Fachbereich Mathematik und Informatik
Westfälische Wilhelms-Universität Münster

Bachelor Thesis

Crystallization in the Wulff shape for triangular and square configurations

Author:
Benedikt Simon Klein
born on 15.08.1997 in Krefeld

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Für meine Großeltern, die mich immer in meinem akademischen Streben unterstützt haben.

First supervisor: Prof. Dr. Manuel Friedrich
Second supervisor: Prof. Dr. Benedikt Wirth

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1 Introduction

Crystalline solids are all around us. From the silicon semiconductors in our modern smartphones up to the ice in the freezer. In many solids the building atoms are arranged in periodic structures, these solids are then called crystals. Although the scientific field of crystallography is more than 100 years old and has made stunning progress in the characterization of crystals and their properties, many fundamental questions are still unanswered. Such as: Why is it at low temperature favorable for atoms to spontaneously arrange themselves in a periodic array? or: Is there a mathematically rigorous way to predict the physical properties and their macroscopic shape in the equilibrium? These are challenging physical questions which are object of intensive research.

This thesis addresses the question if the (ideal) equilibrium shape of a crystal can be approximated based on the knowledge of the interatomic interactions inside the crystal for some simplified models. Here we discuss mainly the work of Yeung, Friesecke and Schmidt [YFS09] and in a minor extend the one of Mainini, Piovano and Stefanelli [MPS14]. During this process we delve deeper into some of the physical and mathematical background, necessary for treating such questions.

The main goal of the first part is to present a mathematical rigorous proof for the approximation (in the sense of weak*-convergence) of the equilibrium state of large monoatomic crystals in the Euclidean plane. The interatomic interaction inside the crystallized phase is modeled by a potential similar to the Heitmann-Radin sticky disk model. This potential allows, in contrast to the one Heitmann and Radin have used, some elastic deformations inside the crystal. We will show that the equilibrium states can be approximated by a hexagonal set.

For achieving this we will prove at first a compactness statement, which asserts some convergence of configurations with low energy while increasing the number of atoms. Then we are going to prove that for a simplified calculation of the surface energies Γ-converges to an appropriate chosen functional occurs, for that the Wulff property holds. With standard arguments from variational calculus then follows that the previously mentioned limit is, for a sequence of ground states, a minimizer of this functional and thus these ground states can be estimated by this minimizer.

It has to be mentioned here that we do not calculate the interfacial interaction energies in a strict physical way. Instead, we assume that in this setting the microscopic atomic structure, is already determining the macroscopic shape and then prove that this assumption indeed holds. We are able to show that in this model the macroscopic shape of the configurations with minimal energy, in which the atoms are arranged almost in a triangular lattice, is approximately a hexagon.

In the second part we will investigate this question for another atomistic model, where the atoms in the crystal form a square lattice. Here a similar statement can be proved by adapting the arguments from Yeung et al. with minor changes. The equilibrium states can be approximated by the unit square $\left[-\frac{1}{2},\frac{1}{2}\right] \times \left[-\frac{1}{2},\frac{1}{2}\right]$.

2 Mathematical Framework

We begin our discussion by giving the mathematical background necessary to cover the results and arguments. This chapter introduces some important definitions and results from functional analysis, measure theory and variational analysis. We only state the results without the proofs, these can be found in various literature on these topics, e.g. [AFP00] and [ABM14].

In the following Ω denotes an arbitrary open subset of $\mathbb{R}^n$, $\mathcal{B}(\Omega)$ the Borel σ-algebra on Ω and $\mathcal{M}(\Omega)$ the space of all finite $\mathbb{R}$-valued Radon measures on Ω. Notice that all open subsets of $\mathbb{R}^n$ are locally compact and σ-compact. λ^n is the Lebesgue measure and $\mathcal{H}^{n-1}$ the $n-1$-dimensional Hausdorff measure. Further we need to introduce the function spaces $C_c^k(\Omega, \mathbb{R}^m)$ for $k \in \mathbb{N}_0 \cup \{\infty\}$, $m \in \mathbb{N}$ and $C_0(\Omega)$.

Definition 2.1.

1. $C_c^k(\Omega)$ is the set of $\mathbb{R}$-valued C^k-functions on Ω, with compact support in Ω.
2. $C_c^k(\Omega, \mathbb{R}^m)$ is the set of all $\mathbb{R}^m$-valued functions such that every component is in $C_c^k(\Omega)$. If $k = 0$ set $C_c(\Omega, \mathbb{R}^m) := C_c^0(\Omega, \mathbb{R}^m)$ and if $m = 1$ is $C_c^k(\Omega) = C_c^k(\Omega, \mathbb{R}^1)$.
3. $C_0(\Omega)$ is the set of the continuous $\mathbb{R}$-valued functions f on Ω such that for every $\epsilon > 0$ there exists a set K_ϵ, compact in Ω and $|f(x)| < \epsilon$ on $\Omega \setminus K_\epsilon$.

Remark 2.2. *$C_0(\Omega)$ is the closure of $C_c(\Omega)$ in the norm $\|f\|_{C_0(\Omega)} := \sup_{x\in\Omega} |f(x)|$.*

2.1 Measure space and weak*-convergence

As mentioned above we want to use weak*-convergence for approximating the shape of the crystals. In this section we give some of the mathematically background of weak*-convergence of measures and point out the connection to functional spaces. Especially we will see that, under the right conditions, this convergence can be identified with the more general concept of weak*-convergence for function spaces, respectively with the weak*-topology in a topological dual space V^*. This identification allows us the usage of certain compactness statements.

Definition 2.3. Let V be a normed space with dual space V^* and $\iota_v : V^* \to \mathbb{R}; f \mapsto f(v)$ for some $v \in V$. Then the coarsest topology on V^* such that all mappings in $(\iota_v)_{v\in V}$ are continuous is called *weak*-topology* wk*.

For every topological space a convergence can be defined. For (V^*, wk^*) this convergence coincides with the following.

Lemma 2.4. *Let V be a normed space and V^* equipped with wk*. A sequence $(f_n)_{n\in\mathbb{N}}$ in V^* converges in the wk*-topology to $f \in V^*$ if and only if the sequences $(f_n(v))_{n\in\mathbb{N}}$ converges to $f(v)$ for all $v \in V$. In this case we say $(f_n)_{n\in\mathbb{N}}$ convergences weakly* to f and write $f_n \overset{*}{\rightharpoonup} f$.*

One of the most important properties of the wk^*-topology is that the unit ball is compact. This result was shown by Banach and Alaoglu.

Theorem 2.5 (Banach-Alaoglu)**.** *Let V be a normed vector space. Then is the unit ball $B_1(V^*) = \{f \in V^* \big| \|f\|_* \leq 1\}$ wk*-compact. $||\cdot||_*$ is the operator norm on V^*.*

If V is a *separable* normed vector spaces then $B_1(V^*)$ is metrizable with respect to wk*. Therefore, compactness implies sequential compactness in the *wk**-topology. If Ω is locally compact, metrizable and σ-compact, then is $C_0(\Omega)$ separable and consequentially follows

Corollary 2.6. *For each bounded sequence in $C_0^*(\Omega)$ a weakly* converging subsequence exists.*

A remarkable feature of the theory of weak*-topology is that it can be applied on certain measure spaces. The advantage is in particular that measures are more intuitive than the in general rather abstract functionals in a dual space. For discussing this in detail, we introduce at first the total variation of a measure.

Definition 2.7. Let μ be a $\mathbb{R}^m$-valued measure on $(\Omega, \mathcal{B}(\Omega))$ and $B \in \mathcal{B}(\Omega)$. The *total variation* $|\mu|(B)$ of μ for B is defined as

$$|\mu|(B) := \sup\left\{\sum_{h=0}^{+\infty} ||\mu(B_h)||, \middle| B_h \in \mathcal{B}(\Omega) \text{ pairwise disjoint}, B = \bigcup_{h=0}^{+\infty} B_h\right\}.$$

Proposition 2.8. *It applies*

1. *For a $\mathbb{R}^m$-valued measure μ on $(\Omega, \mathcal{B}(\Omega))$ is $|\mu|(\cdot)$ a positive finite measure on $(\Omega, \mathcal{B}(\Omega))$.*
2. *The total variation $|\cdot|(\Omega)$ is a norm on a space of measures defined on Ω.*

The following important theorem identifies $\mathcal{M}(\Omega)$ with operator spaces.

Theorem 2.9 (Riesz-Alexandroff representation Theorem)**.** *The topological dual $C_0^*(\Omega)$ of $C_0(\Omega)$ can be isometrically identified with the space of $\mathbb{R}$-valued finite Radon measures. For each bounded linear functional Φ on $C_0(\Omega)$ there exists a unique $\mathbb{R}$-valued finite Radon measure μ on Ω such that for all $f \in C_0(\Omega)$ is*

$$\Phi(f) = \int_\Omega f(x) d\mu(x)$$

and $||\Phi||_* = |\mu|(\Omega)$.

Therefore, the compactness statements from above can be transferred to the measure space.

Definition 2.10. We say a sequence of measures $(\mu_n)_{n\in\mathbb{N}}$ in $\mathcal{M}(\Omega)$ *converges weakly** to $\mu \in \mathcal{M}(\Omega)$ if for all $\phi \in C_0(\Omega)$ is

$$\int_\Omega \phi d\mu_n \longrightarrow \int_\Omega \phi d\mu.$$

Notation: $\mu_n \overset{*}{\rightharpoonup} \mu$

Remark 2.11. *The weakly* convergence in $\mathcal{M}(\Omega)$ corresponds to the weakly* convergence in $C_0^*(\Omega)$. Indeed, the following is equivalent*

(i) $\mu_n \overset{*}{\rightharpoonup} \mu$

(ii) $\Psi(\mu_n) \overset{*}{\rightharpoonup} \Psi(\mu)$

(iii) $\int_\Omega \phi d\mu_n \longrightarrow \int_\Omega \phi d\mu \ \ \forall \phi \in C_0(\Omega)$.

Especially the Banach-Alaoglu theorem and Corollary 2.6 applies to $\mathcal{M}(\Omega)$.

2.2 *BV* spaces

We will often cover a collection of atoms (configurations) with an arrangement of bounded sets. The characteristic functions of these sets are elements of the space of functions with bounded variation. This function space also provides useful compactness statements. In the following section we present the relevant parts of the theory of BV spaces, necessary for understanding the results and proofs. Beginning with the definition of BV spaces.

Definition 2.12. Let $u \in L^1(\Omega)$; we say u is a *function of bounded variation* in Ω if the distributional derivative of u is representable by a $\mathbb{R}^n$-valued finite Radon measure $Du = (D_1u, \ldots, D_nu)$ in Ω i.e. if for all $\phi \in C_c^\infty(\Omega)$ and $i \in \{1, \ldots, n\}$ is

$$\int_\Omega u \frac{\partial \phi}{\partial x_i} d\lambda^n(x) = -\int_\Omega \phi dD_i u.$$

The *vector space of all functions with bounded variation* is denoted by $BV(\Omega) \subset L^1(\Omega)$. Is u locally and not necessarily globally integrable, we define analog the space of functions with *locally bounded variation* $BV_{\mathrm{loc}}(\Omega)$ and we say u is a function of locally bounded variation if (2.12) applies for all open and relative compact subsets A of Ω ($A \subset\subset \Omega$), instead of Ω itself.

It can be shown that the existence of such a measure is equivalent to the fact that the variation of a functions is bounded.

Definition 2.13. Let $u \in L^1_{\mathrm{loc}}(\Omega)$. The *variation* $V(u, \Omega)$ of u in Ω is defined by

$$V(u, \Omega) = \sup \left\{ \int_\Omega u \nabla \phi d\lambda^n \,\middle|\, \phi \in C_c^1(\Omega, \mathbb{R}^n),\ \|\phi\|_\infty \leq 1 \right\}.$$

Proposition 2.14. *Let $u \in L^1(\Omega)$. Then belongs u to $BV(\Omega)$ if and only if $V(u, \Omega) < \infty$. In addition is then $|Du|(\Omega) = V(u, \Omega)$.*

The BV space can be easily equipped with a complete norm.

Proposition 2.15. *$BV(\Omega)$ equipped with the norm*

$$\|u\|_{BV(\Omega)} := \|u\|_{L^1(\Omega)} + |Du|(\Omega)$$

is a Banach space.

In most cases the requirements for a convergence in the norm-topology are too restrictive and so often a weaker concept of convergence is used.

Definition 2.16. Let $u \in BV(\Omega)$ and $(u_n)_{n\in\mathbb{N}}$ a sequence of functions in $BV(\Omega)$. We say $(u_n)_{n\in\mathbb{N}}$ *converges weakly** in $BV(\Omega)$ to u if $(u_n)_{n\in\mathbb{N}}$ converges in L^1 to u and $(Du_n)_{n\in\mathbb{N}}$ converges weakly* to Du, i.e. all components are weakly* converging in $\mathcal{M}(\Omega)$. Notation: $u_n \overset{*}{\rightharpoonup} u$

For this weaker convergence, we get an important compactness statement for $BV_{\mathrm{loc}}(\Omega)$, if Ω satisfies some additional properties.

Theorem 2.17. *Let Ω be an open, relative compact and bounded Lipschitz set and $(u_n)_{n\in\mathbb{N}}$ a sequence of functions in $BV_{loc}(\Omega)$ with*

$$\sup_{N\in\mathbb{N}} \left\{ \|u_n\|_{L^1(A)} + |Du_n|(A) \right\} < \infty,$$

for all open, relative compact sets A in Ω. If the sequence is bounded in $BV(\Omega)$, then there exists a subsequence $(u_{n_k})_{k\in\mathbb{N}}$ that converges weakly and in L^1_{loc} to a function $u \in BV(\Omega)$.*

One problem with this theorem is that the concepts of wk^*- and L^1_{loc}-convergence are sometimes too unwieldy. The next proposition allows then the use of the more convenient L^1-convergence.

Proposition 2.18. *Let $u \in BV(\Omega)$ and $(u_n)_{n\in\mathbb{N}}$ a sequence of functions in $BV(\Omega)$. Then $(u_n)_{n\in\mathbb{N}}$ converges weakly* to u in $BV(\Omega)$ if and only if $(u_n)_{n\in\mathbb{N}}$ is bounded in $BV(\Omega)$ and converges in the L^1-norm to u.*

2.3 Structure of sets of finite perimeter

An important class of BV-functions are the characteristic functions of certain sets. For these sets their variation can be linked with some topological properties in $\mathbb{R}^n$.

Definition 2.19. Let E be a λ^n-measurable subset of $\mathbb{R}^n$. The *perimeter* of E in Ω is defined as the variation of χ_E, i.e.

$$P(E,\Omega) := V(\chi_E,\Omega) = \sup\left\{ \int_E \nabla\phi d\lambda^n \,\middle|\, \phi \in C^1_c(\Omega,\mathbb{R}^n),\ \|\phi\|_\infty \leq 1 \right\}.$$

We say E is a set of *finite perimeter* in Ω if $P(E,\Omega) < \infty$.

Remarkable is the link between the perimeter of E given by (2.19) and the perimeter in a topological sense. For a λ^n-measurable set $E \subset \mathbb{R}^n$ with $\mathcal{H}^{n-1}$-a.e. C^1-boundary and $\mathcal{H}^{n-1}(\Omega \cap \partial E) < \infty$ the Gauss-Green equation

$$\int_E \nabla\phi d\lambda^n = -\int_{\Omega\cap\partial E} \langle \nu_E, \phi\rangle d\mathcal{H}^{n-1}\ \forall \phi \in C^1_c(\Omega,\mathbb{R}^n),$$

where ν_E is the inner unit normal to E, provides that $P(E,\Omega) = \mathcal{H}^{n-1}(\Omega \cap \partial E)$. The sets of finite perimeter have some further convenient properties.

Proposition 2.20. *Let E be a λ^n-measurable subset of $\mathbb{R}^n$. If E has finite mass in Ω, then is E a set of finite perimeter in Ω if and only if $\chi_E \in BV(\Omega) \subset L^1(\Omega)$ and further $P(E,\Omega)$ coincides with $|D\chi_E|(\Omega)$. If E has finite perimeter in Ω, it can be shown that χ_E belongs also to $BV_{loc}(\Omega)$. On the other hand, if $\chi_E \in BV_{loc}(\Omega)$, then E has finite perimeter in any open set $A \subset\subset \Omega$. We call E then a set with locally finite perimeter in Ω.*

For using the sets of finite perimeters E in a physical context we must address an important issue with the topological boundary, because this concept is in many ways not suitable for the physical discussion of surface energies. It is possible that subsets of ∂E exist which are not part of the physical boundary of a body. One example of this is shown in Figure 2.1. The set I is part of the topological boundary but atoms near this line do not interact with the surrounding phase of E and so do not contribute to the surface energy.

Another problem is that for many physical properties a normal vector to the surface, i.e. a vector orthogonal to the surface, is necessary for modeling them. However, the normal vector, how he is commonly constructed, is only defined for sets with a sufficiently smooth boundary. For solving these issues we introduce an improved definition of normal vectors and new boundary concepts, based more on measure theory than on topology. Indeed, we will see that these new concepts are closely related to the concepts generally used in topology and abstract geometry.

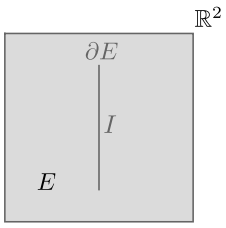

Figure 2.1: Example for a set E where the definition of ∂E as boundary is physically not suitable. The line in the square does not contribute to the surface energy. The definition of $\partial^* E$ asserts that the line will not take into account.

Definition 2.21. Let $E \subset \mathbb{R}^n$ be λ^n-measurable.

- (*Reduced boundary*) Let Ω be the largest open set such that E has locally finite perimeter in Ω. Define the reduced boundary as

$$\mathcal{F}E := \left\{ x \in \operatorname{supp}|D\chi_E| \cap \Omega \;\middle|\; v_E(x) := \lim_{r \searrow 0} \frac{D\chi_E(B_r(x))}{|D\chi_E|(B_r(x))} \text{ exist and } \|v_E(x)\| = 1 \right\}.$$

  The Borel map $v_E : \mathcal{F}E \to \mathbb{S}^{n-1}$ is called *generalized inner normal to* E. Consequently, we define the *generalized outer normal to* E as $\nu_E \equiv -v_E$.

- (*Points of density*) For every $t \in [0,1]$ let

$$E^t := \left\{ x \in \mathbb{R}^n \;\middle|\; \lim_{r \searrow 0} \frac{\lambda^n(E \cap B_r(x))}{\lambda^n(B_r(x))} = t \right\}$$

  be the set of points where E has density t.

- (*Essential boundary*) The set $\partial^* E := \mathbb{R}^n \setminus (E^0 \cup E^1) \subset \partial E$ of points with density neither 0 nor 1 is called essential boundary.

Theorem 2.22 (Federer)**.** *Let E be an arbitrary subset of $\mathbb{R}^n$, λ^n-measurable and with finite perimeter in Ω. Then holds*

1. *The set E has either density 0 or $1/2$ or 1 at $\mathcal{H}^{n-1}$-a.e. $x \in \Omega$.*
2. *The sets $\mathcal{F}E \cap \Omega$, $E^{1/2} \cap \Omega$ and $\partial^* E \cap \Omega$ coincide $\mathcal{H}^{n-1}$-a.e. and $P(E, \Omega) = \mathcal{H}^{n-1}(\partial^* E \cap \Omega)$.*

Remark 2.23. *For sets with C^1-boundary the vector ν_E coincides with the usual definition of the outer normal vector and the essential boundary $\partial^* E$ with the topological boundary ∂E.*

Sets of finite perimeter have many useful properties, one of them is the following approximation.

Theorem 2.24. [B$^+$98, Proposition 4.7] *Let Ω be a Lipschitz set. For a set $E \subset \mathbb{R}^n$ with finite perimeter in Ω there exists a sequence $(E_k)_{k \in \mathbb{N}}$ of sets with finite perimeter in Ω, such that*

$$\lambda^n(E_k \triangle E) \to 0 \text{ and } |D\chi_{E_k}|(\Omega) \to |D\chi_E|(\Omega).$$

as $k \to \infty$. For every open set Ω' with $\Omega \subset\subset \Omega'$ there exists sets E'_k of the class C^∞ in Ω' such that $E'_k \cap \Omega = E_k$.

With this theorem we can derive a continuity statement for certain integral operators.

