

THE GEOMETRY OF OPTIMAL AND NEAR-OPTIMAL
RIESZ ENERGY CONFIGURATIONS

By

Justin Fitzpatrick

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Approved:

Professor Douglas P. Hardin

Professor Edward B. Saff

Professor Gieri Simonett

Professor James H. Dickerson

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This work is dedicated to my two mothers: to Mrs. Cynthia Fitzpatrick, who has suffered more physically and emotionally during my five years of graduate school than any woman ought to suffer in a lifetime; and to the Blessed Virgin Mary, whose help I constantly sought and whose help is truly perpetual.

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CHAPTER I

INTRODUCTION

The problem of placing a fixed number of electrons on the 2-sphere in such a way so that the total electrostatic energy is minimized has been of interest since at least 1904 and Thomson's article ([36]). This problem and subsequently posed associated problems are problems with wide-ranging applications including approximation theory, best-packing, viral morphology, and coding theory, to name just a few.

Given two electrons placed at x_1 and x_2 in \mathbb{R}^3 , the electrostatic potential energy between them is, up to a constant,

$$\frac{1}{|x_1 - x_2|}.$$

Furthermore, the total energy required to assemble a collection of N electrons at x_1, x_2, \dots, x_N in \mathbb{R}^3 is, up to the same constant,

$$\sum_{i=1}^N \sum_{j>i}^N \frac{1}{|x_i - x_j|}. \tag{1}$$

If the points x_1, x_2, \dots, x_N are now constrained to lie in some set A , then the question of what configuration of those points minimizes the quantity in (1) is called a minimal energy problem for the set A ; this is precisely Thomson's problem when $A = S^2 \subseteq \mathbb{R}^3$. Over a century after his posing of the problem, solutions to Thomson's problem are known only for $N = 2, 3, 4, 6, 12$, and more recently $N = 5$ (see ([38]), ([22]), ([1]), ([33])).

The difficulty of the minimal energy problem even for relatively small values of N has led to several different approaches that attempt to circumvent the computational

difficulties. The primary approach considered here is an asymptotic one: Given data about the growth of the total electrostatic energy as the number of electrons grows to infinity, what can be said about the minimal energy configurations themselves?

More generally, one can consider the problem of minimizing over all N -point configurations on a set A the quantity

$$\sum_{i=1}^N \sum_{j>i}^N k(x_i, x_j),$$

where k is a lower semicontinuous function on A called a **kernel**. Of particular interest in this paper is the kernel

$$k(x, y; s) := k_s(x, y) := \frac{1}{|x - y|^s}, \tag{2}$$

which is called the **Riesz kernel of exponent** s for $s > 0$. Notice that taking the s -th root of the **Riesz s -energy**

$$\sum_{i=1}^N \sum_{\substack{j=1 \\ j \neq i}}^N \frac{1}{|x_i - x_j|^s}$$

which is the energy associated to the Riesz kernel of exponent s , and then taking the limit as s goes to infinity leaves only the largest term in (2). In this sense the minimal energy problem approximates the best-packing problem as s approaches infinity.

Fejes-Toth showed in 1940 in ([17]) that the best-packing problem in the plane is solved by the hexagonal lattice; that is, the densest way to pack non-overlapping disks in the plane is to place them so that their centers form a hexagonal lattice. The **density** of a circle-packing indicates the fraction of space covered by the disks used in the packing; Fejes-Toth's result implies that the maximum packing density is $\frac{\pi}{\sqrt{12}}$. Given the solution in dimension two to the best packing problem and the above

remark about how the best-packing problem is, in that sense, approximated by the minimal energy problem, we seek to gain information about minimal Riesz s -energy configurations in subsets of the plane for large values of s ; more precisely, that they share many characteristics with the hexagonal lattice itself.

The following result of Gruber was motivational in our efforts to generate results about the geometry of minimal and near-minimal Riesz energy configurations. In particular, all of the results of Chapter 4 are in the same vein.

