningful estimates for the FCC lattice. The main reason for this failure may lie in the inability of (2.1.2) to construct continuous boundary surfaces that form a proper thickening of the underlying discrete structure. This issue could potentially be resolved by modifying the definition of ζ to allow the rescaled Wulff shape to move along closed two-dimensional polygons that connect neighbouring points in the configuration, rather than restricting it to the straight edges between them. Defining such polygons, however, is challenging: a meaningful local definition would require taking into account the relative positions of all neighbouring points, whereas we would prefer to base our construction only the local datum given by the number of neighbouring points in the given lattice.

For further details on this issue in the case of the FCC lattice, we refer to the Appendix, where we briefly show that Definition 2.1.3 leads to a trivial fluctuation estimate.

Chapter 3

Q-closeness for the discrete Faber-Krahn Inequality

In this chapter, we refer the results obtained in collaboration with M. Cicalese, L. Kreutz, and G.P. Leonardi, which are presented in [14]. In that work, we establish a discrete counterpart of the quantitative inequality of Theorem 3.1.3 for a discrete version of the first eigenvalue functional (3.1.1) via the Q-closeness technique introduced in [13].

In Section 3.1 we motivate our interest in the quantitative discrete Faber-Krahn by summarizing some basic result on the classic inequality and by stating its quantitative estimate. Then, in Section 3.2, we define a discrete functional λ_N that resembles the continuous one and we prove that this functional has good analytical properties and that its definition is well-posed in the sense of Γ-convergence. In Section 3.3, we report some results on the rearrangement of discrete functions, which serves as a key tool in establishing a discrete version of the Faber–Krahn inequality of Theorem 3.1.1. Moreover, we use the this technique to deduce some geometric properties of the minimizers of λ_N. Afterwards, in Section 3.4, we introduce a suitable choice for the discrete-to-continuous map ζ, which ensures that λ_N is Q-close to the continuous functional in (3.1.1) as N goes to $+\infty$, and allows us to apply Proposition 1.5.3. Eventually, in Section 3.5, following appropriate error estimates, we derive the quantitative inequality in Theorem 3.6.1.

Differently from the previous chapter, all definitions, remarks, and computations are made specifically on the d-dimensional square lattice $\mathbb{Z}^d$. Therefore, before proceeding, we fix some useful notation introduced in the previous chapter:

- we denote by $\mathcal{L}_Q = \mathbb{Z}^d$ the d-dimensional square lattice; in the following, we will sometimes omit to specify it when it is clear from the context
- again, we denote by $\{p, q\} \in \mathcal{N}$ an unordered couple of neighbouring points p, q in $\mathbb{Z}^d$ and by $\mathcal{X}_N$ the sets of all the subsets of $\mathbb{Z}^d$ having cardinality N (i.e., $\mathcal{X}_N = \{Y \subset \mathbb{Z}^d : \#Y = N\}$).

3.1 The Quantitative Faber-Krahn Inequality

Given the Dirichlet problem

$$\begin{cases} -\triangle u = \lambda u & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \,, \end{cases}$$

the first eigenvalue problem consist in studying the behaviour of the eigenvalue λ depending on the choice of u and of the domain Ω. For a fixed Ω, the value of the first eigenvalue can be computed by solving the following variational problem:

$$\lambda(\Omega) = \min_{u \in H_0^1(\Omega)} \left\{ \int_\Omega |\nabla u(x)|^2 \, \mathrm{d}x : \ \|u\|_{L^2(\Omega)} = 1 \right\} . \tag{3.1.1}$$

We may also ask under which assumptions on Ω the quantity (3.1.1) is minimized. This problem was solved by Faber and Krahn, who proved Lord Rayleigh's conjecture by showing the following inequality:

Theorem 3.1.1. *Let $\Omega \subset \mathbb{R}^d$ with smooth boundary and let $B_{|\Omega|}$ be the d-dimensional ball such that $\left|B_{|\Omega|}\right| = |\Omega|$. Then,*

$$\lambda\left(B_{|\Omega|}\right) \leq \lambda(\Omega) \tag{3.1.2}$$

and the equality holds if and only if $|\Omega \triangle B_{|\Omega|}| = 0$ (up to translations).

Remark 3.1.2. By (3.1.1), we can infer that the first eigenvalue functional λ satisfies the following scaling law:

$$\lambda(t\Omega) = \frac{1}{t^2}\lambda(\Omega) \qquad \forall t > 0 \,.$$

Thus, it is not restrictive to consider inequality (3.1.2) on sets having unitary measure:

$$\lambda\,(\Omega) \geq \lambda(B_1) \quad \forall \Omega : \ |\Omega| = 1 \,.$$

Moreover, we may also rewrite (3.1.1) by extending u to zero outside the given set Ω and we obtain

$$\lambda(\Omega) = \min_{u \in H^1(\mathbb{R}^d)} \left\{ \int_{\mathbb{R}^d} |\nabla u(x)|^2 \, \mathrm{d}x : \ \|u\|_{L^2(\mathbb{R}^2)} = 1, \ u = 0 \text{ in } \mathbb{R}^d \setminus \Omega \right\}.$$

♣

As for the Euclidean isoperimetric inequality, the ball continues to be the optimal shape also for the first eigenvalue functional (3.1.1). This raised questions about the stability of this solution and brought to quantitative estimates analogously to Theorem 1.2.15 and Theorem 1.2.22. As we mentioned in the Introduction, a first result is due to Fusco, Maggi, and Pratelli in [26], who proved that there exists a purely dimensional non-negative constant C_d such that

$$\inf_{x \in \mathbb{R}^d} \left| \Omega \triangle (x + B_1) \right| \leq C_d \left(\lambda(\Omega) - \lambda(B_1) \right)^{\frac{1}{4}}$$

for $\Omega \mathcal{M}(\mathbb{R}^d)$ such that $|\Omega| = 1$. In 2013, Brasco, De Philippis and Velichkov provided, in [9], the quantitative inequality with sharp exponent:

Theorem 3.1.3 (Brasco, De Philippis, Velichkov)**.** *Let $\Omega \subset \mathbb{R}^d$ such that $|\Omega| = 1$. Then, there exists a purely dimensional constant $C_d > 0$ such that*

$$\inf_{x \in \mathbb{R}^d} \left| \Omega \triangle (x + B_1) \right| \leq C_d \left(\lambda(\Omega) - \lambda(B_1) \right)^{\frac{1}{2}} \tag{3.1.3}$$

Remark 3.1.4. We point out that both the results in [26] and in [9] are more general than the one we stated before: indeed, they involve in (3.1.1)the L^p-norm of ∇u and the L^q-norm of u (with suitable choices of q). However, the formulation given in Theorem 3.1.3 is enough for our purposes. ♣

3.2 The discrete functional

In (3.1.1) we evaluate the L^2-norm of the gradient of given functions. On the $\mathbb{Z}^d$ lattice, we define the gradient of a function $u \colon \mathbb{Z}^d \to \mathbb{R}$ as the difference in function values between adjacent grid points, divided by the distance between them, as it is usually done in the mathematical literature. Hence, we have

Definition 3.2.1. Given a function $u\colon \mathbb{Z}^d \to \mathbb{R}$, we define its **discrete Dirichlet energy** $D(u)$ as

$$D(u) = \sum_{\{i,j\}\in\mathcal{N}} |u(i) - u(j)|^2 .$$

Then, given a discrete set $X \subset \mathbb{Z}^d$ and a function $u\colon \mathbb{Z}^d \to \mathbb{R}$, we define some discrete functionals associated to X and u, which we will consider in the rest of this chapter. In particular, since we will consider lattices that haven't unitary spacing, our definition highlights the dependence on the scaling $N^{-\frac{1}{d}}$, that is the cardinality of $X \in \mathcal{X}_N$.

Definition 3.2.2. Given $X \in \mathcal{X}_N$ and $P(X)$ the discrete perimeter in Definition 1.3.12, then we denote the **scaled discrete perimeter** of X as

$$P_N(X) = N^{-\frac{d-1}{d}} P(X) .$$

Moreover, given $u\colon \mathbb{Z}^d \to \mathbb{R}$ such that $\operatorname{supp}(u) \subset X$, we denote the **scaled discrete Dirichlet energy** as

$$D_N(u) = N^{-\frac{d-2}{d}} D(u) . \tag{3.2.1}$$

Now we are ready to define λ_N, the discrete counterpart of the continuous functional defined in (3.1.1):

Definition 3.2.3. Given $X \in \mathcal{X}_N$, we define the **discrete first eigenvalue functional** $\lambda_N\colon \mathcal{X} \longrightarrow \mathbb{R}^+$ as

$$\lambda_N\big(X\big) = \min\left\{ D_N(u) :\ u(i) = 0 \text{ in } \mathbb{Z}^d \setminus X\,, \quad \frac{1}{N}\sum_{i\in\mathbb{Z}^d} u^2(i) = 1 \right\} . \tag{3.2.2}$$

As in (3.1.1), the functional λ_N in Definition 3.2.3 is scaling-invariant and, if there exists $Y_N \in \mathcal{X}_N$ such that

$$\lambda_N(Y_N) \le \lambda_N(X) \quad \text{for all } X \in \mathcal{X}_N\,,$$

then we call Y_N a minimal set for λ_N and we set

$$m_{\lambda,N} := \inf\{\lambda_N(X)\colon X \in \mathcal{X}_N\} . \tag{3.2.3}$$

Remark 3.2.4. It is not restrictive to assume that the minimal function u in (3.2.2) has constant sign: indeed, since

$$\big|u(i)-u(j)\big| \geq \big||u(i)|-|u(j)|\big| \qquad \forall u(i), u(j) \in \mathbb{R}\,,$$

then $D_N(u) \geq D_N\big(|u|\big)$. Hence we can assume that $u(i) \geq 0$ on $X \in \mathcal{X}_N$ without loss of generality. ♠

3.2.1 Γ-convergence

Definition 3.2.2 is justified by a Γ-convergence viewpoint. Given $X \in \mathcal{X}_N$ and $u\colon \mathbb{Z}^d \to \mathbb{R}$, we set the denote the rescaled lattice and the rescaled periodicity cell respectively as

$$\mathcal{L}_Q^{N,d} := N^{-\frac{1}{d}}\mathbb{Z}^d\,, \qquad Q_{N^{-\frac{1}{d}}}(i) := i + \left(N^{-\frac{1}{d}}\left[-\frac{1}{2},\frac{1}{2}\right]^d\right) \text{ for } i \in \mathcal{L}_Q^{N,d}$$

and then we define the piecewise-constant interpolation of u on $\mathcal{L}_Q^{N,d}$ as

$$\overline{u}_N(x) := u\left(N^{\frac{1}{d}}i\right) \quad \text{for } x \in Q_{N^{-\frac{1}{d}}}(i) \text{ and } i \in \mathcal{L}_Q^{N,d}\,. \tag{3.2.4}$$

Remark 3.2.5. If u is such that $\sum_{i\in\mathbb{Z}^d} u(i)^p = N$, we get that the function in (3.2.4) satisfies

$$\|\overline{u}_N\|_{L^p(\mathbb{R}^d)} = 1\,.$$

Furthermore, if $u = 0$ on $\mathbb{Z}^d \setminus N^{\frac{1}{d}}\Omega$ for some $\Omega \subseteq \mathbb{R}^d$ open and bounded, we have that, for all $N \in \mathbb{N}$

$$\operatorname{supp}(\overline{u}_N) \subset (\Omega)_{N^{-\frac{1}{d}}\sqrt{d}} = \left\{p \in \mathbb{Z}^d :\ \mathrm{d}(p,\Omega) \leq N^{-\frac{1}{d}}\sqrt{d}\right\}$$

♠

Thanks to the interpolation in (3.2.4), we can extend the discrete Dirichlet functional in Definition 3.2.2 to a function on $L^2(\mathbb{R}^d)$, with a slight abuse of notation.

Definition 3.2.6. Given an open and bounded set $\Omega \subset \mathbb{R}^d$, given a function $u\colon \mathbb{Z}^d \to \mathbb{R}$ such that

$$\frac{1}{N}\sum_{i\in\mathbb{Z}^d} u^2(i) = 1 \qquad \text{and} \qquad u = 0 \text{ on } \mathbb{Z}^d \cap \left(\mathbb{R}^d \setminus N^{\frac{1}{d}}\Omega\right)\,,$$

we define

$$\mathscr{D}_N(v,\Omega) = \begin{cases} D_N(u) & \text{if } v = \overline{u}_N \text{ for } u \\ +\infty & \text{otherwise}. \end{cases} \tag{3.2.5}$$

For this functional, thanks to Theorem 1.4.4, Remark 1.4.5 and the properties in Remark 3.2.5, we get the following convergence result:

$$\Gamma\left(L^2(\mathbb{R}^d)\right) \text{ - } \lim_{N\to+\infty} \mathscr{D}_N(v,\Omega) = \begin{cases} \int_{\mathbb{R}^d} |\nabla v|^2 \, \mathrm{d}x & \text{if } \begin{cases} v \in H^1(\mathbb{R}^d) \\ v = 0 \text{ on } \mathbb{R}^d \setminus \Omega \\ \|v\|_{L^2(\mathbb{R}^d)} = 1 \end{cases} \\ +\infty & \text{otherwise on } L^2(\mathbb{R}^d). \end{cases}$$

Remark 3.2.7. By the Fundamental Theorem of Γ-convergence (Theorem 1.4.3), if $X_N = N^{\frac{1}{d}}\Omega \cap \mathbb{Z}^d$ for some bounded and open $\Omega \subset \mathbb{R}^d$, from the previous Γ-convergence result we can also deduce that

$$\lim_{N\to+\infty} \lambda_N(X_N) = \lambda(\Omega),$$

where λ_N, λ are the functions defined respectively in (3.2.2), (3.1.1). ♠

Remark 3.2.8. Similarly, we can obtain a Γ-convergence result also for the scaled perimeter in Definition 3.2.2: indeed, we can argue as before and we can read P_N as defined on $L^1(\mathbb{R}^d)$ (with a slight abuse of notation) as follows:

$$P_N(v) = \begin{cases} P_N(X) & \text{if } v = \overline{u}_N \text{ for } u = \chi_X \text{ and } X \in \mathcal{X}_N, \\ +\infty & \text{otherwise.} \end{cases}$$

Then, thanks to [1, Theorem 4] and the properties of the interpolation described in Remark 3.2.5, we get the following:

$$\Gamma(L^1(\mathbb{R}^d)) \text{ - } \lim_{N\to+\infty} P_N(v) = \begin{cases} \int_{\partial^*\Omega} \|\nu_\Omega\|_{L^1} \, \mathrm{d}\mathcal{H}^{d-1} & \text{if } \begin{cases} v = \chi_\Omega \in BV(\mathbb{R}^d) \\ \|v\|_{L^1(\mathbb{R}^d)} = 1 \end{cases} \\ +\infty & \text{otherwise on } L^1(\mathbb{R}^d). \end{cases}$$