Remark 2.25. [B$^+$98, Remark 4.8] *Let Ω, $(E_k)_{k\in\mathbb{N}}$ and E be as in the previous theorem, then for every $\varphi : \mathbb{S}^{n-1} \to \mathbb{R}$ positive, convex and positively 1-homogeneous we have*

$$\lim_{k\to\infty} \int_{\Omega\cap\partial^* E_j} \varphi(v_{E_j}(x)) d\mathcal{H}^{n-1}(x) = \int_{\Omega\cap\partial^* E} \varphi(v_E(x)) d\mathcal{H}^{n-1}(x).$$

2.4 Γ-convergence and convergence to minimizers

The question we are dealing with, if we want to describe the equilibrium shape of a crystal, is basically a minimization problem, as we will discuss later. We have to find configurations minimizing a functional that models the surface energy of a crystal. This is in general rather complicated, even for simplified models. The approach we are using in this thesis is to look at the sequence of such functionals for an increasing number of particles in the crystal and try to prove some convergences to a functional where the solution is known. The key point is that under this approximation the solutions of the original problems can be estimated by the solution of the new problem.

The assertion that this works is supplied by the theory of Γ-convergence. Indeed, one of the most important results of this theory is that for a family of real-valued functionals $(F_n)_{n\in\mathbb{N}}, F$, some sequentially continuous statements can be obtained for the inf- and argmin-operators. If $(F_n)_{n\in\mathbb{N}}$ is Γ-converging to F then, under a few compactness assumptions, it holds

$$\inf F_n \to \min F \text{ and } u_n \in \operatorname{argmin} F_n \Rightarrow u_n \to u \in \operatorname{argmin} F.$$

Definition 2.26. Let X be a first countable topological space and $(F_n)_{n\in\mathbb{N}}$ a sequence of extended real-valued functions $F_n : X \to \mathbb{R}\cup\{+\infty\}$ for all $n \in \mathbb{N}$ and $F : X \to \mathbb{R}\cup\{+\infty\}$. The sequence $(F_n)_{n\in\mathbb{N}}$ (sequentially) Γ-*converges* to F at $u \in X$ if and only if

(i) (Lower bound) for all sequences $(u_n)_{n\in\mathbb{N}}$ converging to u (in the topology of X), we have that

$$F(u) \le \liminf_{n\to+\infty} F_n(u_n)$$

(ii) (Upper bound) and there exists a sequence $(v_n)_{n\in\mathbb{N}}$ converging to u such that

$$F(u) \ge \limsup_{n\to+\infty} F_n(v_n).$$

If (i) and (ii) hold for all $u \in X$, we say $(F_n)_{n\in\mathbb{N}}$ Γ-converges to F and notate $F = \Gamma - \lim_{n\to+\infty} F_n$.

Condition (ii) is equivalent to

(ii)' there exists a sequence $(v_n)_{n\in\mathbb{N}}$ converging to u such that

$$F(u) = \lim_{n\to+\infty} F_n(v_n).$$

If $(F_n)_{n\in\mathbb{N}}$ Γ-convergences to F the following continuity statement holds.

Theorem 2.27. *Let X be a first countable topological space and $F_n, F : X \to \mathbb{R}\cup\{+\infty\}$ for all $n \in \mathbb{N}$ such that $(F_n)_{n\in\mathbb{N}}$ Γ-converges to F. Let further be $(u_n)_{n\in\mathbb{N}}$ a sequence in X such that $F_n(u_n) \le \inf\{F_n(u) \mid u \in X\} + \epsilon_n$ with $\epsilon_n > 0$ for all $n \in \mathbb{N}$ and $\epsilon_n \to 0$ for $n \to +\infty$. If $A = \{u_n \mid n \in \mathbb{N}\}$ is relatively compact then every cluster point $\bar{u}$ of A is a minimizer of F and*

$$\lim_{n\to+\infty} \inf\{F_n(u) \mid u \in X\} = F(\bar{u}).$$

For using Γ-convergence for a certain problem, we have to prove the lower bound as well as the upper bound. None of these two statements are in general easy to prove. But especially on the issue of the lower bound an extensive theory has been developed in the past decades. One result of this theory is the following lower semicontinuity statement for functionals on $BV(\Omega)$, which we will use in the proof of Theorem 3.6.

Theorem 2.28. [AFP00, Theorem 5.14] *Let $\phi : \mathbb{R}^n \to [0, \infty)$ be an continuous, even, positively 1-homogeneous and convex function with compact image. Let further be $\rho \in \mathbb{R}_{>0}$ and $(E_k)_{k\in\mathbb{N}}$ a family of subsets from Ω L^1-converging to a $E \subset \Omega$. If all E_k and E has finite perimeter in Ω, then is the functional*

$$\mathcal{F} : \rho\chi_{E_k} \mapsto \int_{\partial^* E_k} \phi(\nu_{E_k}(x)) d\mathcal{H}^{n-1}(x),$$

lower semicontinuous in the following sense

$$\mathcal{F}(\rho\chi_E) \leq \liminf_{k\to+\infty} \mathcal{F}(\rho\chi_{E_k}).$$

3 Background and main results

In this chapter we give a short introduction into the physical background of the formation of macroscopic equilibrium shape of crystallized solids. Then we introduce the model of Yeung et al. and list the main results we want to prove in the following chapters.

3.1 Surface energies and Wulff shape

It is a common physical situation that multiple substances in different states of matter are in contact, this is for example the case when crystals grow. The crystallization starts usually from a nucleus in a suitable surrounding phase. Particles from the surrounding gather them self around the nucleus and thus successively forming a crystal. In general, are crystals materials with a regular microscopic structures. That means the building blocks of a crystal (atom, ions, molecules, etc.) are arranged in a periodic structure.

The macroscopic shape and other properties of crystals as well as the growth process itself are rather complicate to predict and so a variety of theories had been developed on these issues. One theoretical approach to work out the shape and morphology of crystals is based on a thermodynamical treatment of the growing process, put forward by Gibbs and Wulff [DBPD10, MS13]. This theory states that the shape of the crystallized phase is determined exclusively by the surface free energy and that the (ideal) equilibrium state of a crystal droplet in a surrounding medium is achieved when this energy term is minimal. The surface (free) energy for a crystallized phase occupying the space G in $\mathbb{R}^n$ can in general be calculated by the *surface energy functional*

$$S(G) = \int_{\partial^* G} \gamma(\nu_G(x)) d\mathcal{H}^{n-1}(x). \tag{3.1}$$

Here is $\gamma : \mathbb{S}^{n-1} \to \mathbb{R}$ the free energy per area at the interface plane perpendicular to ν_G. For many materials γ depends strongly on the orientation (anisotropy), so crystals often have rather shapes, because crystallization occurs mainly along certain directions [MS13, DKS92].

These considerations show that, from a mathematical point of view, the question of the equilibrium shape can be treated as a minimization problem. One has to minimize the functional (3.1) under the constrain that the volume of the crystallized phase (the set G) is fixed. Wulff was the first who recognized that the intersection of half spaces

$$W_\gamma := \left\{ x \in \mathbb{R}^n \,\middle|\, x \cdot \nu \leq \gamma(\nu),\ \forall \nu \in \mathbb{S}^{n-1} \right\}$$

is a solution for this minimization problem, if the crystal has the same volume as W_γ [Wul01]. The convex set W_γ is therefore known as Wulff set or *Wulff shape*. This postulate was later proved and formalized by others like Herring, Taylor and Fonseca [Her51, Tay75, FM91]. Indeed, it can even be shown that *all* solutions with the same volume are of this kind (under some restrictions to γ).

3.2 Triangular model and terminology

As we have seen can determining the equilibrium shape of crystals in a given surrounding be interpreted as solving a minimization problem. The real physical situation during the formation of crystals is in general far too complex for solving this problem directly. Therefore, we want to use another approach for getting information about the shapes of crystalline configurations. We use a simple model for calculating the interactions inside a configuration and interfacial energies and try to show that configurations with minimal energy for this model can be approximated with a set minimizing (3.1), for a suitable γ, i.e. by the Wulff shape of γ.

For this reason, we only study the problem in two dimensions and at zero temperature. The later one allows us to neglect the dynamic of the particles, so that we can assume the energy of the configuration is completely determined by the interatomic potentials and therefore by the microscopic arrangement of the building blocks. We will call these building blocks in the following for simplicity just atoms, although they can also be ions, molecules, etc..

For a mathematically precise treatment of the problem, we consider a system of N identical particles with positions $x_1, \dots, x_N$ in the two-dimensional Euclidean space $\mathbb{R}^2$. We call the set $\{x_1, \dots, x_N\}$ a *configuration of N atoms* $\mathcal{S}_N$, and let $\mathcal{C}_N$ be the set of all these N-particle configurations. The energy of the system is given by the Hamiltonian

$$\mathcal{E}(x_1, \dots, x_N, p_1, \dots, p_N) = \sum_{i=1}^{N} \frac{\|p_i\|^2}{2m} + \sum_{i \neq j} V(\|x_i - x_j\|).$$

Here is m the mass of a particle and p_i the momentum of the i-th particle. The two-body potential $V(\|x_i - x_j\|)$, supplies interaction energy between two particles x_i and x_j. Based on the zero temperature assumption all velocity components vanish, therefore the dynamic part of the Hamiltonian disappears, i.e.

$$\mathcal{E}(\mathcal{S}_N) = \mathcal{E}(x_1, \dots, x_N) = \sum_{i \neq j} V(\|x_i - x_j\|). \tag{3.2}$$

The potential V is chosen in such a way that it only depends on the distances between the according particles. For modeling the potential, we use a generalization of the Heitmann-Radin potential [HR80] (soft Heitmann-Radin potential). We assume that $V : [0, \infty) \to [-1, \infty)$ is satisfying the subsequent properties:

(H1) (minimum at $r = 1$) $V(1) = -1, V(r) > -1$ for all $r \neq 1$.

(H2) (behavior at short and long range) There exist constants $\alpha \in (0, 1]$ and $\beta \in [1, \infty)$ such that $V(r) = +\infty$ for $r < \alpha$ and $V(r) = 0$ for $r > \beta$, V is continuous on (α, β).

(H3) (narrow potential well) The constants α, β from (H2) satisfy the condition that the ball of radius β contains at most six points whose distances from the center and their mutual distances are $\geq \alpha$.

With these properties we can define the intuitive concept of neighborhood for an atom $x \in \mathcal{S}_N$. Formally we define the set of neighbors $\mathcal{N}(x)$ as follows:

Definition 3.1. Let $\mathcal{S}_N$ be a N-particle configuration and $\mathcal{E}$ an energy functional such that V satisfies (H1) – (H3), for some α and β. For an atom $x \in \mathcal{S}_N$ we say $y \in \mathcal{S}_N$ is a *neighbor of* x, if $\|x - y\| \in [\alpha, \beta]$. The set

$$\mathcal{N}(x) = \{y \in \mathcal{S}_N \,\big|\, \|y - x\| \in [\alpha, \beta]\}$$

is therefore the set of all neighbors of x.

The chosen properties allow us to make some simple geometric statements. So is condition (H3) always satisfied if the potential well is narrow enough and α and β are symmetric with respect to 1, i.e. $\alpha = 1-\epsilon$ and $\beta = 1+\epsilon$ for a sufficient small $\epsilon > 0$. Is ϵ small enough holds additionally condition (4.4), as we will discuss in the proof of Theorem 3.4 *(i)*.

Heitmann and Radin [HR80] have proved that for $\alpha = \beta = 1$ the energy of a N-particle configuration is minimal if the configuration (after translation and rotation) is a subset of the triangular lattice

$$\mathcal{L} := \{me_1 + ne_2 \mid m, n \in \mathbb{Z}\}\,,\ e_1 = (1,0)^T\,,\ e_2 = \frac{1}{2}\left(1, \sqrt{3}\right)^T\,.$$

We call such configurations $\mathcal{S}_N$ crystallized, i.e. $\mathcal{S}_N \subset \mathcal{L}$.

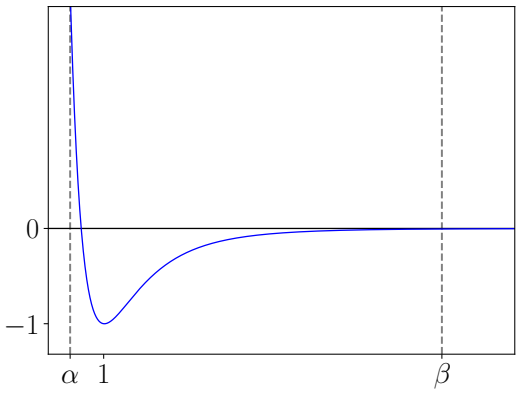

Figure 3.1: Schematic representation of a Heitmann-Radin like interatomic potential.

For crystallized configurations $\mathcal{S}_N$ we define the interfacial energy in the following sense. We assume that the surrounding phase has no specific influence on the interfacial energy. This for example would be the case if the configuration is surrounded by a vacuum. Instead, we calculate this energy with the following algorithm: It is obvious that for every point $z \in \mathcal{L}$ there exist six other points in $\mathcal{L}$ with distance one to z. If now for an atom $x \in \mathcal{S}_N \subset \mathcal{L}$ there are *not* six other atoms from $\mathcal{S}_N$ within the unit ball, then we set the number of "missing" atoms, i.e. difference between six and the actual number of such atoms, times (-1) as the interfacial energy of x. The interfacial energy of the whole configuration is then the sum of all interfacial energies of the atoms in $\mathcal{S}_N$. This shows that this energy can be calculated by $\mathcal{E}(\mathcal{S}_N) + 6\#\mathcal{S}_N$.

3.3 Main results

We now introduce a precise mathematical formulation of the main results. As noted above the key statements are that crystals with an (almost) hexagonal atomic structure have almost a hexagonal macroscopic shape and that an analog statement can be formulated for a potential that asserted an arrangement of the atoms in a square lattice. For proving both statements we need some mathematical groundwork done before we can go to the actual minimization problems.

We have to prove that, for the given potentials, crystallized configurations with N atoms and minimal energy exist for all $N \in \mathbb{N}$ and that some kind of convergence occurs if the number of atoms grows. For the square lattice model these facts can be assumed as settled, thanks to the work of Mainini et al. [MPS14]. Meanwhile, for the triangular model just the existence of crystallized configurations with minimal energy is known [HR80], but no convergence statement for configurations with low energy. Thus

Yeung et al. have also proved such convergence [YFS09]. We will present this proof, before we are going to the actual minimization problem. Therefore, it is necessary that the minimal possible energy for a N-particle configuration is bounded by a term of the order N. So, we begin our discussion with the proof of the later statement.

Theorem 3.2 (Energies for ground states)**.** *The infimum of the energy functional* (3.2)*, where V satisfies (H1) – (H3), for some constants α and β is bounded by*

$$-6N \leq \inf_{\mathcal{S}_N \in \mathcal{C}_N} \mathcal{E}(\mathcal{S}_N) \leq -6N + 4\sqrt{3}\sqrt{N} + 12. \tag{3.3}$$

Here it is important to notice that, if α and β are close enough to one, for all $N \in \mathbb{N}$ there exist configurations $\mathcal{S}_N$ such that the infimum is attained [HR80]. These configurations are called *ground states*. This first theorem proves in particular that the energies of N-particle ground states are bounded from above by a term of the order N. We will later also see (Lemma 4.1) that ground states are always connected in the following sense.

Definition 3.3. Let $\mathcal{E}$ be the energy functional (3.2) such that V satisfies (H1) – (H3) for some α, β. A configuration $\mathcal{S}_N \in \mathcal{C}_N$ is called *connected* if for any two atoms $x, y \in \mathcal{S}_N$ there exists a finite sequence of atoms $x_0, \ldots, x_k$ such that $x_0 = x, x_k = y$ and the distance between successive points is shorter than β. I.e. $\|x_{i+1} - x_i\| \leq \beta$ for all $i \in \{0, \ldots, k-1\}$.

The energy bound and the connectedness assert that the following compactness statement can be applied to sequences of ground states, a fact we will need in the actual approximation argument for the macroscopic shape of the crystals.

Theorem 3.4 (Compactness for low energy configurations)**.** *Suppose that the energy is given by the functional* (3.2) *such that the potential V satisfies the properties (H1) – (H3), for $\alpha = 1-\epsilon$ and $\beta = 1+\epsilon$, where $\epsilon > 0$ is small enough that* (4.4) *holds. (Such an ϵ always exists.) Let $(\mathcal{S}_N)_{N\in\mathbb{N}}$ be a sequence of connected N-particle configurations. We call*

$$\mu_N := \frac{1}{N} \sum_{x \in \mathcal{S}_N} \delta_{\frac{x}{\sqrt{N}}} \in \mathcal{M}(\mathbb{R}^2), \tag{3.4}$$

where δ is the Dirac measure, the re-scaled empirical measures associated to the configuration $\mathcal{S}_N$. If the energy of $\mathcal{S}_N$ satisfies for all $N \in \mathbb{N}$ and a constant C independent of N

$$\mathcal{E}(\mathcal{S}_N) \leq -6N + CN^{1/2}, \tag{3.5}$$

then it holds that

(i) The sequence $(\mu_N)_{N\in\mathbb{N}}$ associated to $(\mathcal{S}_N)_{N\in\mathbb{N}}$ convergences after translation in the sense of weak-convergence to a limit measure $\mu \in \mathcal{M}(\mathbb{R}^2)$, with mass one.*

(ii) This limit measure is of the form

$$\mu(\cdot) = \int_{\cdot} \rho \chi_E d\lambda^2 =: \eta_E(\cdot),$$

for a set of finite perimeter $E \subset \mathbb{R}^2$ with λ^2-volume $1/\rho$, with $\rho = 2/\sqrt{3}$.

Remark 3.5. *Remark that in* (3.4) *we scale the configuration by $\frac{1}{\sqrt{N}}$, this asserts, as we will see later, that the diameter of $\frac{1}{\sqrt{N}}\mathcal{S}_N$ is bounded, which is crucial for proving the theorem.*

While Theorem 3.4 shows that for configurations with sufficient low energy their shapes can be approximated by a set of finite perimeter, it does not provide any information on how this shape looks like. For determining this, we have to study explicit the convergence behavior of ground states.

Theorem 3.6. *Assume that the energy is given by the same functional as in Theorem 3.4 and that a crystallized ground state exists for all $N \in \mathbb{N}$ (as known for $\alpha \approx \beta \approx 1$). Let μ_N be the associated re-scaled empirical measure to a N-particle configuration $\mathcal{S}_N$, minimizing $\mathcal{E}$. Under these conditions the weak*-limit measure μ of $(\mu_N)_{N\in\mathbb{N}}$ is*

$$\mu(\cdot) = \int_{\cdot} \frac{2}{\sqrt{3}} \chi_{h_{\frac{1}{\sqrt{3}}}} d\lambda^2 = \eta_{h_{\frac{1}{\sqrt{3}}}}(\cdot).$$

Here $h_{\frac{1}{\sqrt{3}}}$ is a regular hexagon with edge length $\frac{1}{\sqrt{3}}$, centered at (0,0) and "bottom edge" parallel to e_1.

In general, we define a regular hexagon with edge length $R > 0$ as the closure of a convex hull,

$$h_R = \overline{\operatorname{conv}\{\pm Re_1, \pm Re_2, \pm R(e_2 - e_1)\}}.$$

The set $\overset{\circ}{h_R}$ is the interior of h_R in standard topology on $\mathbb{R}^2$. If this hexagon is rotated by 30° we write h'_R. Further we denote by $h_R(z)$ the according hexagon with the center $z \in \mathbb{R}^2$ and $h'_R(z)$ analogous. A result analog to Theorem 3.6 holds also if the interatomic energies are given by the potential (6.1). In this case a convergence to a squared shape occurs and not to a hexagonal one.

Theorem 3.7. *Let be $\tilde{\mathcal{E}}$ the energy functional (6.1) and $(\mathcal{S}_N)_{N\in\mathbb{N}}$ a sequence of ground states of this functional. Then the associated re-scaled empirical measures $(\mu_N)_{N\in\mathbb{N}}$ are (after translation) converging weakly* to*

$$\mu(\cdot) = \int_{\cdot} \chi_{q_1} d\lambda^2 =: \tilde{\eta}_{q_1}(\cdot),$$

where $q_1 := \left[-\frac{1}{2}, \frac{1}{2}\right] \times \left[-\frac{1}{2}, \frac{1}{2}\right]$ is the square with edge length one and $(0,0)$ as center point.

In general is $q_R(x)$ for $R > 0$ and $x \in \mathbb{R}^2$ the square with edge length R and center at x.