Theorem 10. ([19]) Let $S \subseteq \mathbb{R}^2$ be a finite point set and let $\delta > 0$. A point $p \in S$ is said to be the **center of a regular hexagon in S up to δ** if there are $\sigma > 0$, the **edge length** of the hexagon, and points p_1, \dots, p_6 in S so that

$$S \cap \{x : |x - p| \leq 1.1\sigma\} = \{p, p_1, \dots, p_6\}$$

$$|p - p_i|, |p_{i+1} - p_i| \leq (1 \pm \delta)\sigma, i = 1, \dots, 6,$$

where $(1 \pm \delta)\sigma$ means a quantity between $(1 - \delta)\sigma$ and $(1 + \delta)\sigma$. Now let H be a convex 3-, 4-, 5-, or 6-gon and $\varepsilon > 0$ sufficiently small. Then for all packings of H by m congruent disks of sufficiently small radius and density more than $\frac{\pi}{\sqrt{12}}(1 - \varepsilon)$, the following hold: in the set of centers of these circles, each center, with a set of less than $50\varepsilon^{1/3}m$ exceptions, is the center of a regular hexagon up to $500\varepsilon^{1/3}$. All these hexagons have the same edge length (in the above sense).

To study the geometry of point configurations in the plane, the **Voronoi diagram** associated to a point configuration is introduced. Stated simply, the Voronoi diagram is a collection of Voronoi cells, and a **Voronoi cell** associated to a point x in the configuration is the set of all points that are at least as close to x than to any other

point in the configuration. In the hexagonal lattice, for example, every Voronoi cell is a regular hexagon.

What now follows are the main results of this thesis. The results as stated here will be for minimal Riesz s -energy configurations ω_N^s on the unit square $[0, 1] \times [0, 1] \subseteq \mathbb{R}^2$; they are generalized somewhat later in the paper.

Theorem IV.1.1. Let $\delta(N) = \frac{2}{\sqrt{N\sqrt{12}}}$, $C > 6$ and $\gamma \in (0, 1)$. Then there is s_0 and $N_0 = N_0(s)$ such that for all $N > N_0$,

$$\frac{|A_{N,\gamma}^s|}{N} \leq C\gamma^s$$

for all $s > s_0$, where

$$A_{N,\gamma}^s = \{x \in \omega_N^s : r(x) < \gamma\delta(N)\}$$

and $r(x) = \min \{|x - y| : x \neq y \in \omega_N^s\}$.

Theorem IV.1.2. Let $\delta(N) = \frac{2}{\sqrt{N\sqrt{12}}}$. Fix $\gamma \in (0, 1)$ and $C > 6$. Let $B_{N,\gamma}$ denote the set of points whose Voronoi cell has an inradius of at least $\frac{\gamma\delta(N)}{2}$ but does not have exactly six sides. Then there is a positive constant D such that, for $N = N(s)$ and s sufficiently large,

$$\frac{|B_{N,\gamma}|}{N} \leq D \cdot \left(\frac{1}{\gamma^2} - 1 + C\gamma^s \right).$$

Theorem IV.1.3. Let $\gamma \in (0, 1)$, $\Gamma > 1$ be fixed, and let $D_{N,\gamma,\Gamma}$ denote those points not in $A_{N,\gamma}^s$ whose Voronoi cells are 6-sided and have area more than Γ/N . Then for any $C > 6$, there are $N = N(s)$ and s sufficiently large such that

$$\frac{|D_{N,\gamma,\Gamma}|}{N} \leq \frac{1 - \gamma^2(1 - C\gamma^s)}{\Gamma - \gamma^2}.$$

Given the Voronoi diagram associated to a minimal Riesz s -energy configuration for s sufficiently large, these results indicate that the fraction of Voronoi cells that are hexagonal with at least a certain inradius and at most a certain area is close to 1; in fact, as close to 1 as desired for correct choices of the parameters.

Later in Chapter 4, we go on to give the following improvement of Theorem IV.1.2:

Theorem IV.4.2. Let $C > 6$. Let $B_6 \subseteq \omega_N^s$ denote the set of points in the unit square whose Voronoi cell does not have six sides and does not meet the boundary of the unit square. Then for s sufficiently large, there is $N_0 = N_0(s)$ and a constant D such that for all $N > N_0$,

$$\frac{|B_6|}{N} \leq D \left(C^{\frac{2}{s+2}} - 1 \right).$$

Notice that there is no dependence here on the parameter γ .