Moreover, we also recall that $\|\nu\|_1$ is exactly the anisotropic norm associated to $\mathbb{Z}^d$, as we have already computed in (2.2.1). Hence, as in Remark 3.2.7, we obtain

$$\lim_{N\to+\infty} P_N(X_N) = P_Q(\Omega).$$

♠

3.2.2 Boundedness of minimum value

In the following Lemma we prove that the value $m_{\lambda,N}$ in (3.2.3) assumed by the discrete functional λ_N is finite:

Lemma 3.2.9. *There exists $C_d > 0$ such that, for all $N \in \mathbb{N}$, it holds*

$$m_{\lambda,N} \le C_d \,.$$

Proof. We prove that, for each $N \in \mathbb{N}$, it is possible to construct a competitor $X \in \mathcal{X}_N$ such that

$$\lambda_N(X) \le C_d$$

for some $C_d > 0$ independent of N.
We start by proving the inequality on the sets having $N = (2k+1)^d$ points defined as $X_k = [-k,k]^d \cap \mathbb{Z}^d$ for $k \in \mathbb{N}$, $k \ge 0$. Let $u\colon \mathbb{Z}^d \to \mathbb{R}$ be defined by

$$u(i) = C_{d,N}(k-l) \quad \forall i \in \mathbb{Z}^d : \ \|i\|_\infty = l \text{ and } 0 \le l \le k \,,$$

where $C_{d,N} > 0$ is such that $\sum_{i\in\mathbb{Z}^d} u^2(i) = N$. Since

$$N = \sum_{l=0}^{k} C_{d,N}^2 (k-l)^2 \# \left\{ i \in X_k : \ \|i\|_\infty = l \right\}$$

and $l^{d-1} \le \# \left\{ i \in X_k : \ \|i\|_\infty = l \right\} \le 2dl^{d-1}$, we can infer that

$$N \le 2dC_{d,N}^2 \sum_{l=0}^{k} (k-l)^2 l^{d-1} \le 2dC_{d,N}^2 k^{d+2}$$

and that

$$N \ge C_{d,N}^2 \sum_{l=0}^{k} (k-l)^2 l^{d-1} \ge \hat{c}_d C_{d,N}^2 k^{d+2}$$

for some $\hat{c}_d > 0$. Thus, we can infer that there exists a constant $c_d > 0$ such that

$$\frac{1}{c_d} N^{-\frac{1}{d}} \le C_{d,N} \le c_d N^{-\frac{1}{d}} \,.$$

Then, we obtain that

$$D_N(u) = N^{-\frac{d-2}{d}} \sum_{\{i,j\}\in n} \big|u(i) - u(j)\big|^2 \leq N^{-\frac{d-2}{d}} \sum_{i\in X_k} \sum_{j\in\mathbb{Z}^d \,:\, \{i,j\}\in n} C^2_{d,N}$$
$$\leq N^{-\frac{d-2}{d}} C^2_{d,N} 2dN \leq 2dc_d^2 =: C_d\,.$$

If $N \in \big[(2k+1)^d, (2k+3)^d\big[$ for $k \geq 0$, then it is sufficient to consider, as competitor, the previous set X_k rescaled to keep the mass constraint; the thesis follows since $(2k+3)^d \leq 3^d(2k+1)^d$. □

3.2.3 Uniqueness of the minimizing function

We report here properties of the functions that minimize (3.2.2) We start by the introducing the notion of connectedness of subsets of $\mathbb{Z}^d$.

Definition 3.2.10. We say that $X \subset \mathbb{Z}^d$ is **connected** if, for all $p, q \in X$, there exist $M \in \mathbb{N}$ and points $p_1, \ldots, p_M \in X$ such that

$$\begin{cases} p_0 = p, \quad p_M = q\,, \\ (p_k, p_{k+1}) \in n \quad \forall k = 0, \ldots, M-1\,. \end{cases}$$

Given $X \subset \mathbb{Z}^d$ we call a connected component of X any maximal (with respect to set inclusion) connected subset of X.

Proposition 3.2.11. *Let $X \subset \mathbb{Z}^d$ be a connected set. Then, the following holds:*

(i) *any minimizer u of* (3.2.2) *is such that $u(i) > 0$ for each $i \in X$;*

(ii) *there exists a unique function that minimizes* (3.2.2).

Proof. Proof of (i). By Remark 3.2.4, we can assume that $u(i) \geq 0$ on X and we are only left to prove the strict inequality.
Let us suppose by contradiction that there exists a minimizer u that vanishes on $A \subseteq X$ (maximal with respect to set inclusion) such that $M := \#A < \#X$. Then, for $t \in (0,1)$ we consider $u^t \colon \mathbb{Z}^d \to \mathbb{R}$ defined by

$$u^t(i) := \begin{cases} tu(i) & \text{if } i \in \mathbb{Z}^d \setminus A\,, \\ \sqrt{\frac{N}{M}(1-t^2)} & \text{if } i \in A\,. \end{cases}$$

Let us point out that, for each $t \in (0,1)$, it holds that

$$\begin{aligned}\frac{1}{N}\sum_{i\in\mathbb{Z}^d}(u^t(i))^2 &= \frac{1}{N}\sum_{i\in\mathbb{Z}^d\setminus A} t^2u^2(i) + \frac{1}{N}\sum_{i\in A}\left(\sqrt{\frac{N}{M}(1-t^2)}\right)^2\\ &= t^2 + (1-t^2) = 1\end{aligned}$$

and hence u^t is a competitor for the minimum in (3.2.2). However, the Dirichlet energy of u^t is

$$\begin{aligned}D(u^t) = &\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i,j\in\mathbb{Z}^d\setminus A}} |u^t(i)-u^t(j)|^2 + 2\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i\in\mathbb{Z}^d\setminus A, j\in A}} |u^t(i)-u^t(j)|^2\\ &+ \sum_{\substack{\{i,j\}\in\mathcal{N}\\ i,j\in A}} |u^t(i)-u^t(j)|^2\\ &= t^2\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i,j\in\mathbb{Z}^d\setminus A}} |u(i)-u(j)|^2 + 2\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i\in\mathbb{Z}^d\setminus A, j\in A}} \left|t\,u(i) - \sqrt{\frac{N}{M}(1-t^2)}\right|^2\\ &= t^2D(u) + 2\sqrt{\frac{N}{M}(1-t^2)}\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i\in\mathbb{Z}^d\setminus A, j\in A}}\left(-2t\,u(i) + \sqrt{\frac{N}{M}(1-t^2)}\right).\end{aligned}$$

Note that, since X is connected and A is maximal with respect to set inclusion, there exist $\{i_0, j\} \in \mathcal{N}$ with $i_0 \in \mathbb{Z} \setminus A$ and $j \in A$ such that $u(i_0) > 0$. Since the sum (being finite) on the right-hand side of the previous equation is continuous in t, and for $t = 1$ we have

$$\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i\in\mathbb{Z}^d\setminus A,\, j\in A}} -2u(i) \le -2u(i_0) < 0\,,$$

there exists $t \in (0,1)$ such that

$$2\sqrt{\frac{N}{M}(1-t^2)}\sum_{\substack{\{i,j\}\in\mathcal{N}\\ i\in\mathbb{Z}^d\setminus A,\, j\in A}}\left(-2t\,u(i) + \sqrt{\frac{N}{M}(1-t^2)}\right) < 0\,.$$

This yields a contradiction to the minimality of u.

Proof of (ii). Let us suppose that u, v are both minimizers of $\lambda_N(X)$ in (3.2.2). Thanks to part (i) we can assume that $u, v > 0$ on X. Given $t \in (0,1)$, let us define $w^t \colon \mathbb{Z}^d \to \mathbb{R}$ as

$$w^t(i) := \big(tu^2(i) + (1-t)v^2(i)\big)^{1/2} .$$

Since $\frac{1}{N}\sum_{i\in X}|w_i^t|^2 = 1$, w^t is a competitor for $\lambda_N(X)$. Moreover, for $\{i,j\} \in \mathcal{N}$ it holds that

$$|w^t(i) - w^t(j)|^2 = t\big(u^2(i) + u^2(j)\big) + (1-t)\big(v^2(i) + v^2(j)\big) - 2\Bigg(t^2u^2(i)u^2(j) + (1-t)^2v^2(i)v^2(j) + t(1-t)(u^2(i)v^2(j) + u^2(j)v^2(i))\Bigg)^{\frac{1}{2}}$$

Since

$$0 \le D_N(w^t) - \lambda_N(X) = D_N(w^t) - tD_N(u) - (1-t)D_N(v)\,,$$

by expanding the squares and by the previous calculation, we get that

$$0 = 2\sum_{\{i,j\}\in\mathcal{N}}\Bigg[tu(i)u(j) + (1-t)v(i)v(j) - \Bigg(t^2u^2(i)u^2(j) + (1-t)^2v^2(i)v^2(j) + t(1-t)(u^2(i)v^2(j) + u^2(j)v^2(i))\Bigg)^{\frac{1}{2}}\Bigg].$$

By standard computations, we notice that each term in the last sum is equivalent to

$$-t(1-t)\Bigg(u(i)v(j) - u(j)v(i)\Bigg)^2,$$

and hence we can infer that each term is non-positive and that it equals zero if and only if $u(i)v(j) = u(j)v(i)$. Since X is connected, $u(i) = \alpha v(i)$ for some $\alpha > 0$ and for all i. By the constraint on the norm, we infer that $\alpha = 1$ which concludes the proof of (ii). □

3.3 Discrete rearrangements

The classic proof of the Faber-Krahn inequality (3.1.2) relies on symmetrization arguments, such as the Riesz rearrangement inequality or the Polya-Szego inequality; however, these tools can not be used in the discrete setting and we need to introduce a discrete version of them. In this section, we will report some definitions and results on the discrete Riesz rearrangement that are introduced in [42] and [30].

We start by setting some useful notations:

- we denote by D the set of admissible directions in $\mathbb{Z}^d$

$$D = \Big\{ e_i, e_i + e_j, e_i - e_j \colon i, j = 1, \dots, d \text{ and } i < j \Big\} .$$

  For sake of simplicity, in the following we will sometimes refer to the elements of D as $\{v_1, \dots, v_{d^2}\}$ and, for $k \in \mathbb{N}$, we set $v_k = v_{((k-1) \bmod d^2)+1}$.

- given $e \in D$, we denote with Π_e the hyperplane orthogonal to e:

$$\Pi_e = \begin{cases} \mathbb{Z}^d \cap \{x \colon \langle x, e\rangle = 0\} & \text{if } e = e_k\,, \\ \mathbb{Z}^d \cap \big\{x \colon \langle x, e\rangle \in \{0,1\}\big\} & \text{if } e = e_i \pm e_j\,. \end{cases} \tag{3.3.1}$$

- given $u \colon \mathbb{Z}^d \to [0, +\infty)$ and $q \in \Pi_e$, we denote as $u^{q,e} \colon \mathbb{Z} \to [0, +\infty)$ the restriction of u to the 1-dimensional slice of $\mathbb{Z}^d$ in direction e passing through q, namely

$$u^{q,e}(t) = u(q + te) \quad \text{for } t \in \mathbb{Z}\,.$$

Remark 3.3.1. We notice that, if we fix $e \in D$, then each point of $\mathbb{Z}^d$ can be uniquely written as $i = q + te$ for some $q \in \Pi_e$ and some $t \in \mathbb{Z}$. Hence, we can extend the previous notation to the slices of a given $X \in \mathcal{X}_N$; indeed, we set

$$(X)^{q,e} = \{t \in \mathbb{Z} \colon q + te \in X\}\,.$$

♠

Using the set of directions D we can introduce the notion of convexity for discrete sets and the notion of symmetric decreasing rearrangement of a function. This last one is defined constructively, starting from functions whose domain is contained in $\mathbb{Z}$ and then by extending to domains in $\mathbb{Z}^d$ by slicing; in particular, we refer to the original construction defined in [29, Definition 2.1], [30, Paragraph 2.2] and [30, Definition 4.11].

Definition 3.3.2. Given a direction $e \in D$, we say that $X \subset \mathbb{Z}^d$ is e-**convex** if for every $x \in X$ and $x + Ke \in X$ for some $K \in \mathbb{N}$ we have that $x + ke \in X$

for all $k = 1, \ldots, K-1$. We call a set $X \subset \mathbb{Z}^d$ **direction-convex** if it is e-convex for all $e \in D$.

Definition 3.3.3. Let $u\colon \mathbb{Z} \to [0,+\infty)$ be a function with finite support. Let $\{\alpha_i\}_{i\in\mathbb{N}}$ with $\alpha_i \geq \alpha_{i+1}$ be the values taken by u. We define the **1-dimensional symmetric decreasing rearrangement** of u as

$$u^*(i) = \begin{cases} \alpha_{1-2i} & \text{if } i \leq 0\,, \\ \alpha_{2i} & \text{if } i > 0\,. \end{cases}$$

Given $d \geq 2$, $e \in D$ and $u\colon \mathbb{Z}^d \to [0,+\infty)$ with finite support, we define the **symmetric decreasing rearrangement of u in direction e** as

$$u^{*e}(i) := (u^{q,e})^*(t) \quad \text{for } i = q + te\,,\ q \in \Pi_e\,.$$

Furthermore, setting $u^0 = u$ and $u^k = (u^{k-1})^{*v_k}$, the **symmetric decreasing rearrangement of u** is defined as

$$u^* := \lim_{k\to+\infty} u^k\,.$$

From Definition 3.3.3, the notion of discrete rearrangement of a set immediately follows from the rearrangement of its characteristic function: indeed, given a finite set $X \in \mathcal{X}_N$, its symmetric rearrangement in direction e is defined as

$$R_e(X) := \operatorname{supp}(\chi_X^{*e})\,,$$

while its symmetric rearrangement is defined as

$$R(X) := \operatorname{supp}(\chi_X^{*})\,.$$

Therefore, we say that a finite set $X \in \mathcal{X}_N$ is symmetric if

$$R_e(X) = X \quad \text{for all } e \in D\,.$$

Remark 3.3.4. We remark the following properties of the rearrangement:

(i) In [30] it has been shown that for $u\colon \mathbb{Z}^d \to [0,+\infty)$ with finite support u^* is well-defined and is achieved in a finite number of iteration, namely

$$\exists \hat{k} \text{ such that } u^k = u^{k+1} \qquad \forall k \geq \hat{k}.$$

Obviously, if $X \subset \mathbb{Z}^d$ is a finite set, the same holds for $R(X)$.

(ii) The Cavalieri Principle holds:

$$\sum_{i\in\mathbb{Z}^d} u^2(i) = \sum_{i\in\mathbb{Z}^d} (u(i)^*)^2 .$$

(iii) Note that for $X \in \mathcal{X}_N$ it holds that $\#R_e(X) = \#R(X) = N$.

♣

3.3.1 Discrete Riesz Rearrangement Inequality

Before stating a discrete version of the Riesz rearrangement inequality, we introduce the notion of supermodular function.

Definition 3.3.5. A function $G\colon \mathbb{R}\times\mathbb{R} \to \mathbb{R}$ is said to be **supermodular** if, for any $x, y \in \mathbb{R}$ and for any $s, t > 0$, it holds

$$G(x, y+t) + G(x+s, y) \le G(x+s, y+t) + G(x, y) .$$

If we have a supermodular function, then it is possible to show a Riesz rearrangement inequality; similarly to Definition 3.3.3, this is done by steps, starting from the one-dimensional case and then by generalizing it. As far as we know, the one-dimensional Riesz rearrangement inequality has been proved firstly in [29, Proposition 4.3] via a polarization argument and the higher-dimensional Riesz inequality has been proved in [30, Theorem 1.2].