4 Compactness for low energy configurations

With the groundwork from the last chapters, we can now begin proving the actual results. In this chapter we present the proofs of the Theorems 3.2 and 3.4. The later one asserts that sequences of configurations with a low energy are weak*-converging if the number of atoms is increasing. Theorem 3.2 asserts that this convergence statement can by applied to sequences of ground states. We begin with the proof of this theorem because that is the simpler one.

4.1 Energy bound of low energy configurations

Proof of Theorem 3.2. The inequality on the left-hand side of (3.3) follows imminently from (H3) because each atom can have at most six neighbors with mutual distances and distance to the atom x greater or equal than α. From (H1) follows that the interaction energy between two atoms is minimal if and only if the distance between these atoms is one. We now assume that each of the N atoms has *exactly* six neighbors and the distance between two atoms is always one. The energy of such a configuration would be $-6N$. No configuration can have a lower energy and thus the lower bound for the infimum of the energy functional is $-6N$.

For the second inequality more work is necessary. We have to find one configuration $\tilde{\mathcal{S}}_N$ with N atoms that satisfies the inequality. Choose for $\tilde{\mathcal{S}}_N$ an (quasi)hexagonal configuration, that means $\tilde{\mathcal{S}}_N := \mathcal{L} \cap \Psi$, for a $\Psi \subset \mathbb{R}^2$ with $\mathring{h}_R \subset \Psi \subset h_R$ for an $R \in \mathbb{N}_0$ such that $\partial h_R \cap \tilde{\mathcal{S}}_N \neq \emptyset$ and $\#(\mathcal{L} \cap \Psi) = N$.

Now we consider two different cases to prove the statement. At first suppose $\Psi = h_R$. In this case the number of atoms in ∂h_R is equal to the length of ∂h_R, i.e. $N_s := \#(\tilde{\mathcal{S}}_N \cap \partial h_R) = 6R$. Notice that $\tilde{\mathcal{S}}_N$ can be written as a disjoint union of "hexagonal rings" $\partial h_s,\ s \in \{0, \dots R\}$, see Figure 4.1 and N is the sum of the atoms in these "hexagonal rings", i.e.

$$N = \sum_{r=1}^{R} 6r + 1 = 3R^2 + 3R + 1.$$

Substituting R with $N_s/6$ yields $N_s = \sqrt{12N - 3} - 3$. As mentioned above each atom can interact with maximal six other atoms, at least if the configuration has finite energy. Since the six "corner" atoms in ∂h_R are each "missing" three neighbors and the remaining $N_s - 6$ "surface" atoms are each "missing" two neighbors, the total energy is

$$\mathcal{E}(x_1, \dots x_N) = -6N + 6 \cdot 3 + (N_s - 6) \cdot 2 = -6N + 2\sqrt{12N - 3}.$$

Now we consider the more general case $\mathring{h_R} \subset \Psi \subset h_R$. This configuration has $N + k$ atoms with N atoms inside h_{R-1} and the remaining k atoms in ∂h_R. The number of atoms in this layer ranges from 1

to $6R-1$. We get the following expression for the energy

$$\mathcal{E}(x_1,\dots,x_N,x_N,\dots,x_{N+k}) = \mathcal{E}(x_1,\dots,x_N) + \sum_{l=1}^{k}(-2\cdot\#(\text{neighbors of } x_{N+l} \text{ in } h_{R-1})) + \sum_{l=1}^{k}(-1\cdot\#(\text{neighbors of } x_{N+l} \text{ in } \partial h_R)),$$

where $\mathcal{E}(x_1,\dots,x_N)$ is the energy from the first case. The factor 2 in the sum appears, because we have to count each interaction twice, from the atoms in ∂h_R to h_{R-1} and vice versa, but we only sum over the atoms in the layer ∂h_R. If $k=1$ the claim follows imminently. Is $k\geq 2$ we rearrange the atoms in the layer ∂h_R such that there are at most five "corner" atoms and two "end" atoms, these atoms have each three neighbors (see Figure 4.2). All other atoms in ∂h_R have four neighbors, two in ∂h_R and two in h_{R-1}. Counting the bonds in this way gives us

$$\begin{aligned}\mathcal{E}(x_1,\dots,x_N,x_N,\dots,x_{N+k}) &\leq \mathcal{E}(x_1,\dots,x_N) + 5(-2\cdot 1 - 1\cdot 2) + 2(-2\cdot 2 - 1\cdot 1) + (k-7)(-2\cdot 2 - 1\cdot 2)\\ &= \mathcal{E}(x_1,\dots,x_N) - 6k + 12.\end{aligned}$$

With the calculation of the energy (4.1) in previous case, we get

$$\mathcal{E}(x_1,\dots,x_N,x_N,\dots,x_{N+k}) \leq -6(N+k) + 2\sqrt{12N-3} + 12 \leq -6(N+k) + 2\sqrt{12(N+k)} + 12.$$

This proves the claim. □

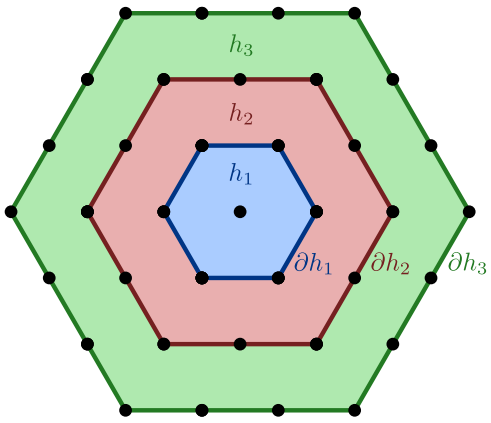

Figure 4.1: Example for a hexagonal configuration with $N=37$. In the darker colors the "hexagonal rings" $\partial h_1, \partial h_2$ and ∂h_3 are shown and in the according brighter color the corresponding hexagons h_1, h_2 and h_3.

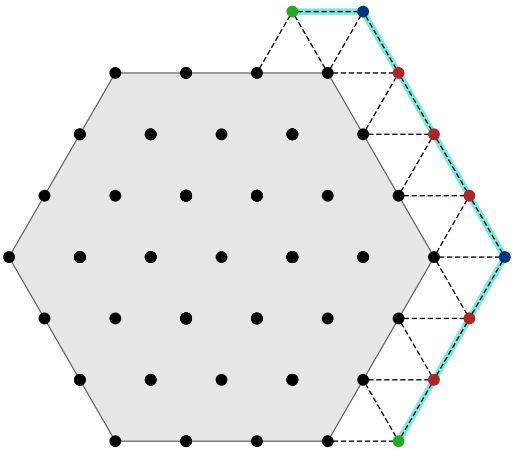

Figure 4.2: Example for a quasihexagonal configuration with $N=46$ and $k=9$ atoms in ∂h_R. The relevant subset of is ∂h_R shown in cyan. The "corner" atoms are shown in dark blue and the "end" atoms in green. The remaining atoms in ∂h_R are red.

One remarking feature of these hexagonal configurations is that they do not just minimize the energy but also are connected. Indeed, it can be shown that each configuration, that minimizes $\mathcal{E}$, is connected.

Lemma 4.1. *Let N be a natural number and $\mathcal{S}_N$ a N-particle ground state of the energy functional $\mathcal{E}$, where the interatomic potential satisfies (H1) - (H3), for some α and β. Then $\mathcal{S}_N$ is connected.*

Proof. Suppose that $\mathcal{S}_N$ consists of two subconfigurations $\mathcal{S}_M$ and $\mathcal{S}_{N-M}$ which are not connected, i.e. for all $x \in \mathcal{S}_M$ and $y \in \mathcal{S}_{N-M}$ their distance is greater than β. The energy of the whole configuration is $\mathcal{E}(\mathcal{S}_M) + \mathcal{E}(\mathcal{S}_{N-M})$. Now move the two subconfigurations so that the distance between the right most point of the left subconfiguration and the left most point right subconfiguration is one. The energy of the new configuration is equal to the energy of $\mathcal{S}_M$ and $\mathcal{S}_{N-M}$ plus the contribution of these two particles, which is negative. That is a contradiction, because the energy of the new configuration is lower than $\mathcal{E}(\mathcal{S}_N)$ and thus $\mathcal{S}_N$ cannot be a ground state of $\mathcal{E}$. □

4.2 Formation of clusters under mass conservation

For the following discussion it is useful to consider not the configuration $\mathcal{S}_N$ itself, but instead a cover of $\mathcal{S}_N$ with bounded sets, such that each set contains exact one atom.

Definition 4.2. Let $\mathcal{S}_N \in \mathcal{C}_N$ be a configuration. For each $x \in \mathcal{S}_N$ the *Voronoi cell* $\mathcal{V}(x)$ of x is

$$\mathcal{V}(x) := \left\{ y \in \mathbb{R}^2 \;\middle|\; \|y - x\| \leq \|y - x'\|,\ \forall x' \in \mathcal{S}_N \setminus \{x\} \right\}.$$

Since $\mathcal{V}(x)$ can be unbounded, we introduce the truncation

$$\mathcal{V}_{\text{trunc}}(x) := \mathcal{V}(x) \cap B_1(x).$$

It is obvious that $(\mathcal{V}_{\text{trunc}}(x))_{x \in \mathcal{S}_N}$ covers $\mathcal{S}_N$. We call $(\mathcal{V}_{\text{trunc}}(x))_{x \in \mathcal{S}_N}$ the truncated Voronoi cover and notate it by

$$\Lambda := \bigcup_{x \in \mathcal{S}_N} \mathcal{V}_{\text{trunc}}(x).$$

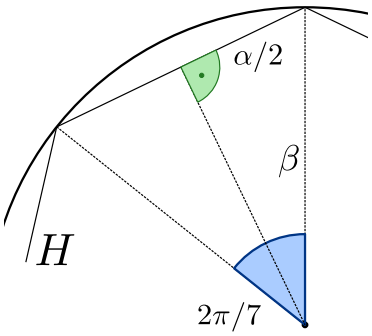

Figure 4.3: The geometric construction for an edge of a regular heptagon H, if it would fit inside a ball of radius β.

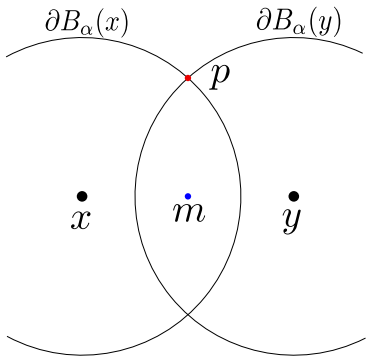

Figure 4.4: Scheme of the geometric situation in the proof of Lemma 4.3.

The following two lemmata refer to important geometric properties of the configurations we are dealing with in Theorem 3.4. They then easily imply the wk*-compactness. The first lemma proves that Λ is connected configurations with finite energy.

Lemma 4.3. *Let $\mathcal{E}$ be the energy functional* (3.2)*, where V satisfies (H1) – (H3), for some constants α and β. Let further $\mathcal{S}_N \in \mathcal{C}_N$ be a connected configuration with $\mathcal{E}(\mathcal{S}_N) < \infty$. Then Λ is connected.*

Proof. Before we are going to the actual proof, we need to establish an elementary geometric statement. Suppose that

$$\sin \frac{\phi}{2} \geq \frac{\alpha/2}{\beta},$$

applies for $\phi = 2\pi/7$. In this case a regular heptagon H would fit inside a ball with radius β such that the edge length and the distances of the corner points to center of the ball are at least α, see Figure 4.3. But this would be a contradiction to the fact (H3), hence

$$\beta < \frac{\alpha}{\sin \phi/2} \approx 1.152382\alpha < \sqrt{2}\alpha.$$

For proving that Λ is connected it is sufficient to verify that for all $(x, y) \in \mathcal{S}_N \times \mathcal{S}_N$ the intersection of $\mathcal{V}_{\text{trunc}}(x)$ and $\mathcal{V}_{\text{trunc}}(y)$ is not empty, if $\|x - y\| \leq \beta$. The fact that $\mathcal{S}_N$ is connected then assures that Λ is also connected. We will show that the midpoint $m = x + \frac{y-x}{2} = \frac{x+y}{2}$ between x and y belongs to $B_1(x) \cap B_1(y)$ and $\mathcal{V}(x) \cap \mathcal{V}(y)$. It is clear that

$$\|m - x\| = \|m - y\| = \frac{1}{2}\|x - y\| \leq \frac{\beta}{2} < \underbrace{\frac{\sqrt{2}}{2}}_{\approx 0.707} \alpha < \alpha.$$

According to (H2) is α less or equal than one and this proves $m \in B_1(x) \cap B_1(y)$. For proving $m \in \mathcal{V}(x) \cap \mathcal{V}(y)$, we use

$$\|x - y\| \leq \beta < \sqrt{2}\alpha \Rightarrow \alpha > \frac{\|x - y\|}{\sqrt{2}},$$

which shows

$$\sqrt{\alpha^2 - \left(\frac{\|x - y\|}{2}\right)^2} > \frac{\|x - y\|}{2}.$$

It is clear that $m \in \mathcal{V}(x) \cap \mathcal{V}(y)$ is equivalent to

$$\|m - x\| \leq \|m - x'\| \; \forall x' \in \mathcal{S}_N \setminus \{x\} \; \wedge \; \|m - y\| \leq \|m - y'\| \; \forall y' \in \mathcal{S}_N \setminus \{y\},$$

which again is equivalent to

$$\frac{1}{2}\|x - y\| \leq \|m - z\| \; \forall z \in \mathcal{S}_N \setminus \{x, y\}. \tag{4.1}$$

A simple geometric construction then establishes that the point p in $\mathbb{R}^2 \setminus B_\alpha(x) \cup B_\alpha(y)$ that is closest to m is element of $\partial B_\alpha(x) \cap \partial B_\alpha(y)$, see Figure 4.4. By the Pythagorean theorem and with (4.2) follows

$$\|p - m\| = \sqrt{\alpha^2 - \left(\frac{\|x - y\|}{2}\right)^2} > \frac{\|x - y\|}{2}.$$

Since $\mathcal{S}_N$ has finite energy are x and y the only atoms in $B_\alpha(x) \cup B_\alpha(y)$. Thus we get $\|z - m\| > \frac{\|x-y\|}{2}$ for all $z \in \mathcal{S}_N \setminus \{x, y\}$. This shows the statement (4.1) and proves that $m \in \mathcal{V}(x) \cap \mathcal{V}(y)$. □

The next lemma states that the diameter of the configurations in that satisfies the conditions in Theorem 3.4 are controlled by a term of order $N^{1/2}$

Lemma 4.4. *Let $\mathcal{E}$ be the same energy functional as in Theorem 3.4. For any connected N-particle configuration $\mathcal{S}_N \in \mathcal{C}_N$ with an energy bounded by*

$$\mathcal{E}(\mathcal{S}_N) \leq -6N + CN^{1/2},$$

the diameter, i.e. the maximum distance between two atoms in the configuration, is of the order $N^{1/2}$. Indeed, there exists a constant D, independent of N such that for all N

$$\text{diam } \mathcal{S}_N := \max_{x,y \in \mathcal{S}_N} \|x - y\| \leq DN^{1/2}.$$

Proof. In the first step we divide the energy functional into a bulk and a boundary part. We say an atom x is in the bulk of $\mathcal{S}_N$, if x has six neighbors ($\#\mathcal{N}(x) = 6$) and in the boundary part if *less* than six. The energy can therefore be written as

$$\mathcal{E}(\mathcal{S}_N) = \sum_{x\in\mathcal{S}_N} \underbrace{\sum_{y\in\mathcal{S}_N\setminus\{x\}} V(\|x-y\|)}_{\mathcal{E}_{\mathrm{loc}}(x)} = \sum_{\substack{x\in\mathcal{S}_N \\ \#\mathcal{N}(x)=6}} \mathcal{E}_{\mathrm{loc}}(x) + \sum_{\substack{x\in\mathcal{S}_N \\ \#\mathcal{N}(x)<6}} \mathcal{E}_{\mathrm{loc}}(x).$$

Remark, that according to (H3) and the finiteness of the energy, every atom x in the configuration has at most six neighbors and so $\mathcal{E}_{\mathrm{loc}}(x) \geq -6$. If an atom is in the bulk part, we can give an even stronger lower bound. Suppose without loss of generality that $N > 6$. If now $\#\mathcal{N}(x) < 6$ so is at least one of the six nearest atoms to x not in $B_{1+\epsilon}(x)$. In this case the energy contribution of this particle to $\mathcal{E}_{\mathrm{loc}}(x)$ is zero. It follows immediately

$$\mathcal{E}_{\mathrm{loc}}(x) \geq -6 + \underbrace{\Delta}_{>0}.$$

Thus

$$-6N + CN^{1/2} \geq \mathcal{E}(\mathcal{S}_N) \geq \sum_{\substack{x\in\mathcal{S}_N \\ \#\mathcal{N}(x)=6}} -6 + \sum_{\substack{x\in\mathcal{S}_N \\ \#\mathcal{N}(x)<6}} (-6+\Delta) \geq -6N + \#\partial\mathcal{S}_N\Delta$$

and consequently

$$\#\partial\mathcal{S}_N \leq \frac{C}{\Delta} N^{1/2}, \tag{4.2}$$

with $\partial\mathcal{S}_N := \{x \in \mathcal{S}_N \,|\, \#\mathcal{N}(x) < 6\}$.

By construction is $\mathcal{V}_{\mathrm{trunc}}(x) \subset B_1(x)$ and both sets are convex for all $x \in \mathcal{S}_N$. From a fundamental property[1] for convex bodies derives that

$$\mathcal{H}^1(\partial\mathcal{V}_{\mathrm{trunc}}(x)) \leq \mathcal{H}^1(\partial B_1(x)) = 2\pi. \tag{4.3}$$

For sufficiently small $\epsilon > 0$ follows from geometric consideration

$$\#\mathcal{N}(x) = 6 \Longrightarrow \partial\Lambda \cap \partial\mathcal{V}_{\mathrm{trunc}}(x) = \emptyset. \tag{4.4}$$

Notice that $\partial\mathcal{V}_{\mathrm{trunc}}(x)$ and $\partial\Lambda$ depends *continuously* on the positions of all atoms in $\mathcal{S}_N$, since for all $y \in \mathcal{S}_N$ can $\partial\mathcal{V}_{\mathrm{trunc}}(x) \cap \partial\mathcal{V}_{\mathrm{trunc}}(y)$ be represented by a support vector s and a direction vector orthogonal to s. Both vectors depend *continuously* on x and y. For $\partial\Lambda$ analog. If all of the six atoms in $\mathcal{N}(x)$ have distance one to each other it is easy to see that the minimal distance $\tilde{d}_{\min}(y)$ between $\partial\Lambda$ and $\partial\mathcal{V}_{\mathrm{trunc}}(x) \cap \partial\mathcal{V}_{\mathrm{trunc}}(y)$ is for all $y \in \mathcal{N}(x)$ greater than zero. This proves that for any small enough positional variation of the atoms in $\mathcal{N}(x) = B_{1+\epsilon}(x) \setminus B_{1-\epsilon}(x)$ the distance $\tilde{d}_{\min}(y)$ is greater than zero for all $y \in \mathcal{N}(x)$. Therefore, it exists an $\epsilon > 0$ such that (4.4) holds.

By negation of (4.4), (4.3) and the fact that $\partial\Lambda \subset \bigcup_{x\in\mathcal{S}_N} \partial\mathcal{V}_{\mathrm{trunc}}(x)$ we get

$$\mathcal{H}^1(\partial\Lambda) \leq \sum_{x\in\mathcal{S}_N \,|\, \partial\Lambda\cap\partial\mathcal{V}_{\mathrm{trunc}}(x)\neq\emptyset} \mathcal{H}^1(\partial\mathcal{V}_{\mathrm{trunc}}(x)) \leq 2\pi\#\partial\mathcal{S}_N. \tag{4.5}$$

According to Lemma 4.3 is Λ connected, giving

$$\operatorname{diam}\mathcal{S}_N \leq \operatorname{diam}\Lambda \leq \frac{1}{2}\mathcal{H}^1(\partial\Lambda). \tag{4.6}$$

[1] [Ste16, p. 1, Eq. 1.1]

Since for any two points in $\partial\Lambda$ the way along the direct line between these two points is shorter than the way along the edge. Combining (4.5) and (4.6) shows

$$\operatorname{diam} \mathcal{S}_N \leq \operatorname{diam} \Lambda \leq \frac{1}{2}\mathcal{H}^1(\partial\Lambda) \leq \pi \# \partial\mathcal{S}_N.$$

Together with (4.2) this proves

$$\operatorname{diam} \mathcal{S}_N \leq \operatorname{diam} \Lambda \leq \frac{1}{2}\mathcal{H}^1(\partial\Lambda) \leq \frac{\pi C}{\Delta} N^{1/2}. \tag{4.7}$$

□

With this lemma we can now prove Theorem 3.4 *(i)* relatively easy.