Denote by $\mathcal{E}_s(A, N)$ the minimal N -point Riesz s -energy on the set A and by $\mathcal{H}_d(\cdot)$ d -dimensional Hausdorff measure normalized so that the measure of the unit cube in \mathbb{R}^d is 1. A result due to Hardin and Saff in ([20]) is that, for a large class of d -dimensional sets A (to be defined later) and for $s > d$,

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}_s(A, N)}{N^{1+\frac{s}{d}}} = \frac{C_{s,d}}{(\mathcal{H}_d(A))^{\frac{s}{d}}},$$

where $C_{s,d}$ is a constant that depends on s and d but not on the set A . This constant is of interest because it is related to the geometry of these minimal s -energy configurations; more will be discussed on this matter later. It was shown in ([3]) that, for all $d > 1$, $\lim_{s \rightarrow \infty} C_{s,d}^{1/s}$ exists and is given by

$$\lim_{s \rightarrow \infty} C_{s,d}^{1/s} = \frac{1}{2} \left(\frac{\Delta_d}{\beta_d} \right)^{\frac{1}{d}},$$

where Δ_d is the greatest sphere packing density in \mathbb{R}^d , and β_d is the measure of the unit ball in \mathbb{R}^d . By removing the need to take the s -th root, in Chapter 3 we will improve upon this result in the case $d = 2$:

Theorem III.2.4.

$$\lim_{s \rightarrow \infty} \frac{C_{s,2}}{\left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}} = 6. \quad (3)$$

One can understand here the 6 as reflecting the fact that most cells are 6-sided, and the $\left(\frac{\sqrt{3}}{2}\right)^{s/2}$ as corresponding to the area of a fundamental cell of the hexagonal lattice raised to the appropriate power $s/2$.

Establishing Theorem III.2.4 has been a goal of the author for some time, and crucial in its proof was the establishment of the two geometric theorems of Chapter 3. Given a convex M -gon P and an interior point p , let $\{r_i\}_{i=1}^M$ be the lengths of its altitudes drawn from p and $A(P)$ be its area. Let $a(n)$ be the area of the regular n -gon of inradius 1. We consider the quantity

$$F(P) := \left(\sum_{i=1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}}$$

Theorem III.1.4. Let $M \in \mathbb{N}$ be given and P be a convex M -gon. Then there is an $s_0 = s_0(M)$ so that for all $s > s_0$, $F(P) \geq Ma(M)^{\frac{s}{2}}$, which is the value of $F(P)$ when P is the regular M -gon and p is the center.

Theorem III.1.6. For any convex M -gon P with interior point p and any $s \geq 2$, we have

$$F(P) \geq \min_{\nu \leq M} \nu a(\nu)^{\frac{s}{2}}.$$

Furthermore, this inequality is strict unless $F(P) = Ma(M)^{\frac{s}{2}}$.

For an M -gon P , now let $\Delta_s(P) := F(P) - Ma(M)^{\frac{s}{2}}$, so that Δ_s gives a measure of difference between the polygon P and the regular M -gon. Then in Chapter 4 we show the following:

Theorem IV.4.4. Let $\{\omega_N^s\}$ be a sequence of s -optimal configurations on the unit square for $s > 2$. Then

$$\limsup_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right) \leq (\zeta_\Lambda(s) - 6)^{\frac{2}{s+2}} \cdot a(6)^{\frac{s}{s+2}}$$

where N' denotes a natural number less than N but that satisfies

$$\lim_{N \rightarrow \infty} \frac{N'}{N} = 1.$$

Further, Λ denotes the hexagonal lattice, and ζ_Λ the associated Epstein zeta function:

$$\zeta_\Lambda(s) = \sum_{\substack{x \in \Lambda \\ x \neq 0}} \frac{1}{|x|^s}.$$

These results indicate the significance of the regular figures in the minimal energy problem, as will be discussed at length in what follows.

The organization of the remainder of this thesis is as follows: In Chapter 2, some background information will be given about minimal energy problems and theorems in plane geometry that are useful in gaining information about minimal energy configurations on two-dimensional sets. In Chapter 3, we present two geometric theorems that give insight into the local structure of minimal energy configurations. In Chapter 4, we demonstrate some new results detailing constraints on the geometry of optimal and near-optimal configurations.