Theorem 3.3.6 (1-dimensional Riesz rearrangement inequality)**.** *Let $u, v : \mathbb{Z} \longrightarrow [0, +\infty)$ be two functions with finite support. Let $H\colon \mathbb{N} \longrightarrow [0, +\infty)$ be non-increasing. Let $G\colon [0, +\infty) \times [0, +\infty) \longrightarrow [0, +\infty)$ be a supermodular function such that $G(0, 0) = 0$. Then,*

$$\sum_{i,j\in\mathbb{Z}} G\left(u(i), v(j)\right) H\left(|i-j|\right) \le \sum_{i,j\in\mathbb{Z}} G\left(u^*(i), v^*(j)\right) H\left(|i-j|\right) .$$

In [29], sufficient conditions for the equality case in Theorem 3.3.6 are also provided. However, since these conditions rely on the injectivity of the functions u and v, which cannot be expected in our setting, we do not report them here. The same consideration applies to the forthcoming d-dimensional inequality.

Theorem 3.3.7 (Riesz rearrangement inequality). *Let $u, v : \mathbb{Z}^d \longrightarrow [0, +\infty)$ be two functions with finite support. Let $H : \mathbb{Z} \longrightarrow [0, +\infty)$ be such that $H(t)$ is non-increasing as $|t|$ increases. Let $G : [0, +\infty) \times [0, +\infty) \longrightarrow [0, +\infty)$ be a supermodular function such that $G(0, 0) = 0$. Then,*

$$\sum_{i,j\in\mathbb{Z}^d} G\left(u(i), v(j)\right) H\left(\|i-j\|_{L^1}\right) \leq \sum_{i,j\in\mathbb{Z}^d} G\left(u^*(i), v^*(j)\right) H\left(\|i-j\|_{L^1}\right) .$$

We remark that Theorem 3.3.7 is stated slightly differently than in [30]: indeed, we replaced the assumption $H(t) = H(|t|)$ with with the requirement that the kernel $H(t)$ must be non-increasing as $|t|$ increases, as this is key property needed for rearrangements along a generic direction $e \in D$. Nevertheless, once we prove that the L^1 distance in Theorem 3.3.7 satisfies the non-increasing hypothesis for H, all the ideas presented in the original article still apply and it is sufficient to follow the scheme used in [30, Lemma 5.6].

Lemma 3.3.8. *Fix $e \in D$ and $q, p \in \Pi_e$. Let $d_{q,p} = \|q-p\|_{L^1}$ and $i, j \in \mathbb{Z}^d$ such that*

$$i \in \sigma^{q,e} = \{q + ke \in \mathbb{Z}^d : \ k \in \mathbb{Z}\}$$
$$j \in \sigma^{p,e} = \{p + le \in \mathbb{Z}^d : \ l \in \mathbb{Z}\} .$$

Then we have:

(i) *for $e = e_n$ with $n \in \{1, \dots, d\}$*

$$\|i-j\|_{L^1} = d_{q,p} + |k-l|$$

(ii) *for $e = e_n \pm e_m$ with $1 \leq n < m \leq d$*

$$\|i-j\|_{L^1} = d_{q,p} + \max\left\{0, |2(k-l) + \langle q-p, e\rangle| - |q_n - p_n| - |q_m - p_m|\right\}$$

Proof of (i). We assume $e = e_n$ for some $n \in \{1, \dots, d\}$; then,

$$\|i-j\|_{L^1} = \left\|(q-p) + (k-l)e_n\right\|_{L^1} = d_{q,p} + |k-l|$$

where the last equality follows from $q - p \in \Pi_{e_n} = e_n^\perp$.

Proof of (ii). We assume that $e = e_n + e_m$ for some $1 \leq n < m \leq d$. By definition, we have

$$\begin{aligned}\|i-j\|_{L^1} &= \sum_{h\in\{n,m\}} |q_h - p_h + (k-l)| + \sum_{h\in\{1,\dots,d\}\setminus\{n,m\}} |q_h - p_h| \\ &= \sum_{h\in\{n,m\}} |q_h - p_h + (k-l)| + \left(d_{q,p} - \sum_{h\in\{n,m\}} |q_h - p_h|\right) \\ &= d_{q,p} + \sum_{h\in\{n,m\}} |q_h - p_h + (k-l)| - |q_h - p_h|\end{aligned}$$

By (3.3.1), we know that $\langle q,e\rangle, \langle p,e\rangle \in \{0,1\}$and hence $\langle q-p,e\rangle \in \{0,1,-1\}$. For sake of clarity, we set $a = q_n - p_n$.
If $\langle q-p,e\rangle = 0$, then $q_n - p_n = p_m - q_m$ and we obtain

$$\begin{aligned}&\sum_{h\in\{n,m\}} |q_h - p_h + (k-l)| - |q_h - p_h| \\ &\qquad = |(k-l)+a| + |(k-l)-a| - 2|a| \\ &\qquad = \max\left\{0, 2|k-l| - 2|a|\right\} .\end{aligned}$$

If $\langle q-p,e\rangle = 1$, then we necessarily have $q_n + q_m = \langle q,e\rangle = 1$ and $p_n + p_m = \langle p,e\rangle = 0$. Therefore, $q_n - p_n = 1 - (q_m - p_m)$. Thus, we have

$$\begin{aligned}&\sum_{h\in\{n,m\}} |q_h - p_h + (k-l)| - |q_h - p_h| \\ &\qquad = |(k-l)+a| + |(k-l)+(1-a)| - |a| - |1-a| \\ &\qquad = \max\left\{0, 2\left|k-l+\frac{1}{2}\right| - |a| - |a-1|\right\} .\end{aligned}$$

Eventually, if $\langle q-p,e\rangle = -1$, then we have $q_n + q_m = \langle q,e\rangle = 0$ and $p_n + p_m = \langle p,e\rangle = 1$. Therefore, $q_n - p_n = -1 - (q_m - p_m)$ and we infer

$$\begin{aligned}&\sum_{h\in\{n,m\}} |q_h - p_h + (k-l)| - |q_h - p_h| \\ &\qquad = |(k-l)+a| + |(k-l)-(1+a)| - |a| - |1+a| \\ &\qquad = \max\left\{0, 2\left|k-l-\frac{1}{2}\right| - |a| - |a+1|\right\} .\end{aligned}$$

To sum up, if $e = e_n + e_m$ for some $1 \le n < m \le d$, then we get

$$\|i-j\|_{L^1} = d_{q,p} + \max\left\{0, |2(k-l) + \langle q-p, e\rangle| - |q_n - p_n| - |q_m - p_m|\right\}$$

By analogous computations, we obtain the same expression for $e = e_n - e_m$ and thus the proof of (ii) is completed. □

Thus, now we can report from [30] the proof of Theorem 3.3.7:

Proof of Theorem 3.3.7. Given a direction $e \in D$, we consider the restriction of u, v on the slices of $\mathbb{Z}^d$ in direction e with respect to basis points on Π_e: namely,

$$u^{q,e}(k), v^{p,e}(l) \quad \text{for} \quad q, p \in \Pi_e\,.$$

Thus, we get

$$\sum_{i,j\in\mathbb{Z}^d} G\left(u(i), v(j)\right) H\left(\|i-j\|_{L^1}\right) = \sum_{q,p\in\Pi_e} \sum_{\substack{i\in(X)^{q,e}\\ j\in(X)^{p,e}}} G\left(u^{q,e}(i), v^{p,e}(j)\right) H\left(\|i-j\|_{L^1}\right)$$

and, since $u^{q,e}(i) = u(q+ke)$ and $v^{p,e}(j) = v(p+le)$, the inner sum is equivalent to

$$\sum_{k,l\in\mathbb{Z}} G\left(u(q+ke), v(p+le)\right) H\left(\left\|q-p+(k-l)e\right\|_{L^1}\right)\,.$$

By Lemma 3.3.8, $\|i-j\|_{L^1}$ depends only on $|k-l|$ since $d_{q,p}$ is a constant; thus, $H(\|i-j\|_{L^1}) = \widetilde{H}(|k-l|)$ is decreasing as $|k-l|$ increases and we can apply Theorem 3.3.6, obtaining

$$\sum_{k,l\in\mathbb{Z}} G\left(u(q+ke), v(p+le)\right)\widetilde{H}\left(|k-l|\right)$$
$$\le \sum_{k,l\in\mathbb{Z}} G\left(u^{*e}(q+ke), v^{*e}(p+le)\right)\widetilde{H}\left(|k-l|\right)\,.$$

Since this does not depend on the choice of the basis points in Π_e, we can sum over q, p and obtain

$$\sum_{i,j\in\mathbb{Z}^d} G\left(u(i), v(j)\right) H\left(\|i-j\|_{L^1}\right) \le \sum_{i,j\in\mathbb{Z}^d} G\left(u^{*e}(i), v^{*e}(j)\right) H\left(\|i-j\|_{L^1}\right)\,.$$

By the first point of Remark 3.3.4, we know that we get u^*, v^* in a finite number of rearrangements, hence the thesis follows by iterating over the directions of the set D. □

From Theorem 3.3.6 and Theorem 3.3.7 we can infer the following:

Corollary 3.3.9. *Let $u\colon \mathbb{Z}^d \to [0,+\infty)$ have finite support.*

(i) *For any $e \in D$, the symmetric decreasing rearrangement of u in direction e satisfies*

$$\sum_{\{i,j\}\in n} |u^{*e}(i) - u^{*e}(j)|^2 \leq \sum_{\{i,j\}\in n} |u(i) - u(j)|^2 .$$

In particular, for any $X \in \mathcal{X}$ it follows that $\lambda_N\big(R_e(X)\big) \leq \lambda_N(X)$.

(ii) *The symmetric rearrangement of u satisfies*

$$\sum_{\{i,j\}\in n} |u^{*}(i) - u^{*}(j)|^2 \leq \sum_{\{i,j\}\in n} |u(i) - u(j)|^2 .$$

In particular, for any $X \in \mathcal{X}_N$, it follows that $\lambda_N\big(R(X)\big) \leq \lambda_N(X)$.

Proof. First, we note that the function $G\colon \mathbb{R}\times\mathbb{R} \to \mathbb{R}$ defined by $G(x,y) = -|x-y|^2$ is supermodular (see Definition 3.3.5) and hence we can apply both Theorem 3.3.6 and Theorem 3.3.7.

Proof of (i). Fixed $e \in D$, the proof make use of Theorem 3.3.6 with $G(x,y) = -|x-y|^2$ and different choices for H, u, and v.
If $e = e_n$ for some $n = 1,\dots,d$, the inequality follows by choosing

- $H(t) = \chi_{\{0,1\}}(t)$ and $u = v = u^{q,e}(t)$ for the interactions in direction e_n,
- $H(t) = \chi_{\{0\}}(t)$, and $u = u^{q,e}(t)$, $v = u^{q+e_k,e}(t)$ for the interactions in direction $e_k \neq e_n$,

with $t \in \mathbb{Z}$ and $q \in \Pi_{e_n}$. If $e = e_n + e_k$ for $1 \leq n < k \leq d$, then we choose

- $H(t) = \chi_{\{0\}}(t)$, $u = u^{q,e}(t)$ and $v = u^{q+e_j,e}(t)$ for the interactions in direction $e_j \neq e_n, e_k$, where $t \in \mathbb{Z}$ and $q \in \Pi_{e_n+e_k}$
- for the interaction in directions e_n, e_k, the result follows from [42, Section 5.2]: indeed, all the lines in direction e are contained in the 2-dimensional plane $\mathrm{span}_{\mathbb{Z}}\{e_n, e_k\}$

Proof of (ii). The thesis follows directly from Theorem 3.3.7 by choosing $G(x,y) = -|x-y|^2$, $H(t) = \chi_{\{0,1\}}(t)$ and $u = v$. □

Point (ii) of Corollary 3.3.9 gives us some kind of discrete Faber-Krahn inequality. Unlike the continuous result, the Riesz Rearrangement does not provide a unique ball having fixed measure as minimizer and we can only infer the existence of a family of optimal sets, each of which satisfies some geometric properties that we present in the next section.

3.3.2 Geometric properties of the optimal sets

Thanks to the results on the discrete rearrangement of sets, we can also infer some properties of the sets minimizing (3.2.2). We begin with a slightly technical geometric Lemma that will be used in the proof of the Proposition 3.3.11.

Lemma 3.3.10. *Let $X, Y \subset \mathbb{Z}^d$ have finite cardinality. Then, there exists $\tau \in \mathbb{Z}^d$ such that there exists a unique pair $(x, y) \in \mathcal{N}$ with $x \in X$ and $y \in Y + \tau$.*

Proof. The proof proceeds in two steps. First we show that for any $X, Y \in \mathbb{Z}^d$ with finite cardinality there exists a translation $\sigma \in \mathbb{Z}^d$ such that

$$\begin{aligned} &\bullet \quad X \cap (Y + \sigma) = \{z\} \text{ for some } z \in \mathbb{Z}^d \\ &\bullet \quad X \subset \{x \in \mathbb{Z}^d \colon x_d \geq z_d\} \quad \text{and} \quad Y + \sigma \subset \{y \in \mathbb{Z}^d \colon y_d \leq z_d\} \end{aligned} \tag{3.3.2}$$

and then the claim of the Lemma follows by choosing $\tau = \sigma - e_d$.
To prove (3.3.2), we proceed by induction on the dimension. Since for $d = 1$ the proof is trivial, we assume that the statement is true for $d - 1$ and we prove it for d. We set

$$m_d(X) := \min_{x \in X} x_d \quad \text{and} \quad M_d(Y) := \max_{y \in Y} y_d$$

and we set X_{d-1}, Y_{d-1} to be, respectively, the $(d-1)$-dimensional slices of X, Y with respect to $\{z \in \mathbb{Z}^d : z_d = m_d\}, \{z \in \mathbb{Z}^d : z_d = M_d\}$. Then, by the induction assumption, we infer that there exists $\hat{\tau}$ such that

$$X_{d-1} \cap (Y_{d-1} + \hat{\tau}) = \{z\} \text{ for some } z \in \mathbb{Z}^d$$

while the second point of (3.3.2) holds by construction. By setting $\tau_d := -M_d(Y) + m_d(X)$, it is sufficient to choose the translation $\tau = (\hat{\tau}, \tau_d)$ to conclude the proof of (3.3.2). ☐

Proposition 3.3.11. *Let $Y_N \in \mathcal{X}_N$ be a minimal set for* (3.2.2). *Then, the following properties hold:*

(i) *Y_N is connected;*

(ii) *Y_N is direction-convex;*

(iii) *there exists $C_d > 0$, independent of $N \in \mathbb{N}$, such that, if $d = 2$ or if $d > 2$ and Y_N is symmetric according to Definition 3.3.3, then*

$$\operatorname{diam}(Y_N) \leq C_d N^{1/d}\,,$$

where $\operatorname{diam}(Y_N) = \max\{\|i - j\|_{L^1} \,:\, i, j \in Y_N\}$.