Proof of Theorem 3.4 (i). For all $N \in \mathbb{N}$ are the measures μ_N non negative and have mass one and thus the sequence $(\mu_N)_{N\in\mathbb{N}}$ is bounded in the norm $|\cdot|(\mathbb{R}^2)$. Since $\mathcal{M}(\mathbb{R}^2)$ and $C_0^*(\mathbb{R}^2)$ are isometric isomorph by Theorem 2.9, there exists a bijection between $(\mu_N)_{N\in\mathbb{N}}$ and a sequence $(\Phi_N)_{N\in\mathbb{N}}$, bounded in $C_0^*(\mathbb{R}^2)$. Corollary 2.6 implies that there exists a wk*-convergent subsequence of $(\Phi_N)_{N\in\mathbb{N}}$. By Definition 2.10 is $(\mu_N)_{N\in\mathbb{N}}$ wk*-convergent in $\mathcal{M}(\mathbb{R}^2)$ to a nonnegative measure μ (at least for a subsequence). It remains to prove that μ has mass one. According to Lemma 4.4 is

$$\operatorname{diam} \frac{1}{\sqrt{N}}\mathcal{S}_N \leq \frac{\pi C}{\Delta},$$

for all $N \in \mathbb{N}$. This asserts that there exists a ball with fixed radius $R \in \mathbb{R}_{>0}$ such that for all N the configurations $\mathcal{S}_N$ (up to translations) are contained in $B_R(0)$. Therefore, $\operatorname{supp}(\mu_N)$ is a subset of B_R for all N. Choose an increasing sequence of function $\phi_n \in C_0(\mathbb{R}^2)$ for all $n \in \mathbb{N}$ with $0 \leq \phi_n \leq 1$ and $\phi_n\big|_{B_{nR}} \equiv 1$. This shows

$$\int_{\mathbb{R}^2} \phi_n d\mu_N = \int_{B_R} \phi_n d\mu_N = 1,$$

for all $n, N \in \mathbb{N}$. The monotone convergence theorem applied to $(\phi_n)_{n\in\mathbb{N}}$ finally yields that

$$\int_{\mathbb{R}^2} d\mu = \lim_{n\to\infty} \int_{\mathbb{R}^2} \phi_n d\mu = \lim_{n\to\infty} \left(\lim_{N\to\infty} \int_{\mathbb{R}^2} \phi_n d\mu_N \right) = \lim_{n\to\infty} 1 = 1$$

This establishes that μ has mass 1 and proves Theorem 3.4 *(i)*.

□

4.3 Formation of clusters with constant density and finite perimeter

The first part of Theorem 3.4 proves the existence of a limit measure μ and asserts the conservation of mass in the limit process. For finishing the proof, it remains to show that μ is of the postulated shape, i.e. the density function (in a Radon-Nikodym sense) of μ is proportional to an indicator function χ_E of a set E.

For this purpose we construct a new sequence of measures $(\tilde{\tilde{\mu}}_N)_{N\in\mathbb{N}}$ with densities $(\tilde{\tilde{d}}_N)_{N\in\mathbb{N}}$ in $BV(\mathbb{R}^2)$. The properties of these configurations allow us the usage of the compactness statements introduced in Section 2.2. This will show that the limit of $(\tilde{\tilde{\mu}}_N)_{N\in\mathbb{N}}$ has the required property and bounding arguments show then that μ_N and $\tilde{\tilde{\mu}}_N$ coincide for N to infinity. This will prove Theorem 3.4 *(ii)* and thus Theorem 3.4 completely.

Proof of Theorem 3.4 (ii).

Step 1 Let $\mathcal{S}_N$ be an arbitrary N-particle configuration. Instead of the empirical measures we use a sequence of auxiliary measures $(\tilde{\tilde{\mu}}_N)_{N\in\mathbb{N}}$ with the densities

$$\tilde{\tilde{d}}_N = \frac{1}{N}\sum_{x\in\mathcal{S}_N}\frac{\chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)}}{\left|N^{-1/2}h'_{1/\sqrt{3}}(x)\right|} = \underbrace{\frac{1}{\left|h'_{1/\sqrt{3}}\right|}}_{\rho}\chi_{N^{-1/2}\Lambda_N} \text{ such that } \tilde{\tilde{\mu}}_N(\cdot) := \int_\cdot \tilde{\tilde{d}}_N d\lambda^2,$$

where $\Lambda_N = \bigcup_{x\in\mathcal{S}_N}\mathcal{V}_{\mathrm{trunc}}(x)$. The densities $(\tilde{\tilde{d}}_N)_{N\in\mathbb{N}}$ have some convenient properties:

1. For all open and relatively compact sets $A\subset\mathbb{R}^2$ is

$$\sup_{N\in\mathbb{N}}\left\|\tilde{\tilde{d}}_N\chi_A\right\|_{L^1(\mathbb{R}^2)} \le \sup_{N\in\mathbb{N}}\left\|\tilde{\tilde{d}}_N\right\|_{L^1(\mathbb{R}^2)} \text{ and } \sup_{N\in\mathbb{N}}P(N^{-1/2}\Lambda_N, A) \le \sup_{N\in\mathbb{N}}P(N^{-1/2}\Lambda_N,\mathbb{R}^2).$$

2. Equation (4.7) shows that the diameter of $N^{-1/2}\Lambda_N$ is bounded for by a constant for all $N\in\mathbb{N}$. The support of $\tilde{\tilde{d}}_N$ is for all N a subset in a ball of fix radius R. This shows that the sequence $(\tilde{\tilde{d}}_N)_{N\in\mathbb{N}}$ is L^1-bounded.

3. Also is according to (4.7) is $\mathcal{H}^1(\partial(N^{-1/2}\Lambda_N))$ bounded by a constant for all $N\in\mathbb{N}$. Thus $N^{-1/2}\Lambda_N$ is a set of bounded perimeter in $\mathbb{R}^2$ and $\tilde{\tilde{d}}_N$ an element of $BV(\mathbb{R}^2)$ and $BV_{\mathrm{loc}}(\mathbb{R}^2)$. Indeed is

$$\mathcal{H}^1(\partial(N^{-1/2}\Lambda_N)\cap\mathbb{R}^2) = N^{-1/2}\mathcal{H}^1(\partial\Lambda_N) \overset{(4.7)}{\le} N^{-1/2}\frac{2\pi C}{\Delta}N^{1/2} < \infty.$$

By Proposition 2.20 $|D\chi_{N^{-1/2}\Lambda_N}|(\mathbb{R}^2)$ and $\mathcal{H}^1(\partial(N^{-1/2}\Lambda_N)\cap\mathbb{R}^2)$ coincide, giving that $(\tilde{\tilde{d}}_N)_{N\in\mathbb{N}}$ is bounded in the BV-norm as

$$\sup_{N\in\mathbb{N}}\left\|\tilde{\tilde{d}}_N\right\|_{BV(\mathbb{R}^2)} \le \sup_{N\in\mathbb{N}}\left\|\tilde{\tilde{d}}_N\right\|_{L^1(\mathbb{R}^2)} + \sup_{N\in\mathbb{N}}P(N^{-1/2}\Lambda_N,\mathbb{R}^2) \le \rho\pi R^2 + \frac{2\pi C}{\Delta} < \infty$$

shows. Because $\tilde{\tilde{d}}_N$ is for all N supported inside a open ball $B_R(a)$, $(\tilde{\tilde{d}}_N)_{N\in\mathbb{N}}$ satisfies the conditions in Theorem 2.17. Therefore, there exists a subsequence converging weakly* to a $\tilde{\tilde{d}}\in BV(\mathbb{R}^2)$. Proposition 2.18 implies immediately that this subsequence also converges to $\tilde{\tilde{d}}$ in the L^1-norm. Furthermore, a fact from functional analysis[2] shows that a subsequence of $(\tilde{\tilde{d}}_N)_{N\in\mathbb{N}}$ exist, converging λ^2-a.e. pointwise to $\tilde{\tilde{d}}$. Since $\tilde{\tilde{d}}_N$ takes only the values 0 and ρ, also $\tilde{\tilde{d}}$ does. Therefore, there is a set $E\subset\mathbb{R}^2$ such that

$$\tilde{\tilde{\mu}}_N \overset{*}{\rightharpoonup} \tilde{\tilde{\mu}}(\cdot) := \int_\cdot \tilde{\tilde{d}}(x)d\lambda^2(x) = \int_\cdot \rho\chi_E d\lambda^2 = \eta_E(\cdot).$$

Proposition 2.20 proves that E is a set of finite perimeter in $\mathbb{R}^2$.

Step 2 In the next steps we approximate μ_N by the measures $\tilde{\tilde{\mu}}_N$. We will prove that $\tilde{\tilde{\mu}}_N$ and μ_N coincide for $N\to\infty$. Again, we need auxiliary sequences

$$\tilde{d}_N = \frac{1}{N}\sum_{x\in\mathcal{S}_N}\frac{\chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)}}{\left|N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)\right|}, \quad \tilde{\mu}_N(\cdot) = \int_\cdot \tilde{d}_N d\lambda^2.$$

We claim that (i) $\tilde{\mu}_N - \mu_N \overset{*}{\rightharpoonup} 0$ and (ii) $\tilde{\tilde{d}}_N - \tilde{d}_N \xrightarrow{L^1} 0$, this would prove that μ_N and $\tilde{\tilde{\mu}}_N$ coincide for

[2] [Els18, p. 252; cor. 2.7 b)]

$N \to \infty$, since is for all $\phi \in C_0(\mathbb{R}^2)$

$$\left| \int_{\mathbb{R}^2} \phi d\tilde{\tilde{\mu}} - \int_{\mathbb{R}^2} \phi d\tilde{\mu}_N \right| = \left| \int_{\mathbb{R}^2} \phi \left(\tilde{\tilde{d}}_N - \tilde{d}_N \right) d\lambda^2 \right| \leq \sup_{z \in \mathbb{R}^2} |\phi(z)| \left\| \tilde{\tilde{d}}_N - \tilde{d}_N \right\|_{L^1(\mathbb{R}^2)} \longrightarrow 0 \ \ (N \to \infty).$$

This shows $\tilde{\tilde{\mu}}_N - \tilde{\mu}_N \overset{*}{\rightharpoonup} 0$ and thus the weak* convergence of $(\mu_N)_{N \in \mathbb{N}}$ to $\tilde{\tilde{\mu}}$.
(i): For all $x_0 \in \mathcal{S}_N$ and $\phi \in C_0(\mathbb{R}^2)$ we have

$$\begin{aligned}
\left| \int_{\mathbb{R}^2} \left(\delta_{x_0/\sqrt{N}} - \frac{\chi_{q_N(x_0)}}{|q_N(x_0)|} \right) \phi d\lambda^2 \right| &= \left| \int_{\mathbb{R}^2} \delta_{x_0/\sqrt{N}} \phi d\lambda^2 - \frac{1}{|q_N(x_0)|} \int_{q_N(x_0)} \phi d\lambda^2 \right| \\
&= \frac{1}{|q_N(x_0)|} \left| \int_{q_N(x_0)} d\lambda^2 \phi(x_0/\sqrt{N}) - \int_{q_N(x_0)} \phi d\lambda^2 \right| \\
&= \frac{1}{|q_N(x_0)|} \left| \int_{q_N(x_0)} \phi(x_0/\sqrt{N}) - \phi d\lambda^2 \right| \\
&\leq \sup_{z \in q_N(x_0)} \left| \phi(x_0/\sqrt{N}) - \phi(z) \right| \\
&\leq \sup_{\|x-y\| \leq N^{-1/2}} |\phi(x) - \phi(y)| ,
\end{aligned}$$

where $q_N(x_0)$ denotes $N^{-1/2}\mathcal{V}_{\text{trunc}}(x_0)$. For the last inequality we have used that $N^{-1/2}\mathcal{V}_{\text{trunc}}(x_0) \subset B_{N^{-1/2}}(x_0)$. Consequently establishes

$$\left| \int_{\mathbb{R}^2} \phi d\mu_N - \int_{\mathbb{R}^2} \phi d\tilde{\mu}_N \right| \leq \frac{1}{N} \sum_{x \in \mathcal{S}_N} \sup_{\|x-y\| \leq N^{-1/2}} |\phi(x) - \phi(y)| = \sup_{\|x-y\| \leq N^{-1/2}} |\phi(x) - \phi(y)| \longrightarrow 0 \ \ (N \to \infty)$$

the statement (i).
(ii): This convergence statement requires more effort. The idea is to look at the bulk and the boundary part of the densities separately. We decompose $\tilde{d}_N$

$$\tilde{d}_N = \tilde{b}_N + \tilde{s}_N, \ \tilde{b}_N = \frac{1}{N} \sum_{x \in \text{int } \mathcal{S}_N} \frac{\chi_{N^{-1/2}\mathcal{V}_{\text{trunc}}(x)}}{\left| N^{-1/2}\mathcal{V}_{\text{trunc}}(x) \right|}, \ \tilde{s}_N = \frac{1}{N} \sum_{x \in \partial \mathcal{S}_N} \frac{\chi_{N^{-1/2}\mathcal{V}_{\text{trunc}}(x)}}{\left| N^{-1/2}\mathcal{V}_{\text{trunc}}(x) \right|},$$

where int $\mathcal{S}_N := \mathcal{S}_N \setminus \partial \mathcal{S}_N$. By $\tilde{\beta}_N$ and $\tilde{\sigma}_N$ we denote the according measures for the densities $\tilde{b}_N$ and $\tilde{s}_N$ respectively. $\tilde{\tilde{d}}_N$ can analogously be splitted and $\tilde{\tilde{\beta}}_N, \tilde{\tilde{\sigma}}_N$ are defined correspondingly.

The key point here is, that the L^1-difference between the bulk parts and the boundary parts respectively gets zero in the limit process. The difference $\left| \tilde{\tilde{s}}_N - \tilde{s}_N \right|$ becomes for large N negligible, because the number of boundary atoms grows according to (4.2) only like $N^{1/2}$, while the volume of $N^{-1/2}\mathcal{V}_{\text{trunc}}(x)$ shrinks by N^{-1}. On the other hand, we will show that for every small deviation $\delta > 0$ the number of atoms x in int $\mathcal{S}_N$, with $|\Phi(x)| \geq \delta$ also grows just with $N^{1/2}$. $\Phi(x)$ is called the *volume excess function* of x and defined by

$$\Phi(x) := \frac{1}{|\mathcal{V}_{\text{trunc}}(x)|} - \frac{1}{\left| h'_{1/\sqrt{3}}(x) \right|}.$$

An argument analog to the boundary case then shows that $||\tilde{\tilde{\beta}}_N - \tilde{\beta}_N||_{L^1(\mathbb{R}^2)}$ is bounded by δ. Because this deviation is arbitrary chosen the difference is negligible.

The first precise argument is that $|x_j - x_i| \geq \alpha$ for all $j \neq i$ and thus $B_{\alpha/2}(x_i)$ is a subset of $\mathcal{V}_{\text{trunc}}(x_i)$.

This results in

$$\begin{aligned}
\left|\tilde{\tilde{s}}_N - \tilde{s}_N\right| &= \left| \frac{1}{N} \sum_{x \in \partial \mathcal{S}_N} \frac{\chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)}}{\left|N^{-1/2} h'_{1/\sqrt{3}}(x)\right|} - \frac{\chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)}}{\left|N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)\right|} \right| \\
&\leq \frac{1}{N} \sum_{x \in \partial \mathcal{S}_N} \chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)} \left| \frac{1}{\left|N^{-1/2} h'_{1/\sqrt{3}}(x)\right|} - \frac{1}{\left|N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)\right|} \right| \\
&\leq \sum_{x \in \partial \mathcal{S}_N} \chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)} \left| \frac{1}{\left|h'_{1/\sqrt{3}}(x)\right|} + \frac{1}{|\mathcal{V}_{\mathrm{trunc}}(x)|} \right| \\
&\leq \sum_{x \in \partial \mathcal{S}_N} \chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)} \underbrace{\left(\frac{1}{\left|h'_{1/\sqrt{3}}(0)\right|} + \frac{1}{\left|B_{\alpha/2}(0)\right|} \right)}_{=:K}.
\end{aligned}$$

Together with (4.2), which bounds $\#\partial\mathcal{S}_N$, we get for the difference of $\tilde{\tilde{\sigma}}_N$ and $\tilde{\sigma}_N$ that

$$\begin{aligned}
\left\|\tilde{\tilde{\sigma}}_N - \tilde{\sigma}_N\right\|_{L^1(\mathbb{R}^2)} = \int_{\mathbb{R}^2} |\tilde{\tilde{s}}_N - \tilde{s}_N| d\lambda^2 &\leq K \# \partial \mathcal{S}_N \max_{x \in \mathcal{S}_N} \left\|\chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)}\right\|_{L^1(\mathbb{R}^2)} \\
&\leq \frac{KC}{\Delta} N^{1/2} \left|B_{N^{-1/2}}(0)\right| \\
&= \frac{KC}{\Delta} N^{-1/2} \left|B_1(0)\right| \to 0 \quad (N \to \infty).
\end{aligned}$$

The next step is to analyze the difference of the bulk parts

$$\tilde{b}_N - \tilde{\tilde{b}}_N = \sum_{x \in \mathrm{int}\ \mathcal{S}_N} \chi_{N^{-1/2}\mathcal{V}_{\mathrm{trunc}}(x)} \underbrace{\left(\frac{1}{|\mathcal{V}_{\mathrm{trunc}}(x)|} - \frac{1}{\left|h'_{1/\sqrt{3}}(x)\right|} \right)}_{=\Phi}.$$

By definition any atom x in int $\mathcal{S}_N$ has six neighbors $y_1, \ldots, y_6$. We assume that y_j are numbered such that $y_j - x = r_j(\cos(\phi_j), \sin(\phi_j))^T, 0 \leq \phi_1 < \phi_2 < \cdots < \phi_6 < 2\pi$. We have

$$\tilde{\mathcal{E}}_{\mathrm{loc}}(x) := \sum_{\mathcal{N}_\epsilon(x)} V(|x-y|) + \sum_{j=1}^{6} V(|y_j - y_{j+1}|) = -12 \Rightarrow |\mathcal{V}_{\mathrm{trunc}}(x)| = \left|h'_{1/\sqrt{3}}(x)\right|.$$

The reason is that the left-hand side is true if and only if the distances between x and all $y \in \mathcal{N}(x)$ as well as all mutual distances between in $y \in \mathcal{N}(x)$ are one. By elementary geometric arguments, the only way to arrange $y_1, \ldots, y_6$ around x with the given distances is forming a regular hexagon.