CHAPTER II

BACKGROUND

II.1 The Riesz Kernel

Let $A \subseteq \mathbb{R}^n$. For $s > 0$, the **Riesz kernel of exponent s** , $k_s(x, y) : A \times A \rightarrow \mathbb{R}$, is defined to be

$$k_s(x, y) = \frac{1}{|x - y|^s}.$$

(We define it to be ∞ in the case $x = y$.) Sometimes for simplicity any such function $k_s(x, y)$, $s > 0$ is simply referred to as the **Riesz kernel**. For an infinite compact set $A \subseteq \mathbb{R}^n$, define the **Riesz s -energy** of a configuration of N points $\omega_N = \{x_1, x_2, \dots, x_N\} \subseteq A$ to be

$$E_s(\omega_N) = \sum_{i=1}^N \sum_{j \neq i=1}^N \frac{1}{|x_i - x_j|^s}. \quad (4)$$

(Notice here that the definition of energy differs by a factor of two from the definition given in the introduction.) For a fixed N , the minimal energy problem on A associated to this kernel is the problem of finding an N -point configuration $\omega_N^s \subseteq A$ that minimizes $E_s(\omega_N)$ as defined above over all N -point configurations $\omega_N \subseteq A$. Recall that when $s = 1$, $n = 3$, and $A = S^2$, this is simply Thomson's problem.

What will be shown first is that, for any infinite compact set A , there is indeed a configuration that minimizes the energy defined in (4).

Proposition II.1.1. Let $A \subseteq \mathbb{R}^n$ be an infinite compact set, $s > 0$ be given, and N be any natural number. Then there is a configuration $\omega_N^s \subseteq A$ that achieves the minimum for the quantity $\{E_s(\omega_N) : \omega_N \subseteq A, |\omega_N| = N\}$.

Proof. Let ω_N be any configuration of N distinct points on A . Since $E_s(\omega_N)$ is finite, choose $\varepsilon > 0$ such that $1/\varepsilon^s > E_s(\omega_N)$. For this value of ε , now set

$$k_s^\varepsilon(x, y) = \begin{cases} \frac{1}{|x-y|^s}, & |x-y| \geq \varepsilon \\ \varepsilon^{-s}, & |x-y| < \varepsilon. \end{cases} \quad (5)$$

Since $E_s(\omega_N) < 1/\varepsilon^s$, we have by the definition of the Riesz kernel that for any configuration ω'_N of energy not more than $E_s(\omega_N)$, all of the points in ω'_N are separated by at least ε . Hence, denoting by E_s^ε the energy associated to the truncated Riesz kernel defined in (5), we have that

$$E_s^\varepsilon(\omega'_N) = E_s(\omega'_N) \quad (6)$$

for all configurations ω'_N of energy not more than $E_s(\omega_N)$. Notice now that the kernel k_s^ε is continuous, and so by the compactness of A , E_s^ε attains a minimum for some N -point configuration, which shall be called ω_N^s . (6) now gives the theorem. □

(The previous result holds in more generality, with the same proof if the energy is defined with any lower semicontinuous kernel. In the proof the lower semicontinuity of the Riesz kernel was used explicitly.)

For a given value of s , configurations ω_N^s that give this minimum will be called **s -optimal configurations**. Notice that s -optimal configurations need not be unique;

for example, when $A = S^1$, if ω_N^s is any s -optimal configuration, then any rotation of ω_N^s is also s -optimal. With the result of Proposition II.1.1, now define

$$\mathcal{E}_s(A, N) = \min \{E_s(\omega_N) : \omega_N \subseteq A, |\omega_N| = N\}.$$

Given $s > 0$ and A , the questions of finding s -optimal configurations ω_N^s on A and $\mathcal{E}_s(A, N)$ quickly become intractable even for modest values of N . This is due to the facts that the system of equations defining this minimum is intractable even when N is small; there is strong evidence that there are many local minima for the energy that are not global minima, and according to this evidence the number of local minima increases exponentially with N . (To view some of this evidence see e.g. ([5]).)

An approach that has generated recent interest is to consider the asymptotics of the energy $\mathcal{E}_s(A, N)$ and the asymptotic distribution of s -optimal configurations ω_N^s . The asymptotic distribution of such configurations depends highly on the value of s , as we will show in the following sections.

II.2 The Continuous Energy Minimization Problem

Following ([12]), a Borel measure μ on \mathbb{R}^n is said to be a **Radon measure** if $\mu(K)$ is finite for every compact set $K \subseteq \mathbb{R}^n$. An equivalent definition of a Radon measure (see [15]) is that the Borel measure must be inner and outer regular; that is, for every measurable set A ,

$$\mu(A) = \sup \{\mu(K) : K \subseteq A \text{ is compact}\} = \inf \{\mu(O) : O \supseteq A \text{ is open}\}.$$

Let $A \subseteq \mathbb{R}^n$ be a compact set of positive d -dimensional Hausdorff measure, and let

μ be a Radon probability measure on A ; that is, a positive Radon measure satisfying $\mu(A) = 1$. For $s > 0$, we define the **Riesz s -energy** I_s of a probability measure μ supported on A :

$$I_s(\mu) := \int_A \int_A \frac{1}{|x - y|^s} d\mu(x) d\mu(y). \quad (7)$$

Similar to the question of minimizing the discrete Riesz s -energy posed in the previous section is the question of minimizing the continuous Riesz s -energy; that is, the question of finding a probability measure μ on a given compact set A that minimizes the quantity in (7) over all probability measures on A . Intuitively this is thought of as finding the continuous distribution of a fixed amount of charge that minimizes the total potential energy on a conductor rather than finding the locations of point charges that minimize this energy.