Remark 3.3.12. We note that, thanks to Corollary 3.3.9, for any $d \geq 2$ and $N \in \mathbb{N}$ there exists a symmetric minimal set $Y_N \in \mathcal{X}_N$. ♠

Proof of Proposition 3.3.11. For the proof of (i) we argue by contradiction, assuming that Y_N is not connected. First, we assume that $Y_N = C^1 \sqcup C^2$ with $C^1, C^2 \subset \mathbb{Z}^d$ two disjoint connected components of Y_N, according to Definition 3.2.10, and we consider a non-negative function u realizing the minimum for $\lambda_N(Y_N)$, that is

$$D_N(u) = \lambda_N(Y_N) \quad \text{and} \quad u = 0 \text{ on } \mathbb{Z}^d \setminus Y_N\,.$$

By Lemma 3.3.10, there exists $\tau \in \mathbb{Z}^d \setminus \{0\}$ such that there exists a unique pair $\{i, j\} \in \mathcal{N}$ with $i \in C^1$ and $j \in \tau + C^2$. Thus, $\hat{Y}_N = C^1 \sqcup (\tau + C^2)$ is a connected set such that $\#\hat{Y}_N = N$.
We define a function $\hat{u}\colon \mathbb{Z}^d \to \mathbb{R}^+$ such that $\hat{u} \equiv 0$ on $\mathbb{Z}^d \setminus \hat{Y}_N$:

$$\hat{u}(i) = \begin{cases} u(i) & \text{if } i \notin C^2 + \tau \\ u(i - \tau) & \text{if } i \in C^2 + \tau\,. \end{cases}$$

Then, $\hat{u}$ is a competitor for $\lambda_N(\hat{Y}_N)$ and it holds that

$$\begin{aligned} D_N(\hat{u}) &= D_N\left(\hat{u}\chi_{C^1}\right) + D_N\left(\hat{u}\chi_{(\tau + C^2)}\right) + \left|\hat{u}(i) - \hat{u}(j)\right|^2 + \left|\hat{u}(i)\right|^2 + \left|\hat{u}(j)\right|^2 \\ &= D_N(u) + \left|u(i) - u(j - \tau)\right|^2 + \left|u(i)\right|^2 + \left|u(j - \tau)\right|^2 \\ &\leq D_N(u) = \lambda_N(Y_N)\,, \end{aligned}$$

where the equality holds if and only if $\min\{u(i), u(j-\tau)\} = 0$. Hence, $\hat{u}$ is a minimizer for $\lambda_N(\hat{Y}_N)$ and, according to Proposition 3.2.11, it satisfies $u(x), u(y-\tau) > 0$, which gives a contradiction to the minimality of Y_N.
If Y_N has more disjoint connected components, then it is sufficient to repeat the same argument iteratively.

Proof of (ii). This is a straightforward consequence of point (i) of Corollary 3.3.9 and point (iii) of Remark 3.3.4.

Proof of (iii). The case $d = 2$ follows from [42, Proposition 6.6] and it remains to prove the case $d > 2$ for Y_N, symmetric and minimal set for λ_N. The thesis follows if we prove that there exists $C_d > 0$ such that for all $i \in Y_N$ there holds

$$|i_n| \leq C_d N^{\frac{1}{d}} \text{ for all } n = 1, \dots, d\,. \tag{3.3.3}$$

We assume that there exists $i \in Y_N$ such that (without loss of generality) $|i_d| \geq \kappa$. We then show that there exists $c_d > 0$ such that

$$\#Y_N \geq c_d \kappa^d\,. \tag{3.3.4}$$

Since $R_{e_d}(Y_N) = Y_N$, there exist $i^* \in Y_N$ such that

$$\begin{cases} i^*_n = i_n & \text{if } n \in \{1, \dots, d-1\}\,, \\ |i^*_d + i_d| \leq 1\,. \end{cases}$$

Since Y_N is direction-convex by the previous step, Y_N contains the segment $\overline{i, i^*} \cap \mathbb{Z}^d$ and we can assume that this segment contains the origin. In fact, if it is not the case, then for all $j \in \overline{i, i^*} \cap \mathbb{Z}^d$ we have $j_k \neq 0$ for an index k in $\{1, \dots, d-1\}$ and we have

$$R_{e_k}\left(\overline{i, i^*} \cap \mathbb{Z}^d\right) = \left\{\left(R_{e_k} j_1, \dots, R_{e_k} j_d\right) \,:\, j \in (\overline{i, i^*} \cap \mathbb{Z}^d)\right\} \subset Y_N\,,$$

where

$$R_{e_k} j_n = \begin{cases} j_n & \text{if } n \neq k\,, \\ -j_k & \text{if } n = k\,. \end{cases}$$

Then, exploiting the direction-convexity of Y_N for the direction e_k, we conclude that $(\overline{i, i^*} \cap \mathbb{Z}^d - i_k) \subset Y_N$ and passes through the origin. Therefore, we can infer that

$$\overline{i, i^*} \cap \mathbb{Z}^d = \big\{ne_d : \ n \in \mathbb{N}\,, |n| \le \kappa - 1\big\} \subset Y_N\,.$$

Again, by symmetry with respect to $e = e_j + e_d$ for $j \neq d$, we have that

$$\big\{ne_j : \ n \in \mathbb{N}\,, |n| \le \kappa - 1\big\} \subset Y_N \qquad \text{for all } j = 1, \dots, d-1\,.$$

Due to the directional-convexity with respect to $e = e_j + e_k$ for all $j \neq k$, we conclude that

$$C := \operatorname{conv}\left(\bigcup_{j=1}^{d} \{ne_j : \ n \in \mathbb{N}\,, |n| \le \kappa - 1\} \right) \cap \mathbb{Z}^d \subset Y_N\,,$$

where $\operatorname{conv}(\Omega)$ denotes the convex envelope of Ω. Since $\#C = C_d \kappa^d$ we obtain (3.3.4) and, since $\#Y_N = N$, this implies (3.3.3). $\square$

3.4 The embedding map ζ

In order to apply the Q-closeness technique to the discrete Faber-Krahn inequality, we have to define a map ζ from $\mathbb{Z}^d$ to $\mathcal{M}(\mathbb{R}^d)$ (see Definition 1.5.2) that gives a suitable continuous competitor for optimizing the Rayleigh quotient. We will properly define this map in Section 3.4, but first we need to introduce a peculiar decomposition of $\mathbb{Z}^d$, the so-called Kuhn decomposition, that also allows us to define a suitable competitor function in (3.1.1).

3.4.1 Kuhn decomposition

The Kuhn decomposition is an useful tool that allows us to establish a well-defined and periodic partition of the periodicity cell $[0,1]^d$ of $\mathbb{Z}^d$ into d-dimensional simplices (for instance, see [3]). For sake of clarity, we denote

$$\mathscr{P}_d = \{\pi : \ \pi \text{ is a permutation of d elements}\}\ .$$

and we recall that $\Omega(x) = x + \Omega$ for $x \in \mathbb{R}^d$ and $\Omega \subset \mathbb{R}^d$.

Definition 3.4.1. Given $\pi \in \mathscr{P}_d$ and given $[0,1]^d$, if we define the d-dimensional simplex $T_\pi \subset [0,1]^d$ as

$$T_\pi = \{x \in \mathbb{R}^d \colon 0 \le x_{\pi(d)} \le x_{\pi(d-1)} \le \cdots \le x_{\pi(1)} \le 1\}\,.$$

then, we define the **Kuhn decomposition** of $[0,1]^d$ as

$$\mathcal{T}\left([0,1]^d\right) = \{T \colon T = T_\pi \text{ for some } \pi \in \mathcal{P}(d)\}.$$

In particular, we define $\mathcal{T} = \mathcal{T}(\mathbb{R}^d)$, the Kuhn decomposition of $\mathbb{R}^d$, as

$$\mathcal{T} = \{T \colon T = T_\pi(z) \text{ for some } z \in \mathbb{Z}^d \text{ and } \pi \in \mathcal{P}(d)\}.$$

Remark 3.4.2. From Definition 3.4.1 it immediately follows that the Kuhn decomposition is periodic of period $[0,1]^d$. Moreover, we can also infer that $\#\mathcal{T}\left([0,1]^d\right) = d!$ (since $\#\mathcal{P}(d) = d!$) and that

$$\mathring{T}_{\pi_1} \cap \mathring{T}_{\pi_2} = \emptyset \quad \text{for } \pi_1, \pi_2 \in \mathcal{P}(d) : \ \pi_1 \neq \pi_2 \,.$$

♣

In the following Proposition, we show some basic properties of the Kuhn decomposition that we will be of use in the forthcoming sections of this chapter.

Proposition 3.4.3. *The Kuhn decomposition satisfies the following properties:*

(i) $\bigcup_{z \in \mathbb{Z}^d} \left\{T \in \mathcal{T} \,:\, T \cap \{z\} \neq \emptyset\right\} = \mathbb{R}^d$

(ii) *For all* $z \in \mathbb{Z}^d$ *and* $\pi \in \mathcal{P}_d$ *we have* $|T_\pi(z)| = 1/d!$*;*

(iii) *For any* $k \in \{1, \dots, d\}$*, there exists a unique edge of the simplex* $T_\pi(z)$ *parallel to* e_k*;*

(iv) *For each* $\{i,j\} \in \mathcal{N}$*, there exist* $d!$ *distinct simplices sharing the segment* $\overline{i,j}$ *as a common edge;*

(v) *For each point* $i \in \mathbb{Z}^d$*, there exist* $(d+1)!$ *distinct elements of* $\mathcal{T}$ *sharing* i *as a common vertex.*

Proof. Properties (i), (ii) and (iii) are a trivial consequence of the definition of $T_\pi(z)$ and Remark 3.4.2.

Proof of (iv). First, we notice that, given an edge $\overline{i,j}$ such that $i, j \in \mathbb{Z}^d$ with $j = i + e_k$ for some $k \in \{1, \dots, d\}$ and given a permutation $\pi \in \mathscr{P}_d$, then there exists a unique $z \in \mathbb{Z}^d$ such that $\overline{i,j} \subset T_\pi(z)$; namely, we have

$$\#\{z \in \mathbb{Z}^d : \overline{i,j} \subset T_\pi(z)\} = 1 . \tag{3.4.1}$$

Indeed, if $z, z' \in \mathbb{Z}^d$ are distinct, then necessarily $T_\pi(z) \cap T_\pi(z')$ is either empty or contains a single point of the lattice. Then by (3.4.1) we conclude the proof of (iv) as

$$\begin{aligned}\#\{(\pi, z) \in \mathscr{P}_d \times \mathbb{Z}^d \colon \overline{i,j} \subset T_\pi(z)\} &= \sum_{\pi \in \mathscr{P}_d} \#\{z \in \mathbb{Z}^d \colon \overline{i,j} \subset T_\pi(z)\} \\ &= \sum_{\pi \in \mathscr{P}_d} 1 = d! .\end{aligned}$$

Proof of (v). We first observe that, since $[0,1]^d$ is the periodicity cell of the decomposition, counting the number of different simplices passing through a point is equivalent to summing the number of times each vertex of $[0,1]^d$ belongs to a different simplex of the Kuhn decomposition of $[0,1]^d$. If we call this number $S(d)$, then we have

$$\begin{aligned}S(d) &= \sum_{i \in \{0,1\}^d} \#\{\pi \in \mathscr{P}_d \colon i \in T_\pi\} = \sum_{i \in \{0,1\}^d} \sum_{\pi \in \mathscr{P}_d} \chi_{T_\pi}(i) \\ &= \sum_{\pi \in \mathscr{P}_d} \sum_{i \in T_\pi \cap \{0,1\}^d} 1 = \sum_{\pi \in \mathscr{P}_d} (d+1) = (d+1)! .\end{aligned}$$

□

3.4.2 Definition of ζ and its properties

In this section, we define the embedding of the discrete problem in the continuum setting through a map ζ, similarly to the embeddings presented in the previous chapter for the lattices $\mathcal{L}_Q, \mathcal{L}_H, \mathcal{L}_T$. To this end, we need to properly extend both sets $X \in \mathcal{X}_N$ and functions $u \colon \mathbb{Z}^d \to \mathbb{R}$ by using the Kuhn decomposition introduced in Section 3.4.1.

Definition 3.4.4. We define the map $\zeta \colon \mathbb{Z}^d \to \mathcal{M}(\mathbb{R}^d)$ as

$$\zeta(X) = \bigcup_{i \in X} \bigcup_{T \in \mathcal{T}(i)} T \qquad \text{for any } X \subset \mathbb{Z}^d , \tag{3.4.2}$$

where $\mathcal{T}(i) = \big\{T \in \mathcal{T} : T \cap \{i\} \neq \emptyset\big\}$.

Definition 3.4.5. Given a function $u\colon \mathbb{Z}^d \to \mathbb{R}$, we define the function $\hat{u}\colon \mathbb{R}^d \to \mathbb{R}$ as the function who is affine on each Kuhn simplex $T \in \mathcal{T}$ and satisfies

$$\hat{u}(i) = u(i) \qquad \forall i \in \mathbb{Z}^d .$$

Remark 3.4.6. Given $X \in \mathcal{X}_N$, and $u\colon \mathbb{Z}^d \to \mathbb{R}$ such that $u(i) \neq 0$ for any $i \in X$, then from Definition 3.4.4 and Definition 3.4.5 we get that $\operatorname{supp}(\hat{u}) = \zeta(\mathring{X})$. ♠

Even if the map ζ has an intuitive formulation, we saw in Chapter 2 that the estimates of its analytical properties can be very hard; in the next lemma we estimate the error in the measure one makes when passing from a discrete set X to its continuum representation $\zeta(X)$.

Lemma 3.4.7. *Let $X \in \mathcal{X}_N$ and let ζ be the map defined in* (3.4.2). *Then, there exists $C_d > 0$ such that*

$$N \leq \left|\zeta(X)\right| \leq N + C_d N^{\frac{d-1}{d}} P_N(X) . \tag{3.4.3}$$

In particular, $\left|\zeta(X)\right| \leq C_d N$.