Now choose an arbitrary $\delta > 0$. Then there exists $\tilde{\Delta}(\delta) > 0$ such that for all $x \in$ int $\mathcal{S}_N$

$$|\Phi(x)| \geq \delta \Longrightarrow \sum_{\mathcal{N}(x)} V(|x-y|) + \sum_{j=1}^{6} V(|y_j - y_{j+1}|) \geq -12 + \tilde{\Delta}.$$

Indeed is -12 the lower bound of $\tilde{\mathcal{E}}_{\mathrm{loc}}(x)$. Every variation (continuous or not) of the positions of $x, y_1, \ldots, y_6$ results in an increase of energy by an increment $\tilde{\Delta}(\delta)$. Since $|\Phi(x)|$ is strictly greater than zero, the atoms cannot form a regular hexagon. With the energy bound required in Theorem 3.2 and the fact that atoms in $\partial\mathcal{S}_N$ have less than six neighbors now follows that

$$
\begin{aligned}
-6N + CN^{1/2} \geq \mathcal{E}(\mathcal{S}_N) \geq \frac{1}{2}\sum_{x\in\mathcal{S}_N} \tilde{\mathcal{E}}_{\mathrm{loc}}(x) &\geq \frac{1}{2}(-12)\#\left\{x\in\mathcal{S}_N \,\middle|\, x\in\partial\mathcal{S}_N \vee |\Phi(x)|<\delta\right\} \\
&\quad + \frac{1}{2}(-12+\tilde{\Delta})\#\left\{x\in\mathcal{S}_N \,\middle|\, x\in \text{int }\mathcal{S}_N \wedge |\Phi(x)|\geq\delta\right\} \\
&\geq -6N + \frac{\tilde{\Delta}}{2}\#\left\{x\in\mathcal{S}_N \,\middle|\, x\in \text{int }\mathcal{S}_N \wedge |\Phi(x)|\geq\delta\right\}
\end{aligned}
$$

and thus

$$
\#\left\{x\in \text{int }\mathcal{S}_N \,\middle|\, |\Phi(x)|\geq\delta\right\} \leq \frac{2C}{\tilde{\Delta}}N^{1/2}.
$$

Remark that the factor $1/2$ is necessary, otherwise each pair of atoms would be counted twice. This shows that for every arbitrary but fixed deviation $\delta > 0$ the number of atoms with $|\Phi(x)| \geq \delta$ is of the order $N^{1/2}$ and that $||\tilde{\tilde{\beta}}_N - \tilde{\beta}_N||_{L^1(\mathbb{R}^2)}$ is bounded in an appropriate way by

$$
\begin{aligned}
\left\|\tilde{\tilde{\beta}}_N - \tilde{\beta}_N\right\|_{L^1(\mathbb{R}^2)} \leq |B_{N^{-1/2}}(0)| \sum_{x\in\text{int }\mathcal{S}_N} |\Phi(x)| &\leq |B_{N^{-1/2}}(0)| \sum_{A_{<\delta}} |\Phi(x)| + |B_{N^{-1/2}}(0)| \sum_{A_{\geq\delta}} |\Phi(x)| \\
&\leq N^{-1}\,|B_1(0)|\left(\delta N + \max_{x\in\text{int }\mathcal{S}_N} |\Phi(x)| \# A_{\geq\delta}\right) \\
&= |B_1(0)|\,\delta + |B_1(0)|\,K\frac{2C}{\tilde{\Delta}}N^{-1/2}.
\end{aligned}
$$

$A_{\geq\delta}$ and $A_{<\delta}$ denote hereby $\left\{x\in\text{int }\mathcal{S}_N \,\middle|\, |\Phi(x)|\geq\delta\right\}$ and $\left\{x\in\text{int }\mathcal{S}_N \,\middle|\, |\Phi(x)|<\delta\right\}$ respectively. Letting $N\to\infty$ gives

$$
\limsup_{N\to\infty} \left\|\tilde{\tilde{\beta}}_N - \tilde{\beta}_N\right\|_{L^1(\mathbb{R}^2)} \leq |B_1(0)|\,\delta.
$$

Since the deviation $\delta > 0$ of the volumes is arbitrary this establishes the L^1-convergence of $\tilde{\tilde{\beta}}_N - \tilde{\beta}_N$ to zero and finally proves that μ_N and $\tilde{\tilde{\mu}}_N$ coincide for $N\to\infty$. Thus

$$
\mu = \tilde{\tilde{\mu}} = \eta_{\tilde{E}},
$$

for some $\tilde{E}\subset\mathbb{R}^2$. Since μ has mass one, $\tilde{E}$ has volume $1/\rho$, which proves Theorem 3.4.

□

5 Convergence to the Wulff shape in the triangular lattice

5.1 Minimizing surface energy by Γ-convergence

In this chapter we finally prove the convergence of ground states to a hexagonal set (Theorem 3.6). The basic idea is that the ground states of the energy functional $\mathcal{E}$ (3.2), i.e. the configurations $\mathcal{S}_N \subset \mathcal{L}$ that minimizes $\mathcal{E}$, converge weakly* to a minimizer of the surface energy functional with a suitable γ. Suitable here means that the according Wulff shape is a set with a hexagonal shape. Using the Wulff property (see Theorem below) proves immediately that the limit is a measure with a density proportional to the indicator function of the Wulff shape. For proving the convergence of these minimizers, we are using the convergence statement Theorem 2.27 for Γ-converging functionals.

Theorem 5.1 (Wulff property)**.** [Tay75, FM91] *Let S be the surface energy functional*

$$S : \tilde{\mathcal{P}}(\mathbb{R}^2) \to \mathbb{R},\ G \mapsto \int_{\partial^* G} \gamma(\nu_G(x)) d\mathcal{H}^1(x), \tag{5.1}$$

where γ is a continuous function on $\mathbb{S}^1$, bounded away from zero and $\tilde{\mathcal{P}}(\mathbb{R}^2) \subset \mathcal{P}(\mathbb{R}^2)$ is the set of all $G \subset \mathbb{R}^2$ with finite perimeter and $\lambda^2(G) = 1$. Then the set $G \in \tilde{\mathcal{P}}(\mathbb{R}^2)$ minimizes S if and only if G agrees up to translation λ^2-a.e. with cW_γ, here is

$$W_\gamma := \left\{x \in \mathbb{R}^2 \middle|\ x \cdot \nu \le \gamma(\nu),\ \forall \nu \in \mathbb{S}^1\right\} = \bigcap_{\nu \in \mathbb{S}^1} \underbrace{\left\{x \in \mathbb{R}^2 \middle|\ x \cdot \nu \le \gamma(\nu)\right\}}_{H_\nu},$$

the Wulff shape and $c > 0$ the normalization constant such that $\lambda^2(cW_\gamma) = 1$.

For γ we are choosing

$$\gamma : \left\{\nu = (-\sin(\phi), \cos(\phi))^T \mid \phi \in [0, 2\pi/6]\right\} \to \mathbb{R};\ \nu \mapsto 2\nu_2 - \frac{2}{\sqrt{3}}\nu_1, \tag{5.2}$$

extended $\frac{2\pi}{6}$-periodically. This function is obviously continuous and bounded away from zero. The Wulff shape of γ is the hexagon $h_{\frac{4}{\sqrt{3}}}(0)$, see Figure 5.2.

If we succeed to show that a set $E \subset \mathbb{R}^2$ with finite perimeter and volume one exists such that a subsequence of $(\mu_n)_{n\in\mathbb{N}}$ converges weakly* to η_E, and $S(dE) = \min\{S(G) \mid G \in \tilde{\mathcal{P}}(\mathbb{R}^2)\}$ for a $d \in \mathbb{R}_{>0}$, then we have proved the theorem. The existence of the cluster point is with Theorem 3.4 almost trivial. According to Lemma 4.1 and Theorem 3.2 ground states are connected and satisfies the energy bound in Theorem 3.4. Therefore, there exists such a set $E \subset \mathbb{R}^2$ with volume $1/\rho$ and $\mu_N \overset{*}{\rightharpoonup} \eta_E$. (At least for a subsequence.)

The crucial part of this proof is the minimization property of η_E. For this purpose, we redefine (5.1) as a functional I_∞ on the space of probability measures $\mathcal{R}(\mathbb{R}^2) := \left\{\mu \in \mathcal{M}(\mathbb{R}^2) \mid \mu \text{ nonnegative and } \mu(\mathbb{R}^2) = 1\right\}$ with

$$I_\infty(\mu) := \begin{cases} \int_{\partial^* E} \gamma(\nu_E(x)) d\mathcal{H}^1(x) = S(E), & \text{if } \mu = \eta_E \text{ for some set } E \text{ of finite perimeter and mass } \frac{\sqrt{3}}{2}. \\ +\infty & \text{otherwise} \end{cases}$$

and define a sequence of functionals $(\tilde{I}_N)_{N\in\mathbb{N}}$ with $\tilde{I}_N = N^{-1/2}(I_N + 6N)$ on $\mathcal{R}(\mathbb{R}^2)$ where

$$I_N(\mu) := \begin{cases} \int_{\mathbb{R}^2\times\mathbb{R}^2\setminus\text{diag}} NV(N^{1/2}\|x-y\|) d(\mu\otimes\mu)(x,y), & \text{if } \mu = \frac{1}{N}\sum_{i=1}^N \delta_{\frac{x_i}{\sqrt{N}}}, \text{ for } \{x_1,\dots,x_N\} \subset \mathcal{L} \\ +\infty & \text{otherwise.} \end{cases}$$

This definition of $\tilde{I}_N$ is for crystallized configurations consistent with the definition of the interfacial energies in Section 3.2, we just introduce additionally the factor $N^{-1/2}$. If $(\tilde{I}_N)_{N\in\mathbb{N}}$ Γ-converges to I_∞ we can apply Theorem 2.27 and see that η_E is a minimizer of I_∞. Indeed, it holds for all $N \in \mathbb{N}$

$$\begin{aligned} \inf\left\{\tilde{I}_N(\mu) \mid \mu \in \mathcal{R}(\mathbb{R}^2)\right\} &= \inf\left\{\left(N^{-1/2}\mathcal{E}(\tilde{\mathcal{S}}_N) + 6N\right) \mid \tilde{\mathcal{S}}_N \in \mathcal{C}_N, \tilde{\mathcal{S}}_N \subset \mathcal{L}\right\} \\ &= N^{-1/2}(\mathcal{E}(\mathcal{S}_N) + 6N) \\ &= \tilde{I}_N(\mu_N), \end{aligned}$$

because for all N exists a configuration $\tilde{\mathcal{S}}_N \subset \mathcal{L}$, minimizing the functional $\mathcal{E}$ and $\mathcal{S}_N$ is a minimizer. Obviously is η_E a cluster point (in the wk*-topology) of the sequence $(\mu_N)_{N\in\mathbb{N}}$ of bounded measures. With arguments from topology follows that the prerequisites of Theorem 2.27 are satisfied and thus η_E is a minimizer of I_∞. The following lemma establishes then that $\sqrt{\rho}E$ is already a minimizer of S. In this case is $\sqrt{\rho}E = cW_\gamma$ and $\lambda^2(cW_\gamma) = 1$, it follows $c = 8^{-1/2}3^{-1/4}$ and so $E = 8^{-1/2}3^{-1/4}\rho^{-1/2}h_{\frac{4}{\sqrt{3}}}(0) = h_{\frac{1}{\sqrt{3}}}(0)$.

Lemma 5.2. *Let $E \subset \mathbb{R}^2$ be an arbitrary set with $\lambda^2(E) = 1/\rho$. If the measure η_E minimizes the functional I_∞ then $\sqrt{\rho}E$ minimizes S, i.e.*

$$\inf\{I_\infty(\mu) \mid \mu \in \mathcal{R}(\mathbb{R}^2)\} = I_\infty(\eta_E) = S(\sqrt{\rho}E).$$

Proof. Let $G \in \tilde{\mathcal{P}}(\mathbb{R}^2)$ be arbitrary and $\tilde{G} := 1/\sqrt{\rho}\, G$, then follows

$$\int_{\partial^* E} \gamma(\nu_E(x)) d\mathcal{H}^1(x) \le \int_{\partial^* \tilde{G}} \gamma(\nu_{\tilde{G}}(x)) d\mathcal{H}^1(x).$$

Using the transformation theorem with $\Phi : \mathbb{R}^2 \to \mathbb{R}^2$; $x \mapsto \sqrt{\rho}x$ as an isomorphism, establishes

$$\int_{\partial^* E} \gamma(v_E(\rho^{-1/2}\Phi(x)))\rho d\mathcal{H}^1(x) \le \int_{\partial^* \tilde{G}} \gamma(v_{\tilde{G}}(\rho^{-1/2}\Phi(x)))\rho d\mathcal{H}^1(x).$$

Thus

$$\int_{\partial^* \sqrt{\rho}E} \gamma(\nu_{\sqrt{\rho}E}(y)) d\mathcal{H}^1(y) \le \int_{\partial^* \sqrt{\rho}\tilde{G}} \gamma(\nu_{\sqrt{\rho}\tilde{G}}(y)) d\mathcal{H}^1(y)$$

giving

$$S(\sqrt{\rho}E) \le S(G).$$

So $\sqrt{\rho}E$ minimizes S on $\tilde{\mathcal{P}}(\mathbb{R}^2)$. In the last step we have used, that for all $a \in \mathbb{R}_{>0}$ and $A \in \tilde{\mathcal{P}}(\mathbb{R}^2)$ is $\nu_A(a^{-1}x) = \nu_{aA}(x)$ where x is an arbitrary element from aA. □

It remains to show that $(\tilde{I}_N)_{N\in\mathbb{N}}$ Γ-converges to I_∞. $\tilde{I}_N$ and I_∞ are constructed such that we only need to prove the upper bound for measures η_E, where E has finite perimeter and $\lambda^2(E) = 1/\rho$. Otherwise I_∞ would be infinite and (ii) in Definition 2.26 applies immediately. Furthermore for (i) we only have

to consider sequences of empirical measures associated to crystalline configurations (at least for N large enough). For all other sequences $\liminf_{N\to+\infty} \tilde{I}_N(\mu_N)$ would be infinite and (i) holds immediately. So we will now proof the lower and upper bound for the remaining cases.

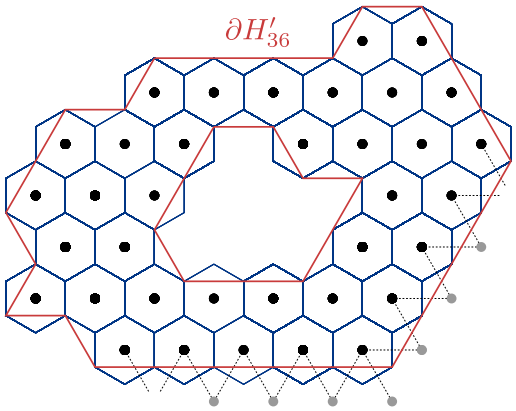

Figure 5.1: Example for covering a configuration with $N = 36$.

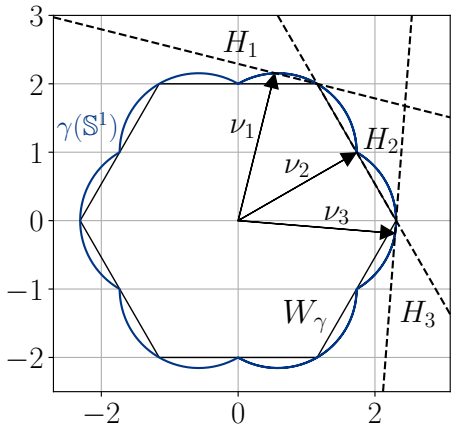

Figure 5.2: The Wulff shape (in black) for γ (5.2), constructed by the intersection of real half-spaces H_ν.

5.2 Lower bound

Our approach for proving the lower bound consists of two parts. At first, we construct a cover H_N for crystalline configurations. Simple geometric arguments prove that the surface energies of these configurations coincide with appropriate integrals over the boundary of this cover. In the next step we will prove that if a sequence of crystalline configurations is wk^*-converging to a limit measure in $\mathcal{R}(\mathbb{R}^2)$, this limit has a density proportional to the indicator function of a set with finite perimeter. Furthermore, we will see that the indicators over the associated covers converge in the L^1-norm to this density. With the representation of the surface energy as an integral and the lower semicontinuity statement Theorem 2.28, follows the lower bound.

Lower bound. Choose an arbitrary probability measure $\mu \in \mathcal{R}(\mathbb{R}^2)$ and a sequence of crystallized configurations $(\mathcal{S}_N)_{N\in\mathbb{N}} \subset \mathcal{L}^{\mathbb{N}}$ converging weakly* to μ. We cover each configuration $\mathcal{S}_N$ with hexagonal sets $h'_{1/\sqrt{3}}(x)$ in the way that

$$\mathcal{S}_N \subset H_N := \bigcup_{x\in\mathcal{S}_N} \overline{N^{-1/2} h'_{1/\sqrt{3}}(x)}.$$

Since $\mathcal{S}_N$ is covered by a finite number of sets, the boundary ∂H_N is a disjoint union of closed polygons $V_1, \dots, V_M$, where $V_j = \bigcup_{i=1}^{m(j)} [v_{i+1,j}, v_{i,j}]$, $[v_{i+1,j}, v_{i,}] := \{v_{i,j} + \lambda(v_{i+1,j} - v_{i,j}) \,|\, \lambda \in [0,1]\}$. The vertices of these polygons $v_{1,j}, \dots, v_{m(j),j}$, $j \in \{1, \dots, M\}$ are on the lattices $\mathcal{A}$ and $\mathcal{B}$, where

$$\mathcal{A} = \left(\frac{1}{3\sqrt{N}}(e_1 + e_2) + \frac{1}{\sqrt{N}}\mathcal{L}\right) \text{ and } \mathcal{B} = \left(\frac{1}{3\sqrt{N}}(2e_2 - e_1) + \frac{1}{\sqrt{N}}\mathcal{L}\right).$$

Since the vertices are alternating between these lattices, we can define for each V_j a closed polygon V'_j with smaller perimeter by skipping every second vertex. From geometric considerations follows that there exists a unique closed set H'_N with $\mathcal{S}_N \subset H'_N$ and $\partial H'_N = \bigcup_{j=1}^{M} V'_j$. The difference in area of H_N and H'_N is obviously equal to a union of small triangles (see Figure 5.1), each with area $\frac{1}{4\sqrt{3}N}$.

A counting argument shows that each atom in $\partial\mathcal{S}_N$ can be assigned to at most three of these triangles,

giving

$$\lambda^2(H_N \triangle H'_N) \leq D\frac{\#\partial\mathcal{S}_N}{N}, \tag{5.3}$$

for a constant $D > 0$ independent of N. If the configuration satisfies (3.5) then (4.2) can be applied, which proves immediately that $\lambda^2(H_N \triangle H'_N)$ is bounded by a term of the order $N^{-1/2}$. Thus $\lambda^2(H_N \triangle H'_N)$ vanishes for $N \to \infty$.

Note that for each boundary segment $[v_{k+1}, v_k] \subset H'_N$ exists two segments in H_N (see Figure 5.1), thus the ratio between the number of segments in ∂H_N and $\partial H'_N$ is two-to-one. It is also obvious that for each segment in ∂H_N there exist $x, y \in \frac{1}{\sqrt{N}}\mathcal{L}$ such that $\|x - y\| = \frac{1}{\sqrt{N}}$ and $x \in \frac{1}{\sqrt{N}}\mathcal{S}_N, y \notin \frac{1}{\sqrt{N}}\mathcal{S}_N$. The number of such atom pairs is equal to $(I_N(\mu_N) + 6N)$ because this is the number of atoms outside the configuration "missing" such that each atom in $\frac{1}{\sqrt{N}}\mathcal{S}_N$ has six neighbors. From the fact that the boundary segments of H'_N are parallel to e_1, e_2 or $e_1 - e_2$ and that γ takes the value two for directions orthogonal to these, it follows that $2\mathcal{H}^1(\partial H'_N)$ can be written as an surface energy integral over γ. Because $\mathcal{S}_N \subset \mathcal{L}$ follows with all this combined

$$F_N := \frac{1}{\sqrt{N}}(I_N(\mu_N) + 6N) = 2\mathcal{H}^1(\partial H'_N) = \int_{\partial H'_N} \gamma(\nu_{H'_N}(x))d\mathcal{H}^1(x). \tag{5.4}$$

Now we define the sequence of normalized densities for the auxiliary sets H_N,

$$d'_N = \frac{1}{N}\sum_{x\in\mathcal{S}_N} \frac{\chi_{N^{-1/2}h'_{1/\sqrt{3}}(x)}}{\left|N^{-1/2}h'_{1/\sqrt{3}}(x)\right|} = \rho\chi_{H_N}.$$

We will see, analog to the proof of Theorem 3.4, that $\int_\cdot d'_N d\lambda^2 \overset{*}{\rightharpoonup} \mu$ and $d'_N \xrightarrow{L^1} \rho\chi_E$, for a subset E in $\mathbb{R}^2$ with volume $1/\rho$ and finite perimeter. This establishes that $\mu = \eta_E$. The proof of the first statement is completely analog the one of Step 2 (i) in Theorem 3.6. The argument for proving the second one is inspired by Step 1, but here the problem occurs that d'_N in general must not be compact supported. The solution is a common truncation argument.