As before, it requires verification that the problem of finding an energy-minimizing measure does have a solution. For $s \in (0, d)$, it is a consequence of Frostman's Lemma and the fact that the Riesz kernel is positive definite that there is a measure that gives a finite minimum for (7). For more details, the reader is referred to ([24]). Therein it is further shown that such a minimizing measure is unique. In this case, the minimizing measure $\mu_{s,A}$ is referred to as the **equilibrium measure** on the set A and its energy $I_s(\mu_{s,A})$ is called the **Wiener energy** of A . The quantity

$$C_s(A) = \frac{1}{I_s(\mu_{s,A})}$$

is called the **s -capacity** of A and has been the subject of considerable study. Loosely speaking, a unit charge will be able to be distributed more sparsely over a larger set, and so such a set will generally have low Wiener energy and high s -capacity. For more details the reader is again referred to ([24]) and also ([35]). Remarks on the case $s \geq d$ will be made in a subsequent section.

For $s \in (0, d)$, define now the s -potential of a probability measure μ at a point $x \in A$ to be

$$U_s^\mu(x) = \int_A \frac{1}{|x - y|^s} d\mu(y).$$

It will also be said that a property holds **(s)-approximately everywhere** on A if the set of points where the property does not hold contains no compact subsets of positive s -capacity.

A result that merits demonstration at this time is one about the potential of the equilibrium measure. As its definition suggests, the equilibrium measure can be thought of as a static distribution of charge; that is, the charge distribution that admits no difference in electrostatic potential from one location to another, so that potential has gradient zero, implying that the location of the charge remains fixed. This intuition is confirmed by the following:

Proposition II.2.1. ([18]) Let $A \subseteq \mathbb{R}^n$ be compact, and $\mathcal{H}_d(A) > 0$. For $s \in (0, d)$, let $\mu_{s,A}$ be the equilibrium measure on A . Then

- $U_s^{\mu_{s,A}} \geq I_s(\mu_{s,A})$ approximately everywhere on A ,
- $U_s^{\mu_{s,A}} \leq I_s(\mu_{s,A})$ everywhere on the support of $\mu_{s,A}$, and
- $U_s^{\mu_{s,A}} = I_s(\mu_{s,A})$ $\mu_{s,A}$ -almost everywhere.

Before proving this proposition, we introduce a Hilbert space structure on the space of probability measures on A . Given two probability measures μ and ν on A , define the following bilinear form:

$$\langle \mu, \nu \rangle = \int_A \int_A \frac{1}{|x - y|^s} d\mu(x) d\nu(y).$$

This bilinear form defines an inner product; for more details, see ([24]). This inner product induces a norm on the space of probability measures in the usual way:

$$\|\mu\|^2 = \langle \mu, \mu \rangle = \int_A \int_A \frac{1}{|x-y|^s} d\mu(x) d\mu(y).$$

It is shown in ([24]) that the space of probability measures is topologically complete with respect to this norm. This is what will be necessary to prove Proposition II.2.1.

Proof of Proposition II.2.1. By Frostman's Lemma, $I_s(\mu_{s,A})$ is finite. Let ν be another probability measure with finite energy, and let $a \in [0, 1]$. Then $\rho_a = a\mu_{s,A} + (1-a)\nu$ is a probability measure, and since $\mu_{s,A}$ is the equilibrium measure, it follows that

$$\|\mu_{s,A}\|^2 \leq \|\rho_a\|^2 = a^2\|\mu_{s,A}\|^2 + 2a(1-a)\langle \mu_{s,A}, \nu \rangle + (1-a)^2\|\nu\|^2,$$

and so

$$\|\mu_{s,A}\|^2 = \lim_{a \uparrow 1} \frac{(1-a^2)\|\mu_{s,A}\|^2 - (1-a)^2\|\nu\|^2}{2a - 2a^2} \leq \langle \mu_{s,A}, \nu \rangle. \quad (8)$$