Proof. If we denote $\mathcal{T}(i) = \left\{T \in \mathcal{T} \,:\, T \cap \{i\} \neq \emptyset\right\}$ and $Q(i) = i + [0,1]^d$ for $i \in \mathbb{Z}^d$, then the lower bound is straightforward since we have

$$Q(i) \subseteq \bigcup_{T \in \mathcal{T}(i)} T .$$

The upper bound is less trivial; we first notice that

$$\zeta(X) \subseteq \bigcup_{i \in (X)_{\sqrt{d}}} Q(i)$$

where we defined $(X)_{\sqrt{d}} = \{i \in \mathbb{Z}^d \colon \operatorname{dist}(i, X) \leq \sqrt{d}\}$. Since the union on the right hand side is a disjoint union, we obtain that

$$|\zeta(X)| \leq \sum_{i \in (X)_{\sqrt{d}}} |Q(i)| = \#X + \#\left((X)_{\sqrt{d}} \setminus X\right) = N + \left((X)_{\sqrt{d}} \setminus X\right) .$$

Then, we can observe that $i \in (X)_{\sqrt{d}} \setminus X$ only if there exists $j \in X$ such that $\mathrm{dist}(i,j) \le \sqrt{d}$ and $\mathrm{val}(j) \ge 1$. Moreover, for each $j \in \mathbb{Z}^d$ there exists a constant $C_d > 0$ (independent of j) such that

$$\#\{i \in \mathbb{Z}^d \setminus X \colon \mathrm{dist}(i,j) \le \sqrt{d}\} \le C_d \,.$$

Hence,

$$\begin{aligned}\#\left((X)_{\sqrt{d}} \setminus X\right) &= \sum_{j \in X \,:\, \mathrm{val}(j) \ge 1} \#\{i \in \mathbb{Z}^d \setminus X \colon \mathrm{dist}(i,j) \le \sqrt{d}\} \\ &\le C_d \sum_{j \in X} \mathrm{val}(j) = C_d N^{\frac{d-1}{d}} P_N(X)\,,\end{aligned}$$

and we conclude the proof of (3.4.3). The last part of the statement follows by construction. □

Differently from Chapter 2, here we have to take into account also the interpolation function $\hat{u}$ in Definition 3.4.5 to compare the Dirichlet energy functionals related of $\hat{u}$ with respect to the one given by $u \colon \mathbb{Z}^d \to \mathbb{R}$. to define the discrete and continuum eigenvalues.

Lemma 3.4.8. *Let $X \in \mathcal{X}_N$ and let $u \colon \mathbb{Z}^d \to \mathbb{R}$ be such that* $\mathrm{supp}(u) = X$*. The function $\hat{u}$ has the following two properties:*

(i)

$$\int_{\mathbb{R}^d} |\nabla \hat{u}(x)|^2 \,\mathrm{d}x = N^{\frac{d-2}{d}} D_N(u)\,,$$

(ii)

$$\int_{\mathbb{R}^d} |\hat{u}(x)|^2 \,\mathrm{d}x \le \sum_{i \in \mathbb{Z}^d} u^2(i) + 2\sqrt{d} \left(\sum_{i \in \mathbb{Z}^d} u^2(i)\right)^{\frac{1}{2}} N^{\frac{d-2}{2d}} D_N(u)^{\frac{1}{2}}\,,$$

$$\int_{\mathbb{R}^d} |\hat{u}(x)|^2 \,\mathrm{d}x \ge \sum_{i \in \mathbb{Z}^d} u^2(i) - 2\sqrt{d} \left(\sum_{i \in \mathbb{Z}^d} u^2(i)\right)^{\frac{1}{2}} N^{\frac{d-2}{2d}} D_N(u)^{\frac{1}{2}}\,.$$

where $D_N(u)$ is the discrete Dirichlet energy defined in (3.2.1).

Proof. Proof of (i). To this end, we can observe that it is sufficient to prove that, for all $k \in \{1, \dots, d\}$, it holds that

$$\sum_{i \in \mathbb{Z}^d} |u(i+e_k) - u(i)|^2 = \int_{\mathbb{R}^d} |\partial_k \hat{u}|^2 \,\mathrm{d}x \,; \tag{3.4.4}$$

indeed, once this equality is proven, (i) follows by summing over $k \in \{1, \dots, d\}$. Let us prove (3.4.4). We fix $k \in \{1, \dots, d\}$, $i \in \mathbb{Z}^d$ and we denote by $\mathcal{T}(i,k)$ the set of simplices of $\mathcal{T}$ that passes through both the points $i, i+e_k$:

$$\mathcal{T}(i,k) = \left\{ T \in \mathcal{T} \,:\, \overline{i,j} \subset T \text{ for } j = i + e_k \right\} .$$

Then, thanks to Proposition 3.4.3(iii), we get that $\#\mathcal{T}(i,k) = d!$ and, thanks to Definition 3.4.5 we have

$$\partial_k \hat{u}(x) = u(i+e_k) - u(i) \quad \forall x \in T \,, T \in \mathcal{T}(i,k) \,.$$

Hence, by Proposition 3.4.3 and the fact that $\mathring{T}_1 \cap \mathring{T}_2 = \emptyset$ for all distinct $T_1, T_2 \in \mathcal{T}$, we obtain

$$\begin{aligned} \int_{\bigcup_{\mathcal{T}(i,k)} T} |\partial_k \hat{u}(x)|^2 \,\mathrm{d}x &= \sum_{T \in \mathcal{T}(i,k)} \int_T |\partial_k \hat{u}(x)|^2 \,\mathrm{d}x = |T| \sum_{T \in \mathcal{T}(i,k)} |u(i+e_k) - u(i)|^2 \\ &= \frac{\#\mathcal{T}(i,k)}{d!} |u(i+e_k) - u(i)|^2 = |u(i+e_k) - u(i)|^2 \,. \end{aligned}$$

By summing over $i \in \mathbb{Z}^d$ we get

$$\sum_{i \in \mathbb{Z}^d} |u(i+e_k) - u(i)|^2 = \sum_{i \in \mathbb{Z}^d} \int_{\bigcup T \in \mathcal{T}(i,k)} |\partial_k \hat{u}(x)|^2 \,\mathrm{d}x = \int_{\mathbb{R}^d} |\partial_k \hat{u}(x)|^2 \,\mathrm{d}x \,,$$

which concludes the proof of (i).

Proof of (ii). Given $T \in \mathcal{T}$, $x \in T$ and $z \in T$ be a vertex of T, by Definition 3.4.5 we have

$$|\hat{u}(x) - u(z)| = |\hat{u}(x) - \hat{u}(z)| \leq \sqrt{d} \, \left|\nabla \hat{u}_{|_T}\right|$$

and, by the triangular inequality, we can infer that

$$u^2(x) \geq \big| |\hat{u}(x) - u(z)| - |u(z)| \big|^2 \geq u^2(z) - 2\sqrt{d} \left|\nabla \hat{u}_{|_T}\right| |u(z)| \,. \tag{3.4.5}$$

Again, by the very definition of $\hat{u}$, we observe that

$$\left|\nabla \hat{u}_{|_T}\right|^2 \leq \sum_{\substack{\{i,j\}\in \mathcal{n} \\ i,j\in\mathbb{Z}^d\cap T}} |u(i)-u(j)|^2 . \tag{3.4.6}$$

Thus, by (3.4.5) and Proposition 3.4.3 we get

$$\begin{aligned}
\int_{\mathbb{R}^d} |\hat{u}(x)|^2 \,\mathrm{d}x &= \sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} \int_{T_\pi(i)} \hat{u}^2(x)\,\mathrm{d}x \\
&\geq \sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} |T_\pi(i)| \left(u^2(i) - 2\sqrt{d}|u(i)|\left|\nabla \hat{u}_{|_{T_\pi(i)}}\right|\right) \\
&= \sum_{i\in\mathbb{Z}^d} u^2(i) - \sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} \frac{2\sqrt{d}}{d!}|u(i)|\left|\nabla \hat{u}_{|_{T_\pi(i)}}\right| .
\end{aligned}$$

By (3.4.6) and the Cauchy-Schwarz inequality, the last quantity can be estimated as follows:

$$\begin{aligned}
\sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} |u(i)|\left|\nabla \hat{u}_{|_{T_\pi(i)}}\right| &\leq \sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} |u(i)| \left(\sum_{\substack{(h,k)\in \mathcal{n} \\ h,k\in\mathbb{Z}^d\cap T_\pi(i)}} |u(h)-u(k)|^2 \right)^{\frac{1}{2}} \\
&\leq \left(\sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} u^2(i)\right)^{\frac{1}{2}} \left(\sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} \sum_{\substack{(h,k)\in \mathcal{n} \\ h,k\in\mathbb{Z}^d\cap T_\pi(i)}} |u(h)-u(k)|^2 \right)^{\frac{1}{2}} \\
&= d! \left(\sum_{i\in\mathbb{Z}^d} u^2(i)\right)^{\frac{1}{2}} \left(\sum_{(h,k)\in \mathcal{n}} |u(h)-u(k)|^2 \right)^{\frac{1}{2}} ,
\end{aligned}$$

where the last equality is due to Proposition 3.4.3(iv) and to

$$\sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d}\sum_{\substack{(h,k)\in\mathcal{N}\\ h,k\in\mathbb{Z}^d\cap T_\pi(i)}} f(h,k) = \sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d}\sum_{(h,k)\in\mathcal{N}} \chi_{T_\pi(i)}(h)\cdot\chi_{T_\pi(i)}(k)f(h,k)$$
$$= \sum_{(h,k)\in\mathcal{N}}\sum_{i\in\mathbb{Z}^d}\sum_{\pi\in\mathscr{P}_d} \chi_{h-T_\pi}(i)\cdot\chi_{k-T_\pi}(i)f(h,k)$$
$$= \sum_{(h,k)\in\mathcal{N}} d!\, f(h,k)\,.$$

Finally, we get that

$$\int_{\mathbb{R}^d} |\hat{u}(x)|^2\,\mathrm{d}x \geq \sum_{i\in\mathbb{Z}^d} u^2(i) - 2\sqrt{d}\left(\sum_{i\in\mathbb{Z}^d} u^2(i)\right)^{\frac{1}{2}}\left(\sum_{\{i,j\}\in\mathcal{N}} |u(i)-u(j)|^2\right)^{\frac{1}{2}}$$

and we obtain the lower bound in (ii). The estimate from above follows the same strategy. □

Remark 3.4.9. In Lemma 3.4.8 there are no conditions on the considered functions apart from its support; thus, if we consider in particular the functions $u\colon \mathbb{Z}^d \to \mathbb{R}$ in (3.2.2), then we have that $\sum_{i\in\mathbb{Z}^d} u^2(i) = N$ and

$$N - 2\sqrt{d}N^{1-\frac{1}{d}}D_N(u)^{\frac{1}{2}} \leq \int_{\mathbb{R}^d} |\hat{u}(x)|^2\,\mathrm{d}x \leq N + 2\sqrt{d}N^{1-\frac{1}{d}}D_N(u)^{\frac{1}{2}}\,.$$

♠

3.5 Computation of the Q-closeness parameters

In the previous paragraphs, we introduced a discrete counterpart of the classical first eigenvalue functional and we proved some of its properties, including a Faber-Krahn-type inequality; then, we defined a discrete-to-continuum map ζ. In order to apply the Q-closeness technique of Proposition 1.5.3 to the quantitative estimate of Theorem 3.1.3 by Brasco, De Philippis and Velichkov, we prove, in the forthcoming Lemma 3.5.1 and Lemma 3.5.4, the two necessary conditions of Definition 1.5.2.

3.5.1 The parameter β_N

In the following Lemma we ensure that condition (1.5.5) holds for the discrete functional (3.2.2) with respect to the continuous one (3.1.1).

Lemma 3.5.1. *Let $N \in \mathbb{N}$ and $X \in \mathcal{X}_N$. Let $\zeta\colon \mathbb{Z}^d \to \mathbb{R}$ the map defined in* (3.4.2)*. Then, it holds that*

$$\lambda\left(\zeta(X)\right) \leq N^{-\frac{2}{d}}\lambda_N(X) + \frac{1}{16d}\,.$$

Proof. For $X \in \mathcal{X}_N$ let $u\colon \mathbb{Z}^d \to \mathbb{R}$ be a minimizer of (3.2.2), that is

$$\lambda_N(X) = D_N(u) = N^{-1+\frac{2}{d}} \sum_{\{i,j\}\in n} |u(i) - u(j)|^2$$

with $\frac{1}{N}\sum_{i\in\mathbb{Z}^d} u^2(i) = 1$ and $u(i) = 0$ for all $i \in \mathbb{Z}^d \setminus X$.
We consider as a competitor for $\lambda(\zeta(X))$ the piecewise-affine interpolation $\hat{u}$ defined in Definition 3.4.5 and we estimate its Rayleigh quotient for N large enough. By Lemma 3.4.8, we obtain

$$\begin{aligned}\frac{\int_{\mathbb{R}^d} |\nabla\hat{u}|^2 \,\mathrm{d}x}{\int_{\mathbb{R}^d} |\hat{u}|^2 \,\mathrm{d}x} &\leq \frac{N^{\frac{d-2}{d}} D_N(u)}{N - 2\sqrt{dN}\left(N^{\frac{d-2}{d}}D_N(u)\right)^{\frac{1}{2}}} = \frac{N^{-\frac{2}{d}}\lambda_N(X)}{1 - 2\sqrt{d}\left(\frac{N^{\frac{d-2}{d}}\lambda_N(X)}{N}\right)^{\frac{1}{2}}} \\ &= N^{-\frac{2}{d}}\lambda_N(X)\frac{1}{1 - 2\sqrt{d}N^{-\frac{1}{d}}\lambda_N^{\frac{1}{2}}(X)}\,.\end{aligned}$$

Furthermore, since $\frac{1}{1-t} \leq 1 + 2t$ for $t \in \left]0, \frac{1}{2}\right[$, we can estimate the last right hand side in the previous inequality as follows

$$\frac{1}{1 - 2\sqrt{d}N^{-\frac{1}{d}}\lambda_N^{\frac{1}{2}}(X)} \leq 1 + 4\sqrt{d}N^{-\frac{1}{d}}\lambda_N^{\frac{1}{2}}(X) \quad \text{for} \quad \lambda_N(X) < \frac{1}{16d}N^{\frac{2}{d}}$$

and, in the end, we get

$$\begin{aligned}\frac{\int_{\mathbb{R}^d} |\nabla\hat{u}|^2 \,\mathrm{d}x}{\int_{\mathbb{R}^d} |\hat{u}|^2 \,\mathrm{d}x} &\leq N^{-\frac{2}{d}}\lambda_N(X) + 4\sqrt{d}N^{-\frac{3}{d}}\lambda_N^{\frac{3}{2}}(X) \\ &< N^{-\frac{2}{d}}\lambda_N(X) + \frac{1}{16d}\,.\end{aligned}$$

The statement of the lemma follows by passing to the infimum over $H^1(\mathbb{R}^d)$ functions which are zero outside $\zeta(X)$ and satisfy $\|u\|_{L^2(\mathbb{R}^d)} = N$. □

Remark 3.5.2. We emphasize that in the proof of Lemma 3.5.1, the inequality $\lambda_N(X) < \frac{1}{16d} N^{\frac{2}{d}}$ is used without being explicitly assumed in the hypothesis. This is justified by Lemma 3.2.9 and the fact that our fluctuation estimate in Theorem 3.6.1 is valid for arbitrarily large N. ♠

3.5.2 The parameter γ_N

Now we check that condition (1.5.6) holds for the discrete functional (3.2.2) with respect to (3.1.1).