We will again use Theorem 2.17. For doing this we must restrict d'_N for all N to $B_R(0)$ with an arbitrary $R > 0$. It can be assumed that a bounded subsequence of $(F_n)_{n\in\mathbb{N}}$ exists, because otherwise the limes inferior is not finite and the lower bound holds anyways. Further exists a constant $d > 0$ such that $\mathcal{H}^1(\partial H_N) \leq d\mathcal{H}^1(\partial H'_N)$. And so, if $(F_N)_{N\in\mathbb{N}}$ is bounded (at least for a subsequence), it follows with (5.4)

$$\sup_{N\in\mathbb{N}} P(H_N, \mathbb{R}^2) = \sup_{N\in\mathbb{N}} \mathcal{H}^1(\partial H_N) \leq d \sup_{N\in\mathbb{N}} \frac{F_N}{2} < \infty,$$

because the edge of H_N is $\mathcal{H}^1$-a.e. smooth. With $\sup_{N\in\mathbb{N}} \|d'_N\|_{L^1(\mathbb{R}^2)} = 1 < \infty$ the Theorem 2.17 and the Proposition 2.18 are proving the L^1-compactness on *all* $B_R(0)$. Since $\|\mu\|_{L^1(\mathbb{R}^2)} = \|\mu_N\|_{L^1(\mathbb{R}^2)} = 1$ for all N follows that $(d'_N)_{N\in\mathbb{N}}$ converges in $L^1(\mathbb{R}^2)$ to $c\chi_E$ for a $E \subset \mathbb{R}^2$ and $c \in \mathbb{R}_{>0}$. Analog to the proof of Theorem 3.4 shows this that $\mu = \eta_E$ and $\lambda^2(E) = 1/\rho$. Furthermore is $\chi_E \in BV(\mathbb{R}^2)$ and thus E has finite perimeter, because $(d'_N)_{N\in\mathbb{N}}$ is bounded in $BV(\mathbb{R}^2)$. Due to the fact that we can assume $(F_N)_{N\in\mathbb{N}}$ as bounded the configurations satisfies (3.5). This yields that $\lambda^2(H_N \triangle H'_N)$ vanishes if N goes to infinity and thus $\left\|\rho\chi_{H'_N} - \rho\chi_E\right\|_{L^1(\mathbb{R}^2)} \to 0$. It is easy to prove that the periodically expansion of γ to $\mathbb{R}$ is even, positively 1-homogeneous, convex and has compact image. This allows us to use the lower semicontinuity statement Theorem 2.28, which finally shows that

$$\int_{\partial^* E} \gamma(\nu_E(x))d\mathcal{H}^1(x) \leq \liminf_{N\to+\infty} \int_{\partial H'_N} \gamma(\nu_{H'_N}(x))d\mathcal{H}^1(x) = \liminf_{N\to+\infty} \frac{1}{\sqrt{N}}(I_N(\mu_N) + 6N).$$

□

5.3 Upper bound

As mentioned above we have to prove the upper bound of the Γ-convergence just for measures η_E where the subset E has finite perimeter and volume $\frac{\sqrt{3}}{2}$. Our approach here is to construct for each of these sets a sequence $(\mu_N)_{N\in\mathbb{N}}$ (recovery sequence) in $\mathcal{R}(\mathbb{R}^2)$ such that $(\mu_N)_{N\in\mathbb{N}} \overset{*}{\rightharpoonup} \eta_E$ and $\lim_{N\to\infty} I_N(\mu_N) = I_\infty(\eta_E)$, thus satisfying condition (ii)' in Section 2.4.

These subsets E can be approximated in an appropriate way with polygonal sets $(\tilde{P}_k)_{k\in\mathbb{N}}$, i.e. sets where $\partial\tilde{P}_k$ is a union of polygons. In this context appropriate means that $\lambda^2(\tilde{P}_k \triangle E) \to 0$ and that the according surface energy functionals satisfies a suitable continuity property, i.e. the surface energy functionals of $\tilde{P}_k$ and E coincide in the limit.

These polygonal sets can be further approximated by sets $P_n \subset \mathbb{R}^2$, where ∂P_n is a polygonal set with all vertices only in $\frac{1}{n}\mathcal{L}$. Geometric arguments for the configurations $\mathcal{S}_{n,N} := \mathcal{L} \cap \sqrt{N}P_n$ show that $N^{-1/2}(I_N(\mu_{n(N),N}) + 6N)$ and $I_\infty(\mu_{n(N),N})$ coincide for N up to infinity, where $n(N)$ is a sequence of natural numbers and $\mu_{n(N),N}$ the empirical measure associated to $\mathcal{S}_{n(N),N}$. A diagonalization argument then allows us to extract the recovery sequence $(P_k)_{k\in\mathbb{N}}$ from these two convergence processes.

Upper bound.

Step 1 Let $n \in \mathbb{N}$ be an arbitrary natural number and P_n a bounded set with polygonal boundary ∂P_n such that all corner points are in the lattice $\frac{1}{n}\mathcal{L}$ and P_n has the volume $\frac{\sqrt{3}}{2} + \alpha_n = \rho^{-1} + \alpha_n$ for a constant α_n. Let $\tilde{\mathcal{S}}_{n,N} := \mathcal{L} \cap \sqrt{N}P_n$ be the configuration of the lattice atoms inside $\sqrt{N}P_n$ and $\mu_{n,N}$ the associated empirical measures. It is easy to see that $\mu_{n,N}$ is weakly* converging to $\int_\cdot \frac{1}{\rho^{-1}+\alpha_n}\chi_{P_n} d\lambda^2$. The configuration $\tilde{\mathcal{S}}_{n,N}$ consists of $M_{n,N} := \#\tilde{\mathcal{S}}_{n,N}$ atoms. Geometric arguments show

$$|M_{n,N} - N| \le c(\alpha_n N + \sqrt{N}) \tag{5.5}$$

for a constant c independent of n and N.

For proving this assume that the set $\sqrt{N}P_n$ is partly covered by parallelograms with area $\frac{\sqrt{3}}{2}$ in the following way: Assign to every atom x inside $\sqrt{N}P_n$ the parallelogram $x + \operatorname{conv}\{e_1, e_2\}$, see Figure 5.3. The absolute value of the difference between the volume of the set covered by the parallelograms C and the volume of the scaled polygonal set is obviously less or equal the volume of the symmetric difference of C and the $\sqrt{N}P_n$. This volume can be bounded by a constant $\tilde{c} \in \mathbb{R}$, independent of n and N, times $\sqrt{N}\mathcal{H}^1(\partial P_n)$. It easily follows the bound (5.5)

$$\begin{aligned}
|M_{n,N} - N|\,\frac{\sqrt{3}}{2} &\le \left|\frac{\sqrt{3}}{2}M_{n,N} - \lambda^2\left(\sqrt{N}P_n\right)\right| + \left|\lambda^2\left(\sqrt{N}P_n\right) - \frac{\sqrt{3}}{2}N\right| \\
&\le \lambda^2\left(\sqrt{N}P_n \triangle C\right) + \left|\frac{\sqrt{3}}{2}N + \alpha_n N - \frac{\sqrt{3}}{2}N\right| \\
&\le \tilde{c}\sqrt{N}\mathcal{H}^1(\partial P_n) + |\alpha_n|\,N
\end{aligned}$$

and thus

$$|M_{n,N} - N| \le \frac{2}{\sqrt{3}} \max\left\{\tilde{c}\mathcal{H}^1(\partial P_n), 1\right\}(|\alpha_n|\,N + \sqrt{N}).$$

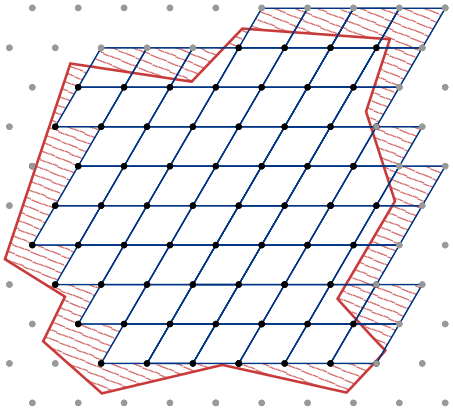

Figure 5.3: Example for partly covering the Polygon $\partial(\sqrt{N}P_n)$ (red) with parallelograms (blue) attached to atoms in $\mathcal{S}_{n,N}$ (black). The triangular lattice outside the configuration is shown in grey.

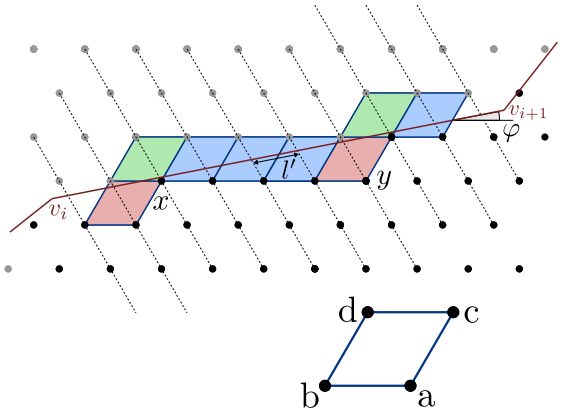

Figure 5.4: Sketch for calculating the surface energy of $\mathcal{S}_{n,N}$ (black) long the edge $[v_i, v_{i+1}]$ with the presented method. For each parallelogram are the verticies named in scheme shown in the bottom right. The color-code for the parallelogram is explained below and the triangular lattice outside the configuration is shown in grey.

Analog to the proof of Theorem 3.4 we can split the surface energy term into a bulk and a boundary part.

$$\begin{aligned}\frac{1}{\sqrt{N}}(I_M(\mu_{n,N}) + 6M_{n,N}) &= \frac{1}{\sqrt{N}} \sum_{\substack{x\in\tilde{\mathcal{S}}_{n,N}\\ \#\mathcal{N}(x)=6}} -6 + \frac{1}{\sqrt{N}} \sum_{\substack{x\in\tilde{\mathcal{S}}_{n,N}\\ \#\mathcal{N}(x)<6}} \left(-6 + R_{\tilde{\mathcal{S}}_{n,N}}(x)\right) + 6\frac{M_{n,N}}{\sqrt{N}} \\ &= \frac{1}{\sqrt{N}} \sum_{x\in\partial\tilde{\mathcal{S}}_{n,N}} R_{\tilde{\mathcal{S}}_{n,N}}(x),\end{aligned} \tag{5.6}$$

where $R_{\tilde{\mathcal{S}}_{n,N}}(x)$ is $\#\left\{x' \in \mathcal{L}\setminus\tilde{\mathcal{S}}_{n,N} \;\middle|\; \|x-x'\| = 1\right\}$. Remark that $\#R_{\tilde{\mathcal{S}}_{n,N}}(x) \leq 6$. We want to find an expression for this sum in dependence of $\mathcal{H}^1(\partial(\sqrt{N}P_n))$. Therefore, we choose an arbitrary segment $s := [v_i, v_{i+1}]$ from $\partial(\sqrt{N}P_n)$ with length $\sqrt{N}L$. L is the length of the edge in the not-scaled polygon P_n. Without loss of generality, we assume that the angle φ between s and e_1 is in the interval $[0, 2\pi/6)$ due to the rotational symmetry of the lattice.

We will prove that the sum $\sum_{x\in\partial\tilde{\mathcal{S}}_{n,N}} l_s(x)$, where $l_s(x) := \{(x,y) \in \tilde{\mathcal{S}}_{n,N} \times (\mathcal{L}\setminus\tilde{\mathcal{S}}_{n,N}) \,|\, \|x-y\| = 1 \text{ and } [x,y]\cap s \neq \emptyset\}$ is equal to two times $\#\mathcal{Z}$ plus an bounded error, where $\mathcal{Z}$ is the set of all atoms with a distance to s of less than one and sufficiently far away from v_i and v_{i+1}. Sufficiently far away in this context means that the ball $B_1(x)$ around an atom $x \in \mathcal{S}_{n,N}$ with minimal distance less than one to s does not intersect with any other segment of $\partial(\sqrt{N}P_n)$. If φ is equal to zero this is obvious, so we only have to consider the case $\varphi \in (0, 2\pi/6)$. For doing that we make the following geometric considerations. (An example is shown in Figure 5.4.) For every atom in $\mathcal{Z}$ there exists *exactly one* line parallel to $t := \{\lambda(e_2 - e_1) \mid \lambda \in \mathbb{R}\}$ (dashed lines), which is intersected by s. Thus $\#\mathcal{Z}$ is equal to the number of such lines, intersected by s up to an error ζ, which is bounded by a constant independent of N.

For each of these atoms exists a *unique* parallelogram such that the atom is at vertex a, see Figure 5.4. The atoms can be sorted into four categories, depending on the orientation of s relative to the corresponding parallelogram. This categorization then also determines the number of neighbors for the according atom.

1. s intersects the segments $e_{ab} := \{a + \lambda(b-a) \mid \lambda \in [0,1)\}$ and e_{ac}. The atom has three neighbors. (green)

2. s intersects the segments e_{bd} and e_{cd}. The atom has five neighbors. (red)

3. s intersects the segments e_{bd} and e_{ac}. The atom has four neighbors. (blue)

4. s intersects the segments e_{ab} and e_{cd}. The atom has four neighbors. (not shown)

Assume now that an atom $x \in \mathcal{Z}$ exists, belonging to case one. Then s intersects the edge e_{ab} of the corresponding parallelogram. If this atom is far enough away from v_{i+1}, there exists a *unique* atom $y \in \mathcal{Z}$, such that s intersects the edge e_{cd} of the corresponding parallelogram. This atom must be of case two or four, since case four is impossible because then this unique atom would coincide with x itself, y must be of case two. Further there exists a set of atoms $\{z_1, \dots, z_k\}$ "between" x and y. These are the atoms uniquely determined by the lines, parallel to t and intersected by s, between the lines x or y lay on. These atoms all belong to case three because s must intersect the edges e_{bd} and e_{ac} of the according parallelograms. It is obvious that the accumulated number of neighbors for all these atoms $(x, y, z_1, \dots, z_k)$ is $4(k+2)$.

If x is not sufficient far enough away from v_{i+1}, no such atom y exists. Consequently for the set of atoms $\{z_1, \dots, z_l\}$ "between" x and v_{i+1} follows that the accumulated number of neighbors is $4(l+1)+\epsilon$, where the error ϵ is bounded. Analog results can be established if x belongs to case two.

Because in the cases three and four the atoms have already four neighbors, it follows that the set $\mathcal{Z}$ can be divided into disjoint subsets $(Z_i)_{i\in\{1,\dots,m\}}$ such that for all $i \in \{1, \dots, m-1\}$ the accumulated number of neighbors for atoms in Z_i is equal to $4\#Z_i$. This shows that $\sum_{x\in\partial\tilde{\mathcal{S}}_{n,N}} l_s(x) = 2\#\mathcal{Z} + \epsilon + \sigma$, where σ is a bounded error, occurring because we have just considered the atoms far enough away from the vertices of s. Further know we that $\#\mathcal{Z}$ can be calculated by the number of lines parallel to t intersected by s. Simple geometric considerations and the addition theorem for sine show that for the length l' (see Figure 5.4) of a segment of s between the parallels to t holds that

$$\frac{1}{l'} = \frac{2}{\sqrt{3}} \sin\left(\frac{\pi}{3} + \varphi\right) = \frac{\gamma(\nu_s)}{2}, \tag{5.7}$$

where ν_s is the outer normal of s. Now it is obvious that the number of lines, parallel to t and intersected by s, is equal to $\sqrt{N}L/l'$, plus an error η bounded independent of N. All these considerations combined lead to the expression

$$\sum_{x\in\partial\tilde{\mathcal{S}}_{n,N}} l_s(x) = 2\#\mathcal{Z} + \epsilon + \sigma = 2\sqrt{N}\frac{L}{l'} + \underbrace{\mathcal{O}(L,\varphi)}_{2\zeta+2\eta+\epsilon+\sigma} = \sqrt{N}\left(\gamma(\nu_s)L + \frac{1}{\sqrt{N}}\mathcal{O}(L,\varphi)\right).$$

The summation over all edges from $\partial(\sqrt{N}P_n) = \cup_{i=1}^{q}[v_i, v_{i+1}]$ shows

$$\sum_{x\in\partial\tilde{\mathcal{S}}_{n,N}} R_{\tilde{\mathcal{S}}_{n,N}}(x) = \sum_{i=1}^{q} \sum_{x\in\partial\tilde{\mathcal{S}}_{n,N}} l_{[v_i,v_{i+1}]}(x).$$

Together with (5.6) we get

$$\left|\frac{1}{\sqrt{N}}(I_{M_{n,N}}(\mu_{n,N}) + 6M_{n,N}) - \int_{\partial P_n} \gamma(\nu_{P_n}(x))d\mathcal{H}^1(x)\right| \le c\left(\alpha_n + \frac{1}{\sqrt{N}}\right), \tag{5.8}$$

for a constant c.

Step 2 Now let $P \subset \mathbb{R}^2$ be a set with polygonal boundary and volume ρ^{-1}. It is easy to see that a sequence of polygonal sets $(P_n)_{n\in\mathbb{N}}$ exist with vertices in $\frac{1}{n}\mathcal{L}$ such that $\lambda^2(P_n) = \rho^{-1} + \alpha_n$ and

$$\lambda^2(P_n \triangle P) = \alpha_n \to 0 \text{ and } \int_{\partial P_n} \gamma(\nu_{P_n}(x))d\mathcal{H}^1(x) \to \int_{\partial P} \gamma(\nu_P(x))d\mathcal{H}^1(x). \tag{5.9}$$

For this purpose, we construct for every vertex $\{v_i\}_{i\in\{1,\dots,k\}}$ of ∂P a sequence $(v_{i,n})_{n\in\mathbb{N}}$ with $v_{i,n} \in \frac{1}{n}\mathcal{L}$ converging to v_i. We define P_n such that ∂P_n is a union of polygons with vertices $\{v_{i,n}\}_{i\in\{1,\dots,k\}}$. Obviously is $\lim_{n\to\infty} \mathcal{H}^1(\partial P_n \triangle \partial P) = 0$, because the segments $[v_i, v_{i+1}]$ depend continuously on v_i and v_{i+1}. Thus ∂P_n and ∂P coincide for $n \to \infty$ and both statements follow imminently.

Choosing now an appropriate $n : \mathbb{N} \to \mathbb{N}$, with $n(N) \to \infty$ for $N \to \infty$ and define $\tilde{\mathcal{S}}_N := \tilde{\mathcal{S}}_{n(N),N}$, $\tilde{\mu}_N := \mu_{n(N),N}$ and $M := M_{n(N),N}$. One important consequence from (5.5) is that

$$\lim_{N\to\infty} \left|\frac{M-N}{N}\right| = \lim_{N\to\infty} \alpha_{n(N)} = 0. \tag{5.10}$$

Further follows

$$\tilde{\mu}_N \overset{*}{\rightharpoonup} \int_\cdot \rho\chi_P d\lambda^2 \text{ and } \frac{1}{\sqrt{N}}(I_M(\tilde{\mu}_N) + 6M) \to \int_{\partial P} \gamma(\nu_P(x))d\mathcal{H}^1(x).$$

The first statement follows, because $\int_\cdot \frac{1}{\rho^{-1}+\alpha_{n(N)}}\chi_{P_N} d\lambda^2$ is weakly* converging to $\int_\cdot \rho\chi_P d\lambda^2$ and the second statement follows from (5.8) and $\alpha_{n(N)} \to 0$.

A problem with the construction in the first step is that configuration $\tilde{\mathcal{S}}_N$ consists in general not of N atoms, so we have to add or remove a configuration with $|N - M|$ atoms but with a negligible surface term for $N \to \infty$. Therefore, set $K := \sqrt{|N-M|}$ and let Q be the parallelogram

$$Q := \lfloor K \rfloor \operatorname{conv}\{e_1, e_2\} \setminus (\{\lambda e_1 + e_2 \,|\, \lambda \in [0, \lfloor K \rfloor]\} \cup \{e_1 + \lambda e_2 \,|\, \lambda \in [0, \lfloor K \rfloor]\}),$$

with edges along e_1 and e_2 but not containing the upper and right edge. The configuration $\tilde{\tilde{\mathcal{S}}} := \mathcal{L} \cap Q$ has $\tilde{K} := (\lfloor\sqrt{|N-M|}\rfloor)^2$ atoms. We are now adding $|N-M| - \tilde{K}$ atoms to $\tilde{\tilde{\mathcal{S}}}$ in the following way: Begin at $\lfloor K \rfloor e_2$ and add an atom. Then go to $\lfloor K \rfloor e_2 + e_1$, add an atom and then go to $\lfloor K \rfloor e_2 + 2e_1$. Continue in that way up to $\lfloor K \rfloor e_2 + \lfloor K \rfloor e_1$, if necessary. If then the configuration has not $|N-M|$ atoms, go to $(\lfloor K \rfloor - 1)e_2 + \lfloor K \rfloor e_1$ and fill the right edge in the same way.