As $\nu(A) = 1$, $\|\mu_{s,A}\|^2 \cdot \nu(A) \leq \langle \mu_{s,A}, \nu \rangle$ for all probability measures ν . Let now $N = \{x \in A : U_s^{\mu_{s,A}}(x) < \|\mu_{s,A}\|^2\}$. Suppose that for some probability measure ν of finite energy that $\nu(N) > 0$. Then since ν is a Radon measure, there is a compact set $K \subseteq N$ with $\nu(K) > 0$. Thus

$$\int_K U_s^{\mu_{s,A}} d\nu < \|\mu_{s,A}\|^2 \cdot \nu(K),$$

which together with (8) implies that ν has infinite energy. This proves the first item in Proposition II.2.1. Letting $\nu = \mu_{s,A}$ in the above argument shows in particular that

$$\mu_{s,A}([U_s^{\mu_{s,A}} < \|\mu_{s,A}\|^2]) = 0.$$

From here it follows that

$$\|\mu_{s,A}\|^2 = \int_{[U_s^{\mu_{s,A}} = \|\mu_{s,A}\|^2]} U_s^{\mu_{s,A}} d\mu_{s,A} + \int_{[U_s^{\mu_{s,A}} > \|\mu_{s,A}\|^2]} U_s^{\mu_{s,A}} d\mu_{s,A}$$

whence $\mu_{s,A}([U_s^{\mu_{s,A}} > \|\mu_{s,A}\|^2]) = 0$. Since $[U_s^{\mu_{s,A}} > \|\mu_{s,A}\|^2]$ is open, it is disjoint from the support of $\mu_{s,A}$, proving the second item of Proposition II.2.1. The third item follows immediately from the first two. □

II.3 Linking the Discrete and Continuous Problems

One can view the discrete problem as a special case of the continuous problem by considering the measure placing a mass of $\frac{1}{N}$ at each point in an N -point configuration ω_N . The question of relating solutions to the continuous and discrete minimum energy problems is a natural one and is the aim of this section.

Let $A \subseteq \mathbb{R}^p$ be compact. For a point $x \in A$, define the probability measure

$$\delta_x(A) = \begin{cases} 1, & x \in A \\ 0, & x \notin A; \end{cases}$$

and for a configuration of points $\omega_N \subseteq A$, define the probability measure

$$\delta_{\omega_N} = \frac{1}{N} \sum_{x \in \omega_N} \delta_x.$$

The following result and proof can be found in e.g. ([24]):

Proposition II.3.1. Let $A \subseteq \mathbb{R}^p$ be a set of positive \mathcal{H}_d -measure and let $s \in (0, d)$. Let $\{\omega_N^s\}$ be a sequence of s -optimal N -point configurations on A for $N \geq 2$. Then

$$\delta_{\omega_N^s} \xrightarrow{*} \mu_{s,A},$$

and

$$\frac{\mathcal{E}_s(A, N)}{N^2} \rightarrow I_s(\mu_{s,A})$$

as $N \rightarrow \infty$.

Proof. Let $\omega_N^s = \{x_{i,N}\}_{i=1}^N$. We will show that the quantity

$$\frac{2}{N(N-1)} E_s(\omega_N^s) \tag{9}$$

is increasing with N . Notice that

$$\sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} = \frac{1}{N-2} \sum_{k=1}^N \sum_{\substack{i < j \\ i \neq k, j \neq k}} \frac{1}{|x_{i,N} - x_{j,N}|^s}.$$

For each k , the inner sum above is the energy associated to an $(N-1)$ -point configuration on A . Therefore, the minimality of $E_s(\omega_{N-1}^s)$ gives

$$\sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} \geq \frac{N}{N-2} \sum_{i < j} \frac{1}{|x_{i,N-1} - x_{j,N-1}|^s}.$$

Multiplying on both sides of the above inequality by $\frac{2}{N(N-1)}$ gives

$$\frac{2}{N(N-1)} \sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} \geq \frac{2}{(N-1)(N-2)} \sum_{i < j} \frac{1}{|x_{i,N-1} - x_{j,N-1}|^s},$$

which establishes that the quantity in (9) is increasing with N . Therefore the limit

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}_s(A, N)}{N^2}$$

exists as an extended real number.