Lemma 3.5.3. *Let $N \in \mathbb{N}$, let $\zeta\colon \mathbb{Z}^d \to \mathbb{R}$ the map defined in* (3.4.2) *and let $m_{\lambda,N}$ be the value defined in* (3.2.3). *Then, there exists $C_d > 0$ such that*

$$m_{\lambda,N} \leq \lambda\big(B_1\big) + C_d N^{-\frac{1}{d}}\,.$$

Proof. We first prove the claim for $N_k := \#(\overline{B}_k \cap \mathbb{Z}^d)$, $k \in \mathbb{N}$. Note that there exists $C_d > 0$ such that

$$|B_1| \left(k^d - C_d k^{d-1}\right) \leq N_k \leq |B_1| \left(k^d + C_d k^{d-1}\right)\,. \tag{3.5.1}$$

In the rest of the proof we omit the dependence of N on k to simplify notation. Let $u \in H_0^1(B_1)$ be such that

$$\int_{B_1} |\nabla u|^2 \,\mathrm{d}x = \lambda(B_1)\,, \quad \int_{\mathbb{R}^d} u^2 \,\mathrm{d}x = 1\,.$$

The following scaling property can be readily checked to hold true:

$$\lambda(B_1) = |B_1|^{-\frac{2}{d}} \lambda(B)\,. \tag{3.5.2}$$

By standard elliptic regularity estimates $u \in C^\infty(\overline{B}_1)$. Hence, for any $m \in \mathbb{N}$ and every multi-index α of order m there exists $C_{d,m} > 0$ such that

$$\|D^\alpha u\|_{L^\infty(\mathbb{R}^d)} \leq C_{d,m}\,. \tag{3.5.3}$$

Let $u_k\colon \mathbb{Z}^d \to \mathbb{R}$ be defined as $u_k(i) = C_{d,k} u\left(\frac{i}{k}\right)$, $i \in \mathbb{Z}^d$, and where $C_{d,k} > 0$ is to be chosen such that $\sum_{i \in \mathbb{Z}^d} u_k^2(i) = N$. Using (3.5.1) and the fact that $u \in H_0^1(B_1)$, we can compute $C_{d,k}$ as follows. We first observe that $\sum_{i\in\mathbb{Z}^d\cap\overline{B}_k} u^2\left(\frac{i}{k}\right) = \sum_{i\in\frac{1}{k}\mathbb{Z}^d\cap\overline{B}_1} u^2(i)$ and then

$$\begin{aligned}\sum_{i\in\frac{1}{k}\mathbb{Z}^d\cap\overline{B}_1} u^2(i) &= \sum_{i\in\frac{1}{k}\mathbb{Z}^d\cap\overline{B}_1}\left(u^2(i) - \fint_{Q_{\frac{1}{k}}(i)} u^2(x)\,\mathrm{d}x\right) + k^d\int_{\mathbb{R}^d} u^2(x)\,\mathrm{d}x \\ &= \sum_{i\in\frac{1}{k}\mathbb{Z}^d\cap\overline{B}_1}\left(u^2(i) - \fint_{Q_{\frac{1}{k}}(i)} u^2(x)\,\mathrm{d}x\right) + \frac{N}{|B_1|} + O(k^{d-1})\,.\end{aligned}$$

By the regularity of u in (3.5.3), we can estimate

$$\sum_{i\in\frac{1}{k}\mathbb{Z}^d\cap\overline{B}_1}\left|u^2(i) - \fint_{Q_{\frac{1}{k}}(i)} u^2(x)\,\mathrm{d}x\right| \le C_d k^{d-1}\|u\|_{L^\infty}\cdot\|\nabla u\|_{L^\infty} \le C_d k^{d-1}\,.$$

This implies that $C_{d,k}$ satisfies

$$|B_1|\left(1-\frac{C_d}{k}\right) \le C_{d,k}^2 \le |B_1|\left(1+\frac{C_d}{k}\right)\,. \tag{3.5.4}$$

Since $u_k(i) = 0$ for all $i \in \mathbb{Z}^d \setminus B_k$, u_k is an admissible competitor for $\lambda_N(X)$ with $X \in \mathcal{X}_N$ given by $X = \overline{B}_k \cap \mathbb{Z}^d$. Therefore we have that

$$m_{\lambda,N} \le \lambda_N(X) \le N^{-1+\frac{2}{d}} \sum_{\{i,j\}\in n} |u_k(i) - u_k(j)|^2 = D_N(u_k)\,. \tag{3.5.5}$$

As a consequence, in order to show the estimate for $m_{\lambda,N}$, it suffices to estimate $D_N(u_k)$. To this end we note that, by the regularity of u given in (3.5.3), there exists $C_d > 0$ such that

$$|u_k(i+e_n) - u_k(i)|^2 \le C_{d,k}^2 k^{d-2}\int_{Q_{\frac{1}{k}}(\frac{i}{k})} \left|\partial_n u(x)\right|^2\,\mathrm{d}x + C_d k^{d-3}\left|Q_{\frac{1}{k}}\left(\frac{i}{k}\right)\right|\,.$$

Summing over $i \in \mathbb{Z}^d$, $n \in \{1,\dots,d\}$ and using (3.5.1),(3.5.2), and (3.5.4), we obtain

$$\begin{aligned}
D_N(u_k) &= N^{-1+\frac{2}{d}} \sum_{\{i,j\}\in n} |u_k(i) - u_k(j)|^2 \\
&\leq N^{-1+\frac{2}{d}} C_{d,k}^2 k^{d-2} \int_{B_1} \left|\nabla u\,(x)\right|^2 \,\mathrm{d}x + C_d N^{-1+\frac{2}{d}} C_{d,k}^2 k^{d-3} \\
&\leq N^{-1+\frac{2}{d}} |B_1| k^{d-2} \int_{B_1} \left|\nabla u\,(x)\right|^2 \,\mathrm{d}x + C_d N^{-1+\frac{2}{d}} k^{d-3} \\
&\leq \lambda(B_1) + C_d N^{-\frac{1}{d}}\,.
\end{aligned}$$

The latter estimate together with (3.5.5) concludes the proof in the case that $N = \#(\overline{B}_k \cap \mathbb{Z}^d)$ for $k \in \mathbb{N}$. To treat the general case we note that for each $N \in \mathbb{N}$ there exists $k \in \mathbb{N}$ such that for $N_k = \#(\overline{B}_k \cap \mathbb{Z}^d)$ we have $0 \leq N - N_k \leq C_d k^{d-1}$. Finally, the estimate in the statement follows by using as a test the function u_k constructed above and $X_N = X \cup Z_N$ where X is set of the previous step and $Z_N \subset \mathbb{Z}^d$ is chosen such that $\#X_N = N$. □

3.5.3 The error on the Fraenkel asymmetry

From Lemma 3.5.1 and Lemma 3.5.3, we have all the necessary estimates to infer that a sequence $(\lambda_N)_N$ as in (3.2.2) is Q-close to (3.1.1) with respect to Definition 1.5.2 and therefore we can prove a quantitative discrete Faber-Krahn inequality via Proposition 1.5.3. Before doing that, we also show the relationship between the discrete Fraenkel asymmetry of $X \in \mathcal{X}_N$ with respect to a (properly discretized) ball and the Fraenkel asymmetry provided by the continuous embedding of the map ζ in (3.4.2).

Lemma 3.5.4. *Let $X \in \mathcal{X}_N$. Then, there exists $C_d > 0$ such that for all $z \in \mathbb{Z}^d$ there holds*

$$\#\left(X\Delta(z + B_{r_N} \cap \mathbb{Z}^d)\right) \leq \left|\zeta(X)\Delta(B_{r_N} + z)\right| + C_d N^{\frac{d-1}{d}} P_N(X)\,,$$

where $r_N > 0$ is such that $|B_{r_N}| = N$.

Proof. Without loss of generality we assume $z = 0$. In order to prove the statement, we claim that for $X, Y \subset \mathbb{Z}^d$ we have

$$\#\,(X\Delta Y) \leq |\zeta(X)\Delta\zeta(Y)| + C_d\left(P(X) + P(Y)\right)\,. \tag{3.5.6}$$

Assuming the claim, we now show how to conclude. If $Y = B_{r_N} \cap \mathbb{Z}^d$, then $|\#Y - N| \leq C_d N^{\frac{d-1}{d}}$ which implies $P(Y) \leq C_d N^{\frac{d-1}{d}}$. Since $X \in \mathcal{X}_N$,

$\#X = N$, hence, by the isoperimetric inequality on $\mathbb{Z}^d$, there exists $C_d > 0$ such that $P(X) \geq C_d N^{\frac{d-1}{d}}$. Thus, we deduce that

$$P(Y) \leq C_d P(X)\,.$$

Arguing as in the proof of Lemma 3.4.7, for $Y = B_{r_N} \cap \mathbb{Z}^d$ it holds that

$$|\zeta(Y)\Delta B_{r_N}| \leq C_d P(Y) \leq C_d P(X)\,. \tag{3.5.7}$$

Since $P(X) = N^{\frac{d-1}{d}} P_N(X)$, the statement of the Lemma eventually follows from (3.5.6), (3.5.7), and the triangular inequality. We now prove the claim (3.5.6). We first observe that (3.5.6) follows from the estimate

$$\#\big(X \setminus Y\big) \leq |\zeta(X) \setminus \zeta(Y)| + C_d P(Y) \tag{3.5.8}$$

by exchanging the roles of X and Y. The proof of (3.5.8) is the consequence of the following two facts. On one hand, by the very definition of ζ in (3.4.2) it follows that

$$\bigcup_{x\in X\setminus\overline{\zeta(Y)}} (x + Q_1) \subset \zeta(X) \setminus \zeta(Y)\,.$$

Hence, we infer that

$$\#\Big(X \setminus \overline{\zeta(Y)}\Big) = \sum_{x\in X\setminus\overline{\zeta(Y)}} |Q_1| = \left|\bigcup_{x\in X\setminus\overline{\zeta(Y)}} (x + Q_1)\right| \leq |\zeta(X) \setminus \zeta(Y)|\,.$$

On the other hand, since any $x \in \overline{\zeta(Y)} \setminus Y$ is a neighbour of a boundary point of Y, it follows that

$$\#\{x \in X \setminus Y : x \in \overline{\zeta(Y)}\} \leq C_d P(Y)\,.$$

Combining these two inequalities, we get (3.5.8) and conclude the proof. □

3.6 The quantitative estimate

Eventually, we can state the quantitative result:

Theorem 3.6.1. *Let $\{\alpha_N\}_N \subseteq (0, +\infty)$ be such that $\sup_N \alpha_N < +\infty$ and let $X \in \mathcal{X}_N$ satisfy*

$$\lambda_N(X) \leq m_{\lambda,N} + \alpha_N\,. \tag{3.6.1}$$

Then, there exists $C_d > 0$ such that

$$\min_{z\in\mathbb{Z}^d} \# \left(X\Delta((B_{r_N}\cap\mathbb{Z}^d)+z)\right) \le C_d N \left(N^{-\frac{1}{2d}} P_N(X)^{\frac{1}{2}} + \alpha_N^{\frac{1}{2}} + N^{-\frac{1}{d}}\right), \tag{3.6.2}$$

where $r_N > 0$ is such that $|B_{r_N}| = N$.
In particular, if the sequence $(X_N)_N$ is such that $\sup_N \mathrm{P}_N(X_N) \le C$, then there holds

$$\min_{z\in\mathbb{Z}^d} \# \left(X_N\Delta((B_{r_N}\cap\mathbb{Z}^d)+z)\right) \le C_d N \left(N^{-\frac{1}{2d}} + \alpha_N^{\frac{1}{2}}\right). \tag{3.6.3}$$

Proof. Before proving the statements, we point out that the value of the constant C_d may change from line to line in what follows. We do not rename it so as not to overburden the notation, unless its value is no longer dimension-dependent.
Using Lemma 3.5.3 and (3.6.1), we have that

$$\lambda_N(X) \le \lambda(B_1) + \alpha_N + C_d N^{-\frac{1}{d}}.$$

From Lemma 3.5.1 and the above estimate we infer that

$$\lambda\left(\zeta(X)\right) \le N^{-\frac{2}{d}}\lambda(B_1) + N^{-\frac{2}{d}}\alpha_N + C_d N^{-\frac{3}{d}}.$$

Furthermore, setting $r_{|\zeta(X)|} > 0$ such that $B_{r_{|\zeta(X)|}} = |\zeta(X)|$, by the scaling properties of λ, Lemma 3.4.7 and the fact that $t \mapsto t^{\frac{2}{d}}$ is concave, we have

$$N^{-\frac{2}{d}}\lambda(B_1) = \left(\frac{|\zeta(X)|}{N}\right)^{\frac{2}{d}} \lambda\left(B_{r_{|\zeta(X)|}}\right) \le \lambda\left(B_{r_{|\zeta(X)|}}\right)\left(1 + \frac{2}{d}C_d N^{-\frac{1}{d}} P_N(X)\right).$$

By Lemma 3.4.7 we have $|\zeta(X)| \le C_d N$ and therefore, again by the scaling properties of λ, we have

$$\begin{aligned}\frac{\lambda\left(\zeta(X)\right) - \lambda\big(B_{r_{|\zeta(X)|}}\big)}{\lambda\big(B_{r_{|\zeta(X)|}}\big)} &\le C_d N^{-\frac{1}{d}} P_N(X) + C_d\alpha_N + C_d N^{-\frac{1}{d}} \\ &\le C_d N^{-\frac{1}{d}} P_N(X) + C_d\alpha_N.\end{aligned}$$

Using the subadditivity of the square-root we obtain

$$\left(\frac{\lambda\left(\zeta(X)\right)-\lambda\big(B_{r_{|\zeta(X)|}}\big)}{\lambda\big(B_{r_{|\zeta(X)|}}\big)}\right)^{\frac{1}{2}} \le C_d\left(N^{-\frac{1}{2d}}P_N(X)^{\frac{1}{2}}+\alpha_N^{\frac{1}{2}}\right).$$

By [9, Main Theorem] there exists $z\in\mathbb{R}^d$ such that

$$\left|\zeta(X)\Delta(B_{r_{|\zeta(X)|}}+z)\right| \le |\zeta(X)|C_d\left(N^{-\frac{1}{2d}}P_N(X)^{\frac{1}{2}}+\alpha_N^{\frac{1}{2}}\right).$$

Combining the latter inequality with the estimate in Lemma 3.4.7, we infer that

$$\left|\zeta(X)\Delta(B_{r_{|\zeta(X)|}}+z)\right| \le C_dN\left(N^{-\frac{1}{2d}}P_N(X)^{\frac{1}{2}}+\alpha_N^{\frac{1}{2}}\right). \tag{3.6.4}$$

Let $\overline{z}\in\mathbb{Z}^d$ be such that $|z-\overline{z}|\le\sqrt{d}$. Then, the triangle inequality gives that

$$\begin{aligned}\left|(B_{r_N}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+z)\right| \le{}& \left|(B_{r_N}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+\overline{z})\right| \\ &+\left|(B_{r_{|\zeta(X)|}}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+z)\right|.\end{aligned}$$

Thanks to Lemma 3.4.7, the first term on the right hand side can be estimated as

$$\left|(B_{r_N}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+\overline{z})\right| \le C_dN^{\frac{d-1}{d}}P_N(X).$$