For the now extended configuration $\tilde{\tilde{\mathcal{S}}}$ we have by induction

$$\#\partial\tilde{\tilde{\mathcal{S}}} \le \mathcal{H}^1(\partial Q) = 4\lfloor K \rfloor = 4\left\lfloor\sqrt{|N-M|}\right\rfloor.$$

Now we are looking at the cases $M < N$ and $M > N$ separately. First assume $M < N$. In this case we arrange the configurations $\tilde{\mathcal{S}}$ and $\tilde{\tilde{\mathcal{S}}}$ such that the minimal distance between them is greater than one. Let μ_N be the re-scaled empirical measure to $\mathcal{S} := \tilde{\mathcal{S}}_N \cup \tilde{\tilde{\mathcal{S}}}$. It follows analog to (5.6) that

$$\begin{aligned}\left|\tilde{I}_N(\mu_N) - \frac{1}{\sqrt{N}}(I_M(\tilde{\mu}_N) + 6M)\right| &= \frac{1}{\sqrt{N}}\left|(\mathcal{E}(\tilde{\tilde{\mathcal{S}}}) + 6(N-M)\right| \\ &= \frac{1}{\sqrt{N}} \sum_{x\in\partial\tilde{\tilde{\mathcal{S}}}} R_{\tilde{\tilde{\mathcal{S}}}}(x) \\ &\le \frac{6}{\sqrt{N}}\left(4\left\lfloor\sqrt{|N-M|}\right\rfloor\right).\end{aligned}$$

Now let $M > N$. Here we are dividing $\tilde{\mathcal{S}}_N$ into a bulk B and a boundary part T (see Figure 5.5) and remove (after translation) the set $\tilde{\tilde{\mathcal{S}}}$ from the bulk part. This is for large enough N always possible.

Indeed, there exists a ball $B_r(x) \subset P$, otherwise P would have volume zero. From (5.10) follows now that $|M-N|/N \to 0$, which implies that for all $\epsilon > 0$, there exists an $\tilde{N} \in \mathbb{N}$ such that for all $N \geq \tilde{N}$ is $\sqrt{|M-N|} \leq \epsilon\sqrt{N}$.

Simple geometric considerations show that a constant $c > 0$ exists such that for all $q, \tilde{r} > 0$ with $q \leq c\tilde{r}$ the parallelogram with edges qe_1 and qe_2 fits (after translation) inside a ball with radius r. This shows that for all sufficient large N, Q will fit inside a ball with radius $\sqrt{N}r$ such that $\tilde{\tilde{\mathcal{S}}}$ is a subset of B. Through the removing of $\tilde{\tilde{\mathcal{S}}}$ we get an additional set of boundary atoms T_a and a new bulk set B_n. Without loss of generality we can choose ϵ so that $T \cap T_a = \emptyset$ and thus $B_n = B \setminus (\tilde{\tilde{\mathcal{S}}} \cup T_a)$.

Let be μ_N the re-scaled empirical measure to $B_n \cup T \cup T_a$. Analog to case $M < N$ we can calculate the difference of the energy functionals

$$\begin{aligned}\left|\tilde{I}_N(\mu_N) - \frac{1}{\sqrt{N}}(I_M(\tilde{\mu}_N) + 6M)\right| &= \frac{1}{\sqrt{N}}\Bigg| -6\#B_n + -6\#T + \sum_{x\in T} R_T(x) - 6\#T_a + \sum_{x\in T_a} R_{T_a}(x) \\ &\qquad - (-6)\#B - \left(-6\#T + \sum_{x\in T} R_T(x)\right) + 6(N-M)\Bigg| \\ &= \frac{1}{\sqrt{N}}\left|-6\underbrace{(\#B_n + \#T_a - \#B)}_{N-M} + \sum_{x\in T_a} R_{T_a}(x) + 6(N-M)\right| \\ &\leq 24\sqrt{\frac{|N-M|}{N}}.\end{aligned}$$

Remark that $\sum_{x\in T_a} R_{T_a}(x) \leq 6\#\partial\tilde{\tilde{\mathcal{S}}}$. In both cases we get

$$\left|\frac{1}{\sqrt{N}}(I_N(\mu_N) + 6N) - \frac{1}{\sqrt{N}}(I_M(\tilde{\mu}_N) + 6M)\right| \leq c\sqrt{\frac{|M-N|}{N}},$$

for a constant c independent of N. This together with (5.8) and (5.10) proves

$$\mu_N \overset{*}{\rightharpoonup} \eta_P \text{ and } \frac{1}{\sqrt{N}}(I_N(\mu_N) + 6N) \to \int_{\partial^* P} \gamma(\nu_P(x))d\mathcal{H}^1(x). \tag{5.11}$$

Here it is important to notice that $\partial^* P$ and ∂P coincides $\mathcal{H}^1$-a.e.. To sum up, we have established that for each polygon P there exists a sequence configurations with empirical measures $(\mu_N)_{N\in\mathbb{N}}$ weakly* converging to η_P such that $(\tilde{I}_N(\mu_N))_{N\in\mathbb{N}}$ is converging to the surface energy of P.

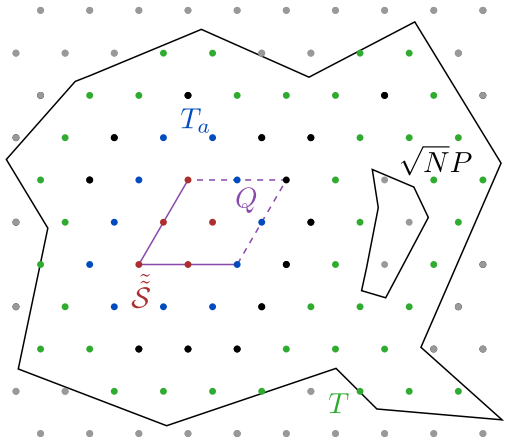

Figure 5.5: Example for removing a configuration with five atoms from the bulk of a configuration. The triangular lattice outside the configuration is shown in grey.

Step 3 It remains to prove that a similar convergence can be obtained for an arbitrary set $E \subset \mathbb{R}^2$ with finite perimeter and $\lambda^2(E) = \frac{\sqrt{3}}{2}$. We want to show that

$$\mu_N \overset{*}{\rightharpoonup} \eta_E \text{ and } \frac{1}{\sqrt{N}}(I_N(\mu_N) + 6N) \to \int_{\partial^* E} \gamma(\nu_E(x))d\mathcal{H}^1(x) = I_\infty(\eta_E). \tag{5.12}$$

At first let $E \subset \mathbb{R}^2$ be a *bounded* set E, with volume $\frac{\sqrt{3}}{2}$ such that $P(E, \mathbb{R}^2) < \infty$. Because E is bounded it can be embedded in an open, relative compact, bounded Lipschitz set Ω. Further is, as mentioned above, γ positive, positively 1-homogeneous and convex. Additionally is $\gamma(x) = \gamma(x + \pi)$ for all $x \in [0, 2\pi/6)$. Therefore, Theorem 2.24 and Remark 2.25 can be applied to our problem. It can then be seen that a sequence of bounded sets $(E_n)_{n\in\mathbb{N}}$ with finite perimeter and C^∞-boundary exists such that

$$\lambda^2(E_n \triangle E) \to 0 \text{ and } \int_{\partial^* E_n} \gamma(\nu_{E_n}(x))d\mathcal{H}^1(x) \to \int_{\partial^* E} \gamma(\nu_E(x))d\mathcal{H}^1(x).$$

The convergence of the symmetric differences shows that $(\lambda^2(E_n))_{n\in\mathbb{N}}$ is bounded. Therefore, it exists (at least for a subsequence of $(E_n)_{n\in\mathbb{N}}$) a sequence $(c_n)_{n\in\mathbb{N}} \to 1$ of nonzero real numbers such that $\lambda^2(c_n E_n) = \frac{\sqrt{3}}{2}$ for all indices large enough. Because we can easily prove $\lambda^2(c_n E_n \triangle E) \to 0$, $\eta_{c_n E_n} \overset{*}{\rightharpoonup} \eta_E$ follows. Analog arguments can be applied to the integral convergence, showing

$$\eta_{c_n E_n} \overset{*}{\rightharpoonup} \eta_E \text{ and } \int_{\partial^* c_n E_n} \gamma(\nu_{c_n E_n}(x))d\mathcal{H}^1(x) \to \int_{\partial^* E} \gamma(\nu_E(x))d\mathcal{H}^1(x). \tag{5.13}$$

The next step is consequently to prove that these $c_n E_n$ can be approximated with polygonal sets, such that the weak*-convergence and a convergence of the surface functional applies in a suitable way. We want to show that for each $n \in \mathbb{N}$ a sequence $(P_{k,n})_{k\in\mathbb{N}}$ of sets with polygonal boundary and volume $\frac{\sqrt{3}}{2}$ exist such that

$$\eta_{P_{k,n}} \overset{*}{\rightharpoonup} \eta_{c_n E_n} \text{ and } \int_{\partial^* P_{k,n}} \gamma(\nu_{P_{k,n}}(x))d\mathcal{H}^1(x) \to \int_{\partial^* c_n E_n} \gamma(\nu_{c_n E_n}(x))d\mathcal{H}^1(x). \tag{5.14}$$

It is a commonly known fact that bounded sets of finite perimeter with C^∞-boundary can be approximated by polygonal sets. With the continuity of γ follows then the convergence statement for the surface functionals. We assume in the following without loss of generality that $c_n = 1$ for all n and choose an arbitrary E_n from $(E_n)_{n\in\mathbb{N}}$.

The main idea for the proof is that ∂E_n is a compact set and as such can be covered for every $\epsilon > 0$ with a finite number $N := N(\epsilon)$ of balls $B_{r_i}(x_i)$ with $r_i < \epsilon$ for $i \in \{1, \dots, N\}$ such that $B_{r_i}(x_i) \cap \partial E_n$ can be written as graph of a C^∞-function for all $i \in \{1, \cdots, N\}$.

Choose now for every $\epsilon > 0$ a polygon ∂P_k with $k := k(\epsilon)$ vertices $y_1, \dots, y_k$ such that $y_i \in \partial E_n$ for all $i \in \{1, \dots k\}$ and $\|y_{i+1} - y_i\| \leq \epsilon$, for all $i \in 1, \dots, k$, where $y_{k+1} = y_1$. Assume further that $\partial P_k \subset \bigcup_{i=1}^N B_{r_i}(x_i)$ and $\mathcal{H}^1(\partial^* P_{k(\epsilon)}) < \mathcal{H}^1(\partial^* P_{k(\tilde{\epsilon})})$ for all $\epsilon, \tilde{\epsilon} > 0$ with $\tilde{\epsilon} < \epsilon$.

In this construction it is easy to see that $\mathcal{H}^1(\partial^* P_k)$ is growing monotonously and is bounded by $\mathcal{H}^1(\partial^* E)$, thus $\lim_{k\to\infty} \mathcal{H}^1(\partial^* P_k) = \mathcal{H}^1(\partial^* E_n)$. It is clear that $\limsup_{\epsilon\to 0} |N(\epsilon)\epsilon| =: C < \infty$, since the union of balls with diameter less than 2ϵ covers $\partial^* E_n$ and $\mathcal{H}^1(\partial^* E_n)$ is finite. Further, it is obvious that $\lambda^2((P_k \triangle E_n) \cap B_{r_i}(x_i)) < \pi\epsilon^2$ for all $i \in \{1, \cdots, N\}$ and $k \in \mathbb{N}$. This shows

$$\lim_{\epsilon\to 0} \lambda^2(P_{k(\epsilon)} \triangle E_n) = \lim_{k\to\infty} \lambda^2(P_k \triangle E_n) \leq \lim_{\epsilon\to 0} \sum_{i=1}^{N(\epsilon)} \pi\epsilon^2 = \pi C \lim_{\epsilon\to 0} \epsilon = 0,$$

which proves the weak*-convergence in (5.14) and that the polygon ∂P_k approximates ∂E. The fact that γ is continuous on $\mathbb{S}^1$ gives then the convergence of the surface integrals. A scaling argument analog to

the one above shows that these convergence statement also applied to polygonal sets scaled such that they have volume $\frac{\sqrt{3}}{2}$ which proves (5.14). A diagonalization argument applied to the sequences defined by (5.13) and (5.14) allows us to extract a sequence of polygonal sets $(\tilde{P}_k)_{k\in\mathbb{N}}$, with $\lambda^2(\tilde{P}_k) = \frac{\sqrt{3}}{2}$ for all $k \in \mathbb{N}$ such that

$$\eta_{\tilde{P}_k} \overset{*}{\rightharpoonup} \eta_E \text{ and } \int_{\partial^* \tilde{P}_k} \gamma(\nu_{\tilde{P}_k}(x)) d\mathcal{H}^1(x) \to \int_{\partial^* E} \gamma(\nu_E(x)) d\mathcal{H}^1(x). \tag{5.15}$$

Applying the same argument to this new sequence and the sequence $(\mu_N)_{N\in\mathbb{N}}$ defined by (5.11), proves (5.12), if E is bounded.

In the case of unbounded sets E we can use a truncation argument to reduce the problem to the case of bounded sets. Construct a sequence $(E_n)_{n\in\mathbb{N}}$ with $((E \cap B_n(0))_n)_{n\in\mathbb{N}}$. The weak*-convergence follows from the *coarea formel*[3]

$$\lambda^2(E) = \int_E d\lambda^2 = \int_0^\infty \mathcal{H}^1(\partial B_r \cap E) dr,$$

proving that $\lim_{n\to\infty} \lambda^2(B_n \cap E) = \lambda^2(E)$. Due to the fact that E_n is a subset of E for all $n \in \mathbb{N}$ and that $\lambda^2(E) < \infty$ this proves $\lim_{n\to\infty} \lambda^2(E_n \triangle E) = 0$ and thus the weak*-convergence. At last, we have to prove that

$$\int_{\partial^* E_n} \gamma(\nu_{E_n}(x)) d\mathcal{H}^1(x) \to \int_{\partial^* E} \gamma(\nu_E(x)) d\mathcal{H}^1(x).$$

It is easy to see that these integrals coincide on $E_n \cap E$ for all n. Simple geometric considerations also show that $\mathcal{H}^1(\partial^* E_n \triangle \partial^* E)$ vanishes for $n \to \infty$, thus a partition of these integrals proves the convergence. Similar to the cases above this convergence holds also after scaling E_n with appropriate factors.

Applying now again a diagonalization argument proves finally (5.12) for an unbounded set E. To sum up, we can find for every measure η_E, where E is a set of finite perimeter and volume $\frac{\sqrt{3}}{2}$, a sequence of measures $(\mu_N)_{N\in\mathbb{N}}$, weakly* converging to η_E and $\tilde{I}_N(\mu_N) \to I_\infty(\eta_E)$. With the considerations in Section 5.1 this proves the upper bound and thus that $\tilde{I}_N \overset{\Gamma}{\to} I_\infty$. This finishes the proof of Theorem 3.6.

□

[3]Derived from [AFP00, p. 102, Eq. 2.74]

6 Convergence to the Wulff shape in the square lattice

The Theorem 3.6 works just for a rather specific potential. If it is possible to show such a statement for other potentials is an unsolved question. The aim of this section is therefore to prove that an analog result (Theorem 3.7) can be shown at least for the potential presented by Mainini et al. [MPS14]. Especially the connection between the macroscopic shape and the microscopic structure can be reproduced. For this new potential we will see that the atoms in the crystal are arranging into square structure and that the macroscopic shape can be approximated by a square.

Indeed, we will also see that not only such statement can be derived but also that the arguments for achieving this are almost identical to the one presented in Chapter 5. So maybe it is possible to develop a proof for a more general potential based on the arguments presented by Yeung et al.

6.1 Square model

The new energy functional we are dealing with in this section consists of two real-valued functions $V_2 : [0,\infty) \to [-1,\infty]$ and $V_3 : [0,2\pi] \to [0,\infty)$. V_2 is the distance depended part of the potential, i.e. the contribution of this part depends *only* on interatomic distances. Different to the Heitmann-Radin like potential in Section 3.2 a second, angle depended, component V_3 exist. Remark that we again analyze the behavior only at zero Kelvin and therefore no dynamic contribution to energy

$$\tilde{\mathcal{E}}(\mathcal{S}_N) := \tilde{\mathcal{E}}(x_1,\dots,x_N) = \sum_{i\neq j} V_2(\underbrace{\|x_i - x_j\|}_{l_{ij}}) + \sum_{(i,j,k)\in\mathcal{A}} V_3(\theta_{ijk}), \tag{6.1}$$

occurs. For the short-ranged two-body potential V_2 we have

$$V_2(l) := \begin{cases} +\infty, & \text{if } l < 1, \\ -1, & \text{if } l = 1, \\ v(l), & \text{if } 1 < l < l^*, \\ 0, & \text{if } l \geq l^*, \end{cases}$$

where v is an arbitrary, negative-valued function, with $v((-1,l^*)) \subseteq (-1,0)$ and l^* a scalar in $(1,\sqrt{2})$. Therefore, it is assumed that two atoms, which are more than $\sqrt{2}$ units apart, do not interact with each other. $\mathcal{A}$ is the set of all tripels in $\mathcal{S}_N \times \mathcal{S}_N \times \mathcal{S}_N$, where l_{ij} and l_{ik} are in the range $[1,l^*)$ ($\mathcal{A} = \{(i,j,k) \,|\, l_{ij}, l_{ik} \in [1,l^*)\}$). θ_{ijk} is then the angle between the lines through (x_i,x_j) and (x_i,x_k) respectively.

For modeling V_3 we define at first the set G. Let be $\sigma \in (0,\pi/8)$ a constant and let G be defined as

$$G := G_1 \cup G_2 \cup G_3, \text{ where } G_k = \left[\frac{k\pi}{2} - \sigma, \frac{k\pi}{2} + \sigma\right] \text{ for } k \in \{1,2,3\}.$$

We demand that V_3 is convex on G_1, symmetric with respect to π and vanishes at $\theta \in \{k\pi/2 \,|\, k \in \{1,2,3\}\}$.

Additionally, it should hold that

$$
\begin{aligned}
&V_3(\theta) > 8 \text{ if } \theta \in \left(\theta_{\min}, \frac{2\pi}{5}\right], \\
&V_3(\theta) > 4 \text{ if } \theta \notin G, \\
&V_3(\theta) = V_3\left(\theta + \frac{\pi}{2}\right) = V_3\left(\theta + \pi\right) \text{ if } \theta \in G_1, \\
&V'_{3,-}\left(\frac{\pi}{2}\right) := \lim_{t \nearrow 0} \frac{V_3(t + \pi/2)}{t} < -\frac{2}{\pi},
\end{aligned}
$$

where the angle $\theta_{\min}$ is defined as $2\arcsin\big(1/(2\sqrt{2})\big) \approx 0.23\pi$. Analog to the definitions above we call a configuration $\mathcal{S}_N$ crystallized if $\mathcal{S}_N \subset \mathbb{Z}^2$ and define the set of neighbors $\mathcal{N}(x)$ for an atom x as

$$
\mathcal{N}(x) := \{y \in \mathcal{S}_N \mid \|y - x\| \in [1, l^*)\}.
$$

For *crystallized configurations* $\mathcal{S}_N$ it is clear that every atom can have at most four neighbors. Indeed, it is in contrast to the hexagonal lattice no interaction along the axis $\tilde{e}_2 - \tilde{e}_1$ possible, where $\tilde{e}_1 := (1,0)^T$ and $\tilde{e}_2 := (0,1)^T$, because l^* is less than $\sqrt{2}$. We define for this potential the sets $\partial\mathcal{S}_N$ and int $\mathcal{S}_N$ as follows

$$
\partial\mathcal{S}_N := \{x \in \mathcal{S}_N \mid \#\mathcal{N}(x) < 4\}, \text{ int } \mathcal{S}_N := \mathcal{S}_N \setminus \partial\mathcal{S}_N
$$

and calculate accordingly the interfacial energy as $\tilde{\mathcal{E}}(\mathcal{S}_N) + 4\#\mathcal{S}_N$, analog to the model in Section 3.2. With these definitions we can now prove Theorem 3.7.

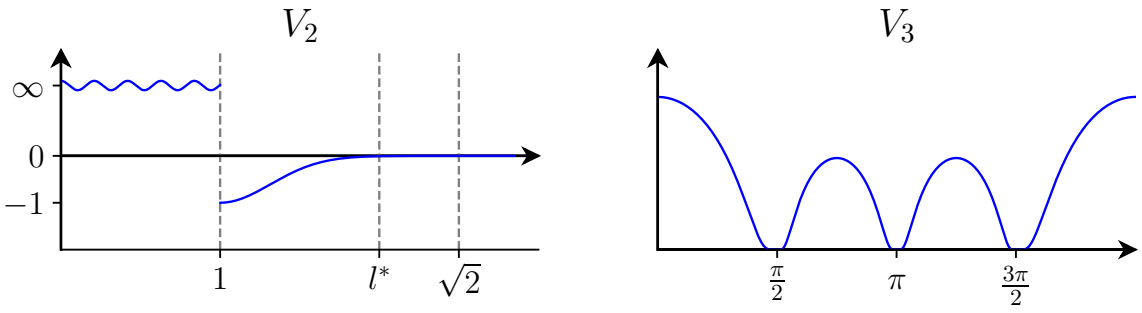

Figure 6.1: Schematic representation of the functions V_2 and V_3.