Now let $\{y_i\}_{i=1}^N$ be an arbitrary configuration of N points on A . Then again by the minimality of $E_s(\omega_N^s)$ we have

$$\sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} \leq \sum_{i < j} \frac{1}{|y_i - y_j|^s}.$$

Let μ be a probability measure on A . Integrating both sides with respect to $d\mu(y_1) \dots d\mu(y_n)$ gives

$$\sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} \leq \sum_{i < j} \int_A \int_A \frac{1}{|y_i - y_j|^s} d\mu(y_i) d\mu(y_j),$$

since only the terms containing y_i or y_j are affected by integration with respect to $d\mu(y_i)$ and $d\mu(y_j)$. Notice that each double integral in the sum above is the same, whence

$$\sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} \leq \frac{N(N-1)}{2} \int_A \int_A \frac{1}{|y_a - y_b|^s} d\mu(y_a) d\mu(y_b).$$

In particular, choosing μ to be the equilibrium measure $\mu_{s,A}$ and letting N tend to infinity gives

$$\lim_{N \rightarrow \infty} \frac{2}{N(N-1)} \sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} \leq \int_A \int_A \frac{1}{|y_a - y_b|^s} d\mu_{s,A}(y_a) d\mu_{s,A}(y_b). \quad (10)$$

Now fix $\varepsilon > 0$ and consider

$$\int_A \int_A k_s^\varepsilon(x, y) d\delta_{\omega_N^s}(x) d\delta_{\omega_N^s}(y).$$

Notice that, for ε sufficiently small, nonzero terms arising from distinct points in the integral above are bounded above by ε^{-s} , and terms arising from the same points give a value of ε^{-s} . Therefore, we have

$$\begin{aligned} \int_A \int_A k_s^\varepsilon(x, y) d\delta_{\omega_N^s}(x) d\delta_{\omega_N^s}(y) &= \frac{1}{N^2} \sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} + \frac{\varepsilon^{-s}}{N} \\ &\leq \frac{2}{N(N-1)} \sum_{i < j} \frac{1}{|x_{i,N} - x_{j,N}|^s} + \frac{\varepsilon^{-s}}{N}. \end{aligned}$$

It is known (see e.g. ([24])) that the space of probability measures forms a weak-star compact subspace of the space of all Radon measures on A . Therefore, we can choose a weak-star cluster point ν of $\{\delta_{\omega_N^s}\}$, and a subsequence of the natural numbers $\{N_i\}$ so that $\delta_{\omega_{N_i}^s} \xrightarrow{*} \nu$ as $i \rightarrow \infty$. Letting N_i tend to infinity and using (10) gives

$$\int_A \int_A k_s^\varepsilon(x, y) d\nu(x) d\nu(y) \leq \int_A \int_A \frac{1}{|y_a - y_b|^s} d\mu_{s,A}(y_a) d\mu_{s,A}(y_b).$$

Now let ε decrease to 0. Since the Riesz kernel is integrable for $s < d$, we have

$$I_s(\nu) \leq I_s(\mu_{s,A}),$$

and the uniqueness of the equilibrium measure now gives the result. \square

The previous proposition holds in greater generality for other kernels that have a unique equilibrium measure, optimal discrete configurations, and can be approximated by continuous functions; for more details see ([7]), ([14]), and ([18]).

II.4 The Case $s > d$

In the previous section it was seen how the continuous minimal energy problem can provide insight into the asymptotics of the discrete minimal energy problem. It was critical for this analysis that the exponent s of the Riesz kernel was less than the Hausdorff dimension d of the set on which the minimal energy problem is being considered; indeed, when $s \geq d$, the continuous minimal energy problem does not make sense in that the s -energy of any probability measure on a set of Hausdorff dimension d is infinite. What follows is a proof of this fact for sets with finite d -dimensional Hausdorff measure.

Theorem II.4.1 (Theorem 8.7 in ([26])). If $\mathcal{H}_s(A) < \infty$, then $I_s(\mu) = \infty$ for all probability measures μ supported on A .