The second term on the right hand side can be estimated by evaluating the measure of the symmetric difference between a ball of radius $r_{|\zeta(X)|}+\sqrt{d}$ and a ball of radius $r_{|\zeta(X)|}-\sqrt{d}$ and then by using Lemma 3.4.7:

$$\begin{aligned}\left|(B_{r_{|\zeta(X)|}}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+z)\right| &\le |\zeta(X)|\left(\left(1+\frac{\sqrt{d}}{r_{|\zeta(X)|}}\right)^d-\left(1-\frac{\sqrt{d}}{r_{|\zeta(X)|}}\right)^d\right) \\ &\le C_d|\zeta(X)|\left(\frac{2d\sqrt{d}}{r_{|\zeta(X)|}}\right)\le C_d\frac{|\zeta(X)|}{N^{\frac{1}{d}}} \\ &\le C_dN^{\frac{d-1}{d}}\left(1+C_dN^{-\frac{1}{d}}P_N(X)\right).\end{aligned}$$

We can thus write that

$$\left|(B_{r_N}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+z)\right| \le C_dN^{\frac{d-1}{d}}P_N(X). \tag{3.6.5}$$

Combining the estimate in Lemma 3.5.4 and (3.6.5), we obtain

$$\begin{aligned}
\#\left(X\Delta(\mathbb{Z}^d\cap B_{r_N}+\overline{z})\right) &\le |\zeta(X)\Delta(B_{r_N}+\overline{z})| + C_d N^{\frac{d-1}{d}} P_N(X)\\
&\le \left|\zeta(X)\Delta(B_{r_{|\zeta(X)|}}+z)\right| + \left|(B_{r_N}+\overline{z})\Delta(B_{r_{|\zeta(X)|}}+z)\right|\\
&\quad + C_d N^{\frac{d-1}{d}} P_N(X)\\
&\le \left|\zeta(X)\Delta(B_{r_{|\zeta(X)|}}+z)\right| + C_d N^{\frac{d-1}{d}} P_N(X)\,.
\end{aligned}$$

Eventually, by (3.4.3) and (3.6.4), we infer that

$$\begin{aligned}
\#\left(X\Delta(\mathbb{Z}^d\cap B_{r_N}+\overline{z})\right) &\le |\zeta(X)\Delta(B_{r_{|\zeta(X)|}}+z)| + C_d N^{\frac{d-1}{d}} P_N(X)\\
&\le C_d N\left(N^{-\frac{1}{2d}} P_N(X)^{\frac{1}{2}} + \alpha_N^{\frac{1}{2}}\right) + C_d N^{\frac{d-1}{d}} P_N(X)\\
&\le C_d N\left(N^{-\frac{1}{2d}} P_N(X)^{\frac{1}{2}} + \alpha_N^{\frac{1}{2}} + N^{-\frac{1}{d}}\right)\,,
\end{aligned}$$

where in the last inequality we used that, by the very definition of P_N, it holds that $P_N(X)\le C_d N^{\frac{1}{d}}$. To conclude, we observe that $\sup_N \alpha_N < +\infty$ yields (3.6.2). The inequality (3.6.3) follows from the assumptions on X_N and the estimate (3.6.2). □

Remark 3.6.2. In the statement of Theorem 3.6.1 we have a perimeter contribution in the estimate: from (3.6.2) we get

$$\min_{z\in\mathbb{Z}^d}\#\left(X\Delta((B_{r_N}\cap\mathbb{Z}^d)+z)\right)\le C_d N\left(N^{-\frac{1}{2d}}P_N(X)^{\frac{1}{2}}+\dots\right)$$

One may expect that it is possible to adjust the hypothesis of Theorem 3.6.1 and avoid this term since $\#X = N$, but, *a priori*, we lack information on the geometry: indeed, we are not considering minimizer of (3.2.2), for which we can infer connectedness and convexity by Proposition 3.3.11, but only sets which are quasi-minimizers (by (3.6.1)). Moreover, even in the continuous setting, we cannot expect a quasi-minimizer of (3.1.1) to have a bounded perimeter: for instance, we can consider a ball having long thin tentacles with negligible measure and negligible Dirichlet energy. ♠

3.7 An alternative version of the Q-closeness

We observe that, in our computations, it was necessary to estimate the approximation error introduced in constructing the continuous domain through the map ζ. However, neither Definition 1.5.2 nor Proposition 1.5.3 accounts for this parameter; therefore, we propose a slightly modified version of both statements that incorporates this approximation error. On a lattice $\mathscr{L} \subset \mathbb{R}^d$, we consider

- a sequence $(\mathcal{E}_N)_N$ of functionals as in (1.5.1),
- a functional $\mathcal{E}\colon \mathcal{M}(\mathbb{R}^d) \to [0, +\infty]$,
- a set $W_v \subset \mathcal{M}(\mathbb{R}^d)$ that satisfies (1.5.2),
- a map $\zeta\colon \mathscr{L} \to \mathcal{M}(\mathbb{R}^d)$ such that $|\zeta(X)| \geq N$ for any $X \subset \mathscr{L}$ such that $\#X = N$

and then we have the followings:

Definition 3.7.1. We say that $(\mathcal{E}_N)_N$ is **Q-close** $\mathcal{E}$ with respect to ζ and to the non-negative parameters α_N, β_N, γ_N, δ_N if, for every $X \subset \mathscr{L}$ such that $\#X = N$ and

$$\mathcal{E}_N(X) \leq \inf_{Y \in \mathcal{X}_N} \mathcal{E}_N(Y) + \alpha_N\,,$$

the following three hold:

$$\mathcal{E}\left(\zeta(X)\right) \leq \mathcal{E}_N(X) + \beta_N\,,$$

$$\inf_{Y \in \mathscr{L}\,:\,\#Y=N} \mathcal{E}_N(Y) \leq \mathcal{E}\left(W_{|\zeta(X)|}\right) + \gamma_N\,,$$

$$\inf_{z \in \mathscr{L}} \frac{|X \Delta (z + W_N \cap \mathscr{L})|}{N} \leq \inf_{z \in \mathbb{R}^d} \frac{\left|\zeta(X) \Delta \left(z + W_{|\zeta(X)|}\right)\right|}{|\zeta(X)|} + \delta_N\,.$$

Corollary 3.7.2. *Let $(\mathcal{E}_N)_N$ be Q-close to a functional $\mathcal{E}$, with respect to Definition 3.7.1, that satisfies* (1.5.2) *and* (1.5.3). *Then, for any $X \in \mathcal{X}_N$, the following holds:*

$$\inf_{z \in \mathscr{L}} |X \Delta (z + W_N \cap \mathscr{L})| \leq |\zeta(X)| \varphi \left(\frac{\alpha_N + \beta_N + \gamma_N}{\mathcal{E}(W_{|\zeta(X)|})} \right) + \delta_N\,.$$

Proof. From Proposition 1.5.3 we have

$$\inf_{z\in\mathbb{R}^d} \left|\zeta(X)\Delta\left(z+W_{|\zeta(X)|}\right)\right| \le |\zeta(X)|\varphi\left(\frac{\alpha_N+\beta_N+\gamma_N}{\mathcal{E}\left(W_{|\zeta(X)|}\right)}\right).$$

Then, from the third condition of Definition 3.7.1, we can infer that

$$\begin{aligned}\inf_{z\in\mathbb{R}^d} \left|\zeta(X)\Delta\left(z+W_{|\zeta(X)|}\right)\right| &\ge \frac{|\zeta(X)|}{N}\inf_{z\in\mathcal{L}}\left|X\Delta(z+W_N\cap\mathcal{L})\right|-\delta_N\\ &\ge \inf_{z\in\mathcal{L}}\left|X\Delta(z+W_N\cap\mathcal{L})\right|-\delta_N\end{aligned}$$

and the thesis follows. □

Appendix A

Q-closeness for the FCC lattice

The face-centred cubic (FCC) lattice is a periodic structure made by an infinite foliation of 2-dimensional triangular lattices $\mathcal{L}_T$ (see Figure A.1), where the vertices of each layer are projected onto the centroid of the triangles in the layer below, following a three-layers periodic pattern. If we assume

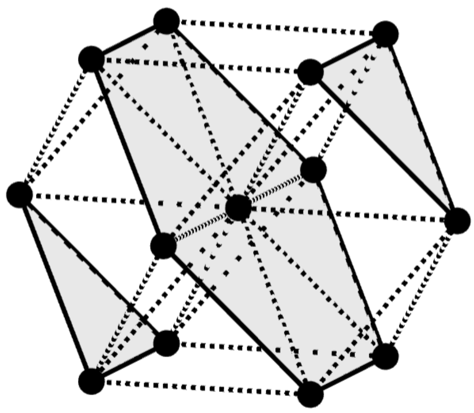

Figure A.1: A portion of $\mathcal{L}_{FCC}$. The layers of the 2-d triangular lattices are highlighted in gray.

that the lattice has uniform unitary spacing, then the FCC lattice can be mathematically described as a Bravais lattice:

$$\mathcal{L}_{FCC} = \frac{1}{\sqrt{2}} span_{\mathbb{Z}} \{e_1 + e_2, e_1 + e_3, e_2 + e_3\} \ . \tag{A.0.1}$$

We report from [12] the value of the anisotropic norm associated to $\mathcal{L}_{FCC}$ and of its Wulff shape, computed thanks to Theorem 1.3.14: we have

$$\|\nu\|_{FCC} = \sum_{1\le i<j\le 3} |\nu_i + \nu_j| + |\nu_i - \nu_j|\,,$$

while the Wulff shape associated to $\mathcal{L}_{FCC}$ is the truncated octahedron

$$W_{FCC} = \left\{ x \in \mathbb{R}^3 : \; \max\left\{ \frac{\|x\|_\infty}{4}, \frac{\|x\|_1}{6} \right\} \le 1 \right\}. \tag{A.0.2}$$

In particular, the value of the anisotropic norm on the outer unit normal to W_{FCC} is

$$\big\|\nu(x)\big\|_{FCC} = \begin{cases} 2\sqrt{3} & \text{if } x \text{ belongs to an hexagonal face of } W_{FCC} \\ 4 & \text{if } x \text{ belongs to a square face of } W_{FCC}\,. \end{cases}$$

A.1 Behaviour of ζ on optimal discrete sets

Since the Wulff shape (A.0.2) does not satisfies the tangential property necessary for the map (2.1.3), we rescale it by a factor equal to $\frac{\sqrt{2}}{12}$ and we denote it as

$$\Theta := \frac{\sqrt{2}}{12} W_{FCC} \quad \text{and} \quad \Theta(p) = p + \Theta \quad \forall p \in \mathcal{L}_{FCC}\,.$$

Then, we consider the discrete-to-continuum map $\zeta\colon \mathcal{L}_{FCC} \to \mathcal{M}(\mathbb{R}^3)$ such that

$$\zeta(X) = \Theta \oplus \left(\bigcup_{\substack{p\in X \\ \mathrm{val}(p)=12}} \{p\} \cup \bigcup_{\substack{p,q\in\mathcal{L}_T \\ \{p,q\}\in\mathcal{N}}} \overline{p,q} \right). \tag{A.1.1}$$

Moreover, we cannot take the Voronoi cells of $\mathcal{L}_{FCC}$ as Minkowski neighbourhoods, since

$$\Theta \oplus \overline{p,q} \not\subset V(p) \cup V(q)$$

for any $p, q \in \mathcal{L}_{FCC}$ such that $\{p,q\} \in \mathcal{N}$. Thus, according to Definition 2.1.5, we need to consider

$$U(p) = \bigcup_{\substack{q\in\mathcal{L}_{FCC} \\ \{p,q\}\in\mathcal{N}}} \left(\Theta \oplus \frac{\overline{p,q}}{2} \right). \tag{A.1.2}$$

A representation of (A.1.2) is given in Figure A.2.

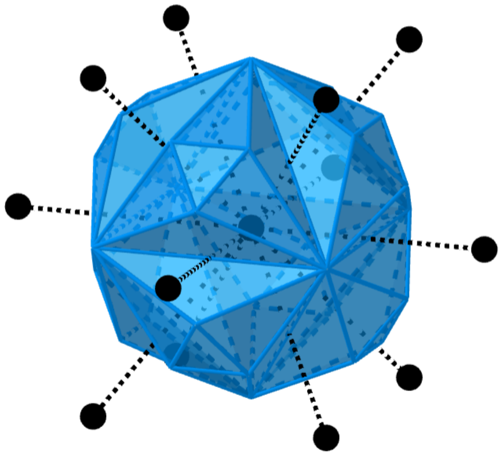

Figure A.2: The Minkowski neighbourhood $U(p)$ of $\mathscr{L}_{FCC}$

Definition A.1.1. Up to translations, we define **optimal discrete sets** for $\mathscr{L}_{FCC}$ the elements of the sequence constructed as follows: $X_0 = \{0\}$ and, for $k \geq 1$,

$$X_k = X_{k-1} \cup \{q \in \mathscr{L}_{FCC} \setminus X_{k-1} : \{p,q\} \in \mathcal{N} \text{ for some } p \in X_{k-1}\}.$$

Remark A.1.2. Roughly speaking, the sets defined in Definition A.1.1 are the 3-dimensional analogue of those defined in the proof of Lemma 2.4.7. ♠

Remark A.1.3. If we denote as p the central point of X_k and we embed the lattice in $\mathbb{R}^3$, then we can visualize X_k as the points of $\mathscr{L}_{FCC}$ contained in the truncated octahedron (see Figure A.3) given by

$$TO = \left\{ x \in \mathbb{R}^3 : \|x-p\|_1 \leq \sqrt{2}k, \quad \|x-p\|_\infty \leq \frac{\sqrt{2}}{2}k \right\}. \tag{A.1.3}$$

We can also characterize the boundary points of X_k, for $k \geq 1$: there are

- 12 points having valence equal to 7 (the vertices of (A.1.3)),
- $24(k-1)$ points having valence equal to 5 (the points contained in each boundary edge of (A.1.3)),

- $6(k-1)^2$ points having valence equal to 4 (the points in the interior of each square face of (A.1.3)),
- for $k \geq 3$, $8\sum_{i=1}^{k-2} i$ points having valence equal to 3 (the points in the interior of each triangular face of (A.1.3)).

In the end, we can also infer that the followings hold (their proof is a straightforward consequence of Definition A.1.1 and of the characterization above):

(i) $P(X_k) = 12(3k^2 + 3k + 1)$.

(ii) $\#\left\{p \in X_k : \operatorname{val}(p) > 0\right\} = 2(5k^2 + 1)$ for $k \geq 1$.

(iii) $\#X_k = \frac{10}{3}k^3 + 5k^2 + \frac{11}{3}k + 1$.

♠

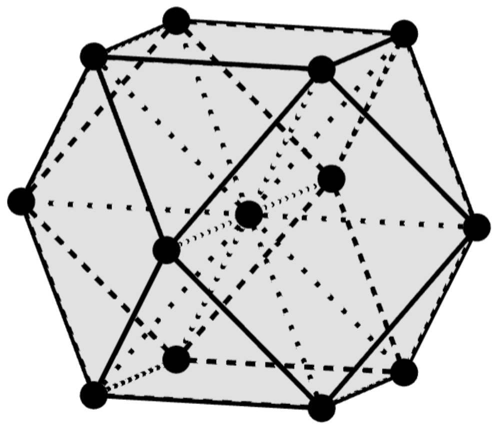

Figure A.3: The convex hull of X_1, coinciding with (A.1.3) for $k = 1$.