6.2 Lower bound and upper bound in the square model

Before we are going to the actual proof, it should be noted that for all $N \in \mathbb{N}$ ground states $\mathcal{S}_N$ exist and that all these are square, i.e. $\mathcal{S}_N \subset \mathbb{Z}^2$. Further can be proved that the associated empirical measures $(\mu_N)_{N\in\mathbb{N}}$ are always converging weakly* to $\tilde{\eta}_E$, for an set $E \subset \mathbb{R}^2$ and $\lambda^2(E) = 1$. Indeed, we even know that the measures are converging to $\tilde{\eta}_{q_1}$, where $q_1 = \left[-\frac{1}{2}, \frac{1}{2}\right] \times \left[-\frac{1}{2}, \frac{1}{2}\right]$. These results have been derived in [MPS14], see there Proposition 4.1, Theorem 5.1 and the explanation to Theorem 8.1.

The idea is to show that the considerations from last chapter can be adapted with minor changes to new functionals adjusted for the potential (6.1). Especially the function γ in (5.1) has to be changed in such a way that the resulting Wulff shape is the square q_1. It turns out that the arguments from Yeung et al. can be relatively easy applied to the new crystal lattice. The most significant change is that atoms in the crystallized configurations have at most four neighbors. Thanks to the new regulation regarding the maximum number of neighbors, all calculations have to be adjusted accordingly.

We begin our discussion by defining appropriate energy functionals on $\mathcal{R}(\mathbb{R}^2)$, analog for the one for the triangular lattice

$$J_\infty(\mu) := \begin{cases} \int_{\partial^* E} \tilde{\gamma}(\nu_E(x)) d\mathcal{H}^1(x) = S(E), & \text{if } \mu = \tilde{\eta}_E \text{ for some set } E \text{ of finite perimeter and mass one.} \\ +\infty & \text{otherwise} \end{cases}$$

$$J_N(\mu) := \begin{cases} \int_{\mathbb{R}^2\times\mathbb{R}^2\setminus \mathrm{diag}} NV_2(N^{1/2}\|x-y\|) d(\mu\otimes\mu)(x,y), & \text{if } \mu = \frac{1}{N}\sum_{i=1}^N \delta_{\frac{x_i}{\sqrt{N}}}, \text{ for } \{x_1,\dots x_N\} \subset \mathbb{Z}^2 \\ +\infty & \text{otherwise,} \end{cases}$$

where $\tilde{\gamma} : \mathbb{S}^1 \to \mathbb{R}$ is continuous and bounded away from zero. An important point to notice here is, that only the distance-depended potential V_2 appears in the integral and not the angle-depended potential V_3. That is a direct result form the fact that for crystallized configurations of the new potential the atoms are on the square lattice $\mathbb{Z}^2$ and therefore the contribution of V_3 to the total energy is zero for all angles, i.e. all angles in $\mathcal{A}$ are in $\{k\pi/2 \,|\, k \in \{1,2,3\}\}$. The angle-energies V_3 assert that the ground states are subsets of the square lattice but the angles are not relevant for calculating the surface energies. The surface energies can, in the same way as for the Heitmann-Radin potential, be determined by counting the "missing" atoms. So we define analog the sequence $(\tilde{J}_N)_{N\in\mathbb{N}}$ with $\tilde{J}_N := N^{-1/2}(J_N + 4N)$. The correction term for calculating the surface part of the energy is not $6N$ but only $4N$.

As in Section 5.1 we choose an appropriate $\tilde{\gamma}$ for the functional (5.1). This time we choose the function as

$$\tilde{\gamma} : \left\{\nu = (-\sin(\phi), \cos(\phi))^T \mid \phi \in [0, \pi/2]\right\} \to \mathbb{R};\ \nu \mapsto -\nu_1 + \nu_2, \tag{6.2}$$

extended $\frac{\pi}{2}$-periodically, so that the Wulff shape is the square $[-1,1]\times[-1,1]$, see Figure 6.2. It is easy to verify that $\tilde{\gamma}$ satisfies the proprieties required in Theorems 2.24, 2.28 and 5.1.

Corresponding to Lemma 5.2 follows that if $\tilde{\eta}_E$ for $E \in \tilde{\mathcal{P}}(\mathbb{R}^2)$ minimizes J_∞ then E minimizes S. It remains to show that the cluster point $\tilde{\eta}_E$ of $(\mu_n)_{n\in\mathbb{N}}$ is in $\operatorname{argmin} J_\infty$. In this case it is easy to see that the factor c in Theorem 5.1 is $\frac{1}{2}$. Since E has already volume one follows then $E = [-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}]$.

We want to use again Theorem 2.27, so we have to check that $(\tilde{J}_N)_{N\in\mathbb{N}}$ is indeed Γ-converging to J_∞. It is important to notice that for a ground state $\mathcal{S}_N$ and the associated empirical measure μ_N applies that

$$\inf\left\{\tilde{J}_N(\mu) \mid \mu \in \mathcal{R}(\mathbb{R}^2)\right\} = N^{-1/2}(\tilde{\mathcal{E}}(\mathcal{S}_N) + 4N) = \tilde{J}_N(\mu_N),$$

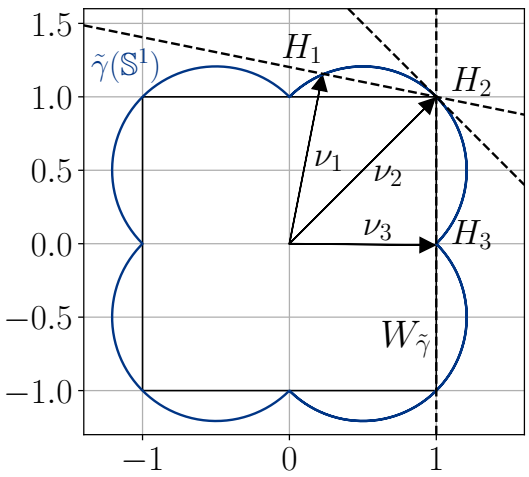

Figure 6.2: The Wulff shape (in black) for $\tilde{\gamma}$ (6.2), constructed by the intersection of real half-spaces.

because $\mathcal{S}_N$ is crystallized and the contribution of V_3 to the energy is zero.

The approach for showing Γ-convergence is the same as for $(\tilde{I}_N)_{N\in\mathbb{N}}$. Especially we can make the same simplification such that we just have to verify the lower bound for sequences of empirical measures for crystallized configurations and the upper bound for measures of the kind $\tilde{\eta}_E$, for an appropriate E.

The proof of the lower bound for the new potential is easier than the one discussed in Section 5.2. The reason is that we get immediately a one-to-one ratio between the number of segments $[x, y]$, with $x, y \in \frac{1}{\sqrt{N}}\mathbb{Z}^2$ such that $\|x - y\| = \frac{1}{\sqrt{N}}$ and $x \in \frac{1}{\sqrt{N}}\mathcal{S}_N, y \notin \frac{1}{\sqrt{N}}\mathcal{S}_N$ and the edgelength of a cover with primitive shapes, with edges orthogonal to $\tilde{e}_1$ or $\tilde{e}_2$. So we can immediately write $\tilde{J}_N$ as an integral over the edge of this cover and do not have to prove an equivalent to (5.3).

Lower bound. Let be $\mu \in \mathcal{R}(\mathbb{R}^2)$ an arbitrary probability measure and $(\mathcal{S}_N)_{N\in\mathbb{N}}$ configurations in $\mathbb{Z}^2$ with associated empirical measures $(\mu_N)_{N\in\mathbb{N}}$ weakly* converging to μ. Choose now as cover

$$Q_N := \bigcup_{x\in\mathcal{S}_N} \overline{N^{-1/2}q_1(x)}.$$

For the same reasons as in Section 5.2 follows that

$$\tilde{F}_N := \frac{1}{\sqrt{N}}(J_N(\mu_N) + 4N) = \mathcal{H}^1(\partial Q_N) = \int_{\partial Q_N} \tilde{\gamma}(\nu_{Q_N}(x))d\mathcal{H}^1(x). \tag{6.3}$$

The second equality follows analog to the triangular lattice. All segments of ∂Q_N are parallel to $\tilde{e}_1$ or $\tilde{e}_2$ and $\tilde{\gamma}$ take the value one for all vectors orthogonal to $\tilde{e}_1$ or $\tilde{e}_2$. For the first equality notice that if for $x \in \frac{1}{\sqrt{N}}\mathcal{S}_N$ a point $y \in \frac{1}{\sqrt{N}}\mathbb{Z}^2$, $y \notin \frac{1}{\sqrt{N}}\mathcal{S}_N$ exists with $\|x - y\| = \frac{1}{\sqrt{N}}$, then the segment $[x, y]$ intersects *exactly one* edge of the square $q_{N^{-1/2}}(x)$ at $x + \frac{1}{2}(y - x)$. On the other hand, there exists for every segment $[a, b] \subset \partial q_{N^{-1/2}}(z) \subset \partial Q_N$ *exactly one* $(x, y) \in \frac{1}{\sqrt{N}}\mathbb{Z}^2 \times \frac{1}{\sqrt{N}}\mathbb{Z}^2$ with the same properties such that $[x, y]$ intersects $[a, b]$. So the number of such segments in ∂Q_N is equal to number of such pairs (x, y). This establishes the first equation.

Now we want to repeat the compactness proof for the triangular configurations by applying them to square configurations. We define the normalized densities for Q_N

$$\tilde{d}'_N = \frac{1}{N}\sum_{x\in\mathcal{S}_N} \frac{\chi_{N^{-1/2}q_1(x)}}{\left|N^{-1/2}q_1(x)\right|} = \chi_{Q_N}.$$

We will see that $\int_\cdot \tilde{d}'_N d\lambda^2 \overset{*}{\rightharpoonup} \mu$, $\tilde{d}'_N \xrightarrow{L^1} \chi_E$ for $E \subset \mathbb{R}^2$, with $\lambda^2(E) = 1$ and $P(E, \mathbb{R}^2) < \infty$, thus proving $\mu = \tilde{\eta}_E$. Theorem 2.28 then establishes immediately the lower bound

$$\int_{\partial^* E} \tilde{\gamma}(\nu_E(x))d\mathcal{H}^1(x) \le \liminf_{N\to+\infty} \int_{\partial Q_N} \tilde{\gamma}(\nu_{Q_N}(x))d\mathcal{H}^1(x) = \liminf_{N\to+\infty} \frac{1}{\sqrt{N}}(J_N(\mu_N) + 4N).$$

The first convergence statement follows analog to Theorem 3.4 Step 2 (i), exactly like in Section 5.2. For proving the second we choose without loss of generality a bounded subsequence of $(\tilde{F}_N)_{N\in\mathbb{N}}$. Equation (6.3) proves that the perimeters of $(Q_N)_{N\in\mathbb{N}}$ are bounded. Because $\int_\cdot \tilde{d}'_N d\lambda^2$ has for all N mass one, it follows that $\tilde{d}'_N \xrightarrow{L^1} \chi_E$, for a set E of finite perimeter and volume one. We use here the same restriction argument with balls of arbitrary radius as in the proof for the hexagonal configurations. □

Upper bound. For proving the upper bound for the new potential, we have only to prove that the arguments in the first two steps of Section 5.3 can be adapted. For Step 3 is this obvious, because $\tilde{\gamma}$ is just like γ, even, positive, positively 1-homogeneous, convex, continuous and it applies $\tilde{\gamma}(x) = \tilde{\gamma}(x + \pi)$ for all $x \in [0, 2\pi/4)$. Thus the arguments in Step 3 can be adapted unchanged to the new surface energy functional and so we get the following convergence statement. For every set E with finite perimeter and

$\lambda^2(E) = 1$ exists a sequence of sets $(\tilde{P}_k)_{k\in\mathbb{N}}$ with polygonal boundary and volume one such that the convergences

$$\tilde{\eta}_{\tilde{P}_k} \overset{*}{\rightharpoonup} \tilde{\eta}_E \text{ and } \int_{\partial^* \tilde{P}_k} \tilde{\gamma}(\nu_{\tilde{P}_k}(x)) d\mathcal{H}^1(x) \to \int_{\partial^* E} \tilde{\gamma}(\nu_E(x)) d\mathcal{H}^1(x). \tag{6.4}$$

apply.

It remains to prove Step 1 and Step 2 in an analog way. We are beginning by choosing for an arbitrary $n \in \mathbb{N}$ a bounded set P_n with volume $1 + \beta_n$ and a polygonal boundary such that the verticies of ∂P_n are in $\frac{1}{n}\mathbb{Z}^2$. For the crystallized configurations $\mathcal{S}_{n;N}$ inside these scaled sets, i.e. $\mathcal{S}_{n;N} := \mathbb{Z}^2 \cap \sqrt{N} P_n$, it is clear that $\mu_{n,N} \overset{*}{\rightharpoonup} \int_\cdot \frac{1}{1+\beta_n} \chi_{P_n} d\lambda^2$ and we get

$$|M_{n,N} - N| \leq \left| M_{n,N} - \lambda^2 \left(\sqrt{N} P_n \right) \right| + |N + \beta_n N - N| \leq \tilde{\tilde{c}} \sqrt{N} \mathcal{H}^1(\partial P_n) + |\beta_n| \, N, \tag{6.5}$$

where $M_{n,N} := \#(\mathbb{Z}^2 \cap \sqrt{N} P_n)$ and $\tilde{\tilde{c}}$ a constant independent of n and N. The proof is basically identical to the one of (5.5). In this case we cover $\sqrt{N} P_n$ with squares $[0,1]^2$ such that every atom in $\mathcal{S}_{n;N}$ is the bottom left corner of such a square. The Lebesgue measure of the symmetric difference of $\sqrt{N} P_n$ and the cover can again be bounded by the Hausdorff measure of $\partial(\sqrt{N} P_n)$ times a constant, thus proving (6.5).

The same considerations as in Section 5.3 proves a result analog to (5.8)

$$\left| \frac{1}{\sqrt{N}} (J_M(\mu_{n,N}) + 4M) - \int_{\partial P_n} \tilde{\gamma}(\nu_{P_n}(x)) d\mathcal{H}^1(x) \right| \leq c \left(\beta_n + \frac{1}{\sqrt{N}} \right), \tag{6.6}$$

for a constant c. The arguments can be adapted with some insignificant changes. At first, it is obvious that we must choose φ from $(0, 2\pi/4)$ instead of $(0, 2\pi/6)$ and that the lines t are now defined by $\tilde{e}_2 - \tilde{e}_1$, i.e. $t := \{\lambda(\tilde{e}_2 - \tilde{e}_1) \mid \lambda \in \mathbb{R}\}$ and not $e_2 - e_1$ anymore. Accordingly, we assign to every atom a unit square, such that the atom is at the vertex a. (Same name-scheme as in Section 5.3). The second difference is the number of neighbors depending on the categorization of these squares. For the square configurations the atoms have in each case one neighbor less. So if an atom belongs to case one, it has two neighbors and not three and so on. The reason for this is that atoms can not interact along the direction $\tilde{e}_2 - \tilde{e}_1$ as it is possible in the triangular configurations along $e_2 - e_1$, due to $l^* \in (1, \sqrt{2})$. The third important difference is that we get

$$\frac{1}{l'} = \frac{1}{\sqrt{2}} \sin\left(\frac{\pi}{4} + \varphi \right) = \tilde{\gamma}(\nu_s)$$

as expression for l'. This takes into account that the distance between the lines t have changed. With these changes the geometric arguments can be adapted and this proves (6.6).

The next step is to use this for the approximation of the surface energy of an arbitrary polygon P. Let $P \subset \mathbb{R}^2$ be a polygonal set with volume one. Precisely as in Section 5.3 we can construct a sequence of polygonal sets $(P_n)_{n\in\mathbb{N}}$ with vertices in $\frac{1}{n}\mathbb{Z}^2$, volume $1+\beta_n$ and chose an appropriate sequence $(n(N))_{N\in\mathbb{N}}$ of natural numbers such that

$$\tilde{\mu}_N \overset{*}{\rightharpoonup} \int_\cdot \chi_P d\lambda^2 \text{ and } \frac{1}{\sqrt{N}} (I_M(\tilde{\mu}_N) + 4M) \to \int_{\partial P} \tilde{\gamma}(\nu_P(x)) d\mathcal{H}^1(x),$$

where $\tilde{\mu}_N := \mu_{n(N),N}$ and $M := M_{n(N),N}$. It is important to notice that this just works because $|M - N|/|N| \to 0$ holds again.

For this construction the same problem occurs as before, that in general we have $M \neq N$. The idea of a correction configuration with $|N - M|$ atoms and a disappearing surface term for $N \to \infty$ works also for this setting, due to (6.5). We use the same construction but this time we start with a half-open square

instead of a parallelogram. Set $K := \sqrt{|N-M|}$ and $\tilde{Q} := [0, \lfloor K \rfloor)^2$. We define again a configuration $\tilde{\tilde{\mathcal{S}}} := \mathbb{Z}^2 \cap \tilde{Q}$ with $(\lfloor K \rfloor)^2$ atoms and add atoms in the same way as for the parallelogram Q. Start in the top left corner of $\tilde{Q}$ and go along the upper and right edges until the configuration consists of $|N-M|$ atoms. Obviously is after adding the necessary atoms to $\tilde{\tilde{\mathcal{S}}}$

$$\#\partial\tilde{\tilde{\mathcal{S}}} \leq \mathcal{H}^1(\partial\tilde{Q}) = 4\lfloor K \rfloor = 4\left\lfloor \sqrt{|N-M|} \right\rfloor.$$

For $M < N$ we get analog to the triangular case immediately

$$\left| \tilde{J}_N(\mu_N) - \frac{1}{\sqrt{N}}(J_M(\tilde{\mu}_N) + 4M) \right| \leq \frac{4}{\sqrt{N}} \left(4 \left\lfloor \sqrt{|N-M|} \right\rfloor \right).$$

For $M > N$ the arguments are also identical. Obviously a constant $\tilde{c}$ exists, such that for all $q, \tilde{r} > 0$ with $q \leq \tilde{c}\tilde{r}$ the square $[0,q]^2$ fits after translation inside a ball with radius $\tilde{r}$. It is clear that a radius $r > 0$ exists such that a ball $B_r(y)$ is a subset of P. Then $|M-N|/|N| \to 0$ asserts that for all large enough N is $[0, \lceil K \rceil)^2 \subset B_{\sqrt{N}r}(y) \subset \sqrt{N}P$. This proves that the configuration $\tilde{\tilde{\mathcal{S}}}$ can be chosen as a subset of the bulk of $\tilde{\mathcal{S}}_N := \tilde{\mathcal{S}}_{n(N),N}$. This allows us to decompose $\tilde{\mathcal{S}}_N \setminus \tilde{\tilde{\mathcal{S}}}$ in the same way as in Section 5.3 and so is

$$\begin{aligned}\left| \tilde{J}_N(\mu_N) - \frac{1}{\sqrt{N}}(J_M(\tilde{\mu}_N) + 4M) \right| &\leq \frac{1}{\sqrt{N}} \left| -4 \underbrace{(\#B_n + \#T_a - \#B)}_{N-M} + \sum_{x \in T_a} R_{T_a}(x) + 4(N-M) \right| \\ &\leq 16\sqrt{\frac{|N-M|}{N}}\end{aligned}$$

and together we get

$$\left| \frac{1}{\sqrt{N}}(J_N(\mu_N) + 4N) - \frac{1}{\sqrt{N}}(J_M(\tilde{\mu}_N) + 4M) \right| \leq c\sqrt{\frac{|M-N|}{N}}.$$

Thus

$$\mu_N \overset{*}{\rightharpoonup} \tilde{\eta}_P \text{ and } \frac{1}{\sqrt{N}}(J_N(\mu_N) + 4N) \to \int_{\partial^* P} \tilde{\gamma}(\nu_P(x)) d\mathcal{H}^1(x). \tag{6.7}$$

Because Step 3 is, as discussed above, completely analog, expect for an other function modeling the interfacial energy (6.4) follows. A diagonalization argument applied to (6.4) and (6.7) proves the Γ-convergence of $\tilde{J}_N$ to J_∞ in $\mathcal{R}(\mathbb{R}^2)$ and thus Theorem 3.7.

□

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