In the following result we provide a formula for computing the anisotropic perimeter of $\zeta(X_k)$. For sake of conciseness, we omit its proof, which merely relies on the weighted sum over the points of X_k, according to the four types of boundary points described in Remark A.1.3.

Lemma A.1.4. *Let $(X_k)_k$ be the sets of Definition A.1.1 and let $\zeta\colon \mathcal{L}_{FCC} \to \mathcal{M}(\mathbb{R}^3)$ be the function defined in* (A.1.1). *Then,*

$$P_{FCC}\left(\zeta(X_k)\right) = \frac{31}{27}P(X_k) - \frac{4}{3}k - \frac{124}{9}\,.$$

A.2 Q-closeness for X_k

We can try to apply the Q-closeness technique on the sets given by Definition A.1.1. As usual, we define the continuous functional as $\mathcal{E}\colon \mathcal{M}(\mathbb{R}^3) \to [0,+\infty]$ such that

$$\mathcal{E}(\Omega) = P_{FCC}(\Omega) \quad \forall \Omega \in \mathcal{M}(\mathbb{R}^3)\,. \tag{A.2.1}$$

Thanks to Lemma A.1.4, we have that the parameter β in (1.5.5) is null if we define the the discrete functionals as $\mathcal{E}_N \colon \mathcal{L}_{FCC} \to [0,+\infty]$

$$\mathcal{E}_N(X) = \frac{31}{27} P(X) \quad \forall X \in \mathcal{X}_N\,. \tag{A.2.2}$$

In order to apply Proposition 1.5.3, it is left to estimate the parameter γ_N of (1.5.6).

Lemma A.2.1. *Let the functionals $\mathcal{E}_N$, $\mathcal{E}$ be the ones defined respectively in* (A.2.2), (A.2.1) *and let X_k be a set defined as in Definition A.1.1. If we set $N = \#X_k$, then there exists $\hat{c} > 0$ such that*

$$\inf_{Y\colon \#Y=N} \mathcal{E}_N(Y) \le \inf_{\substack{\Omega\in\mathbb{R}^3\\ |\Omega|=|\zeta(X_k)|}} \mathcal{E}(\Omega) + \hat{c}k^2\,.$$

Proof. By Remark A.1.3, we can infer that

$$\inf_{Y\colon \#Y=N} \mathcal{E}_N(Y) = \mathcal{E}_N(X_k) = \frac{31}{27} P(X_k) = \frac{124}{3}\left(k^2 + k + \frac{1}{3}\right)\,. \tag{A.2.3}$$

On the other hand, we have

$$\inf_{\substack{\Omega\in\mathbb{R}^3\\ |\Omega|=|\zeta(X_k)|}} \mathcal{E}(\Omega) = 3\,|W_{FCC}|^{\frac{1}{3}}\left|\zeta(X_k)\right|^{\frac{2}{3}} = 12\left(2|\zeta(X_k)|\right)^{\frac{2}{3}}$$

and we can estimate $|\zeta(X_k)|$ by the usual local-to-global approach. By Remark A.1.3, we know that the number of points having valence greater or equal than 5 in X_k is of order k; thus (we omit the precise computations for sake of simplicity), we get

$$\left|\zeta(X_k)\cap U(p)\right| = \begin{cases} \frac{\sqrt{2}}{2} & \text{if } \mathrm{val}(p)\in\{0,3\}\,,\\ \frac{173\sqrt{2}}{324} & \text{if } \mathrm{val}(p)=4\,,\\ C_1 & \text{if } \mathrm{val}(p)=5\,,\\ C_2 & \text{if } \mathrm{val}(p)=6\,.\end{cases}$$

By Remark A.1.3 and by summing up, we obtain

$$\begin{aligned}|\zeta(X_k)| &= \frac{\sqrt{2}}{2}\left(\frac{10}{3}k^3-k^2-\frac{25}{3}k+7\right)+\frac{173\sqrt{2}}{324}6(k-1)^2+\widetilde{C_1}k\\ &= \frac{5\sqrt{2}}{3}\left(k^3+\frac{73}{45}k^2-\frac{571}{90}k+\frac{181}{45}+\widetilde{C_2}k\right)\end{aligned}$$

and then we can infer that

$$\inf_{\substack{\Omega\in\mathbb{R}^3\\ |\Omega|=|\zeta(X_k)|}} \mathcal{E}(\Omega) = 24\left(\frac{5}{3}\right)^{\frac{2}{3}}\left(k^3+\frac{73}{45}k^2-\frac{571}{90}k+\frac{181}{45}+\widetilde{C_2}k\right)^{\frac{2}{3}}\,. \tag{A.2.4}$$

By (A.2.3) and (A.2.4), there exists $\hat{c}>0$ such that

$$\inf_{Y:\,\#Y=N}\mathcal{E}_N(Y)-\inf_{\substack{\Omega\in\mathbb{R}^3\\ |\Omega|=|\zeta(X_k)|}}\mathcal{E}(\Omega)\le \hat{c}k^2\,,$$

□

Remark A.2.2. We can infer that map ζ in (A.1.1) brings to a meaningless fluctuation estimate on the FCC lattice: indeed, by the Q-closeness technique we get an error of the same order of the measure of the set.
If we set $N=\#X_k$ and if we assume that (A.2.2) is Q-close to (A.2.1) with parameters $\alpha_N\ge 0$, then, by Lemma A.1.4, Lemma A.2.1 and Proposition 1.5.3, we get

$$\begin{aligned}\inf_{x\in\mathbb{R}^3}\left|\zeta(X_k)\triangle(x+W_{FCC,|\zeta(X_k)|})\right| &\lesssim \left(\alpha_N+\hat{c}k^2\right)^{\frac{1}{2}}|\zeta(X_k)|^{\frac{2}{3}}\\ &\lesssim \left(\alpha_N+N^{\frac{2}{3}}\right)^{\frac{1}{2}}N^{\frac{2}{3}}\simeq N\,.\end{aligned}$$

♣

Remark A.2.3. If we choose $\zeta\colon \mathcal{L}_{FCC} \to \mathcal{M}(R^3)$ to be the map that associates the Voronoi cells to the points of $\mathcal{L}_{FCC}$, then we obtain that

$$\left|\zeta(X)\right| = \frac{\sqrt{2}}{2}\#X \qquad \text{and} \qquad P_{FCC}\left(\zeta(X)\right) = \frac{3}{2}P(X)$$

for every $X \subset \mathcal{L}_{FCC}$. By choosing $\mathcal{E}_N(X) = \frac{3}{2}P(X)$ as the discrete functional and (A.2.1) as the continuous functional, we can try to estimate the value of γ_N on the sets X_k, analogously to Lemma A.2.1.
By setting $\#X_k = N$, we get that

$$\inf_{Y\colon \#Y=N} \mathcal{E}_N(Y) = \frac{3}{2}P(X_k) = 54\left(k^2 + k + \frac{1}{3}\right)$$

$$\inf_{\substack{\Omega\in\mathbb{R}^3 \\ |\Omega|=|\zeta(X_k)|}} \mathcal{E}(\Omega) = 12\left(\sqrt{2}N\right)^{\frac{2}{3}} = 24\left(\frac{5}{3}\right)^{\frac{2}{3}}\left(k^3 + \frac{3}{2}k^2 + \frac{11}{10}k + \frac{3}{10}\right)^{\frac{2}{3}}$$

and we obtain that, for some $\hat{c} > 0$, it holds that

$$\inf_{Y\colon \#Y=N} \mathcal{E}_N(Y) - \inf_{\substack{\Omega\in\mathbb{R}^3 \\ |\Omega|=|\zeta(X_k)|}} \mathcal{E}(\Omega) \leq \hat{c}k^2\,.$$

As in Remark A.2.2, if we apply Proposition 1.5.3, then we obtain a quantity which still has the wrong scaling to provide a meaningful fluctuation estimate.

♠

List of Figures

Bibliography

[1] R. Alicandro, A. Braides, and M. Cicalese. “Phase and anti-phase boundaries in binary discrete systems: a variational viewpoint”. In: *Networks and Heterogeneous Media* (2006).

[2] R. Alicandro and M. Cicalese. “A general integral representation result for continuum limits of discrete energies with superlinear growth”. In: *SIAM journal on mathematical analysis* 36 (2004).

[3] R. Alicandro, G. Lazzaroni, and M. Palombaro. “On the effect of interactions beyond nearest neighbours on non-convex lattice systems”. In: *Calc. Var.* 56 (2017).

[4] L. Ambrosio, N. Fusco, and D. Pallara. *Functions of Bounded Variation and Free Discontinuity Problems*. Clarendon Press, Oxford, 2000.

[5] Y. Au Yeung, G. Friesecke, and B. Schmidt. “Minimizing atomic configurations of short range pair potentials in two dimensions: crystallization in the Wulff shape”. In: *Calc. Var.* 44 (2012).

[6] X. Blanc and M. Lewin. “The crystallization conjecture: a review”. In: *EMS Surv. Math. Sci. 2* 164 (2015).

[7] A. Braides. *Gamma-convergence for Beginners*. Oxford University Press, Oxford, 2002.

[8] Andrea Braides. *A handbook of* Γ*-convergence*. cvgmt preprint. 2006. URL: `http://cvgmt.sns.it/paper/57/`.

[9] L. Brasco, G. De Philippis, and B. Velichkov. “Faber - Krahn inequalities in sharp quantitative form”. In: *Duke Math. J.* 164 (2015).

[10] X. Cabré. “Elliptic PDEs in probability and geometry: Symmetry and regularity of solutions,” in: *Discrete and Continuous Dynamical Systems* 20 (2008).

[11] A. Chambolle and L. Kreutz. “Crystallinity of the homogenized energy density of periodic lattice systems”. In: *Multiscale Modeling & Simulation* 21 (2023).

[12] M. Cicalese, L. Kreutz, and G.P. Leonardi. "Emergence of Wulff-Crystals from Atomistic Systems on the FCC and HCP Lattices". In: *Communications in Mathematical Physics* 402 (2023).

[13] M. Cicalese and G.P. Leonardi. "Maximal fluctuations on periodic lattices: an approach via quantitative Wulff inequalities". In: *Communications in Mathematical Physics* 375 (2020).

[14] M. Cicalese et al. "The quantitative Faber-Krahn inequality for the combinatorial Laplacian in Z^d". In: *ArXiv* (2025).

[15] J. Conway and Sloane N.J.A. *Sphere Packings, Lattices and Groups 3rd ed.* Springer, 1999.

[16] G. Dal Maso. *An Introducion to Gamma-convergence.* Birkhäuser, 1993.

[17] E. Davoli, P. Piovano, and U. Stefanelli. "Sharp $N^{\frac{3}{4}}$ law for the minimizers of the edge-isoperimetric problem on the triangular lattice," in: *J. of Nonlinear Science* (2017).

[18] E. De Giorgi. "Nuovi teoremi relativi alle misure $(r-1)$-dimensionali in uno spazio ad r-dimensioni". In: *Ricerche Mat.* (1955).

[19] E. De Giorgi. "Su una teoria generale della misura $(r-1)$-dimensionale in uno spazio ad r-dimensioni". In: *Ann. Mat. Pura Appl.* (1954).

[20] E. De Giorgi. "Sulla proprietá isoperimetrica dell'ipersfera, nella classe degli insiemi aventi frontiera orientata di misura finita". In: *Atti Accad. Naz. Lincei Mem. Cl. Sci. Fis. Mat. Nat.* (1958).

[21] W. E and D Li. "On the Crystallization of 2D Hexagonal Lattices". In: *Commun. Math. Phys.* 286 (2009).

[22] L.C. Evans and R.F. Gariepy. *Measure Theory and Fine Properties of Functions.* CRC Press, 1991.

[23] G. Faber. "Beweis, dass unter allen homogenen Membranen von gleicher Fläche und gleicher Spannung die kreisförmige den tiefsten Grundton gibt". In: *Sitzungsber. Bayer. Akad. Wiss. München, Math.-Phys* (1923).

[24] A. Figalli, F. Maggi, and A. Pratelli. "A Mass Transportation Approach to Quantitative Isoperimetric Inequalities". In: *Invent. math.* (2010).

[25] B. Fuglede. "Stability in the isoperimetric problem for convex or nearly spherical domains in $\mathbb{R}^n$". In: *Trans. Amer. Math. Soc.* (1989).

[26] N. Fusco, F. Maggi, and A. Pratelli. "Stability estimates for certain Faber-Krahn, Isocapacitary and Cheeger inequalities". In: *Ann. Sc. Norm. Super. Pisa* (2009).

[27] N. Fusco, F. Maggi, and A. Pratelli. "The Sharp Quantitative Isoperimetric inequality". In: *Ann. Math.* (2008).

[28] R.J. Gardner. "The Brunn-Minkowkski inequality". In: *Bull. Am. Math. Soc.* 39 (2002).

[29] H. Hajaiej. "Rearrangement inequalities in the discrete setting and some applications". In: *Nonlinear Analysis* 71 (2010), pp. 1140–1148.

[30] H. Hajaiej, F. Han, and B. Hua. "Discrete Schwarz rearrangement in lattice graphs". In: *preprint on arXiv* (2022).

[31] R.R. Hall. "A quantitative isoperimetric inequality in n-dimensional space". In: *J. Reine Angew. Math.* (1992).

[32] R.R. Hall, W.K. Hayman, and A.W. Weistman. "On asymmetry and capacity". In: *J. d'Analyse Math.* (1991).

[33] W. Hansen and N. Nadirashvili. "Isoperimetric inequalities in potential theory". In: *Potential Anal.* (1994).

[34] R.C. Heitmann and C. Radin. "The ground state for sticky disks." In: *J. Stat. Phys.* (1980).

[35] E. Krahn. "Über eine von Rayleigh formulierte Minimaleigenschaft des Kreises". In: *Math. Ann.* (1925).

[36] F. Maggi. *Sets of Finite Perimeter and Geometric Variational Problems.* Cambridge University Press, 2012.

[37] E. Mainini et al. "$N^{\frac{3}{4}}$ Law in the Cubic Lattice". In: *J. Stat. Phys* (2019).

[38] A.D. Melas. "The stability of some eigenvalue estimates". In: *J. Differential Geom.* (1992).

[39] R. Osserman. "Bonnesen-style isoperimetric inequalities". In: *Amer. Math. Monthly* (1979).

[40] A R Pruss. "Discrete convolution-rearrangement inequalities and the Faber-Krahn inequality on regular trees". In: *Duke Mathematical Journal* 91 (1998).

[41] B. Schmidt. "Ground states of the 2D sticky disc model: fine properties and $N^{\frac{3}{4}}$ law for the deviation from the asymptotics Wulff shape". In: *J. Stat. Phys* (2013).

[42] Y. Shlapentokh-Rothman. "An asymptotic Faber-Krahn inequality for the combinatorial laplacian on $\mathbb{Z}^2$". In: *preprint on arXiv* (2010).

[43] F. Theil. "A proof of Crystallization in Two Dimensions". In: *Commun. Math. Phys.* 262 (2006).

[44] G. Wulff. "Zur Frage der Geschwindigkeit des Wachstums und der Auflösung der Kristallflächen". In: *Zeitschrift für Kristallographie* (1901).