Proof. The proof is by contradiction. Suppose that for a probability measure μ supported on a set A of Hausdorff dimension d , $\mathcal{H}_s(A) < \infty$ and $I_s(\mu) < \infty$. (Recall that, by definition of the Hausdorff measure \mathcal{H}_s , when $s > d$, $\mathcal{H}_s(A) = 0$.) Since

$$I_s(\mu) = \int \int \frac{1}{|x - y|^s} d\mu(x) d\mu(y) < \infty,$$

Tonelli's theorem implies that the inner integral is finite for μ -a.a. x in A . It follows from the Lebesgue Differentiation Theorem (see e.g. p. 38 of [26]) that, for these x ,

$$\lim_{r \downarrow 0} \int_{B(x,r)} \frac{1}{|x - y|^s} d\mu(y) = 0.$$

Now apply Egorov's Theorem to select $A_0 \subseteq A$ such that $\mu(A_0) > 1/2$ and the above limit is uniform on the set A_0 . Fix $\varepsilon > 0$. Then by the uniformity of the above limit we may find r_0 such that, for all $x \in A_0$ and $r < r_0$, it follows that

$$\mu(B(x, r)) \cdot r^{-s} \leq \int_{B(x, r)} \frac{1}{|x - y|^s} d\mu(y) < \varepsilon,$$

whence $\mu(B(x, r)) < \varepsilon r^s$. Using the construction of the Hausdorff measure, there is a collection of sets $\{U_i\}_{i=1}^{\infty}$ satisfying:

$$(a) \quad A_0 \subseteq \bigcup_{i=1}^{\infty} U_i,$$

$$(b) \quad A_0 \cap U_i \neq \emptyset \text{ for all } i,$$

$$(c) \quad \text{diam } U_i < r_0,$$

$$(d) \quad \sum_{i=1}^{\infty} (\text{diam } U_i)^s < \mathcal{H}_s(A_0) + 1.$$

Now select from each U_i a point x_i lying also in A_0 , and let $r_i = \text{diam } U_i$. Then one has

$$\frac{1}{2} < \mu(A_0) \leq \varepsilon \sum_{i=1}^{\infty} r_i^s < \varepsilon (\mathcal{H}_s(A_0) + 1).$$

As ε is arbitrary, it follows that $\mathcal{H}_s(A_0)$ is infinite, contradicting the assumption. □

Since it follows from this result (and Proposition II.3.1) that

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}_s(A, N)}{N^2} = \infty,$$

it follows that the order of growth of the N -point minimal energy is larger than N^2 when s is larger than the Hausdorff dimension of A . Intuitively one can think of this as the Riesz kernel having an increasingly local character as s increases (a remark along these lines is made in the introduction). Alternatively, one can also view this as an extension of the non-integrability of

$$\int_{B(0,1)} \frac{1}{|x|^s} dx,$$

where dx denotes Lebesgue measure in \mathbb{R}^d . For this reason the case $s \geq d$ is often referred to as the hypersingular case, while the case $s < d$ is referred to as the potential theory case.

Results for the asymptotics of the energy in the case $s > d$ came later. These results are for a class of sets that are defined below. For more information on sets of this type, the reader is referred to ([13]).

Definition II.4.2. A set A is said to be a **d -rectifiable manifold** if it can be written

$$A = \bigcup_{i=1}^n \phi_i(K_i)$$

where K_i is a d -dimensional compact set and ϕ_i is a bi-Lipschitz function on an open set $G_i \supseteq K_i$.

Definition II.4.3. A set A is said to be a **d -rectifiable set** if it is a Lipschitz image of a bounded set in \mathbb{R}^d .

In ([20]), Hardin and Saff were able to show the following:

Theorem II.4.4. ([20], Theorem 2.4) If $A \subseteq \mathbb{R}^p$ is a d -rectifiable manifold that is also a compact subset of a d -dimensional C^1 -manifold, then

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}_d(A, N)}{N^2 \log N} = \frac{\mathcal{H}_d(\mathcal{B}^d)}{\mathcal{H}_d(A)}, \quad (11)$$

where \mathcal{B}^d is the closed unit ball in \mathbb{R}^d . Furthermore, if $\mathcal{H}_d(A) > 0$, then for any sequence $\{\omega_N^d\}$ of configurations on A satisfying (11), we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{x \in \omega_N^d} \delta_x = \frac{\mathcal{H}_d(\cdot)|_A}{\mathcal{H}_d(A)},$$

where the convergence above is understood in the weak-star topology of measures; that is, for every continuous function f on A ,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{x \in \omega_N^d} f(x) = \frac{1}{\mathcal{H}_d(A)} \int_A f(x) d\mathcal{H}_d(x).$$

Theorem II.4.5. ([20], Theorem 2.4) If $A \subseteq \mathbb{R}^p$ is a d -rectifiable manifold, then for $s > d$,

$$\lim_{N \rightarrow \infty} \frac{\mathcal{E}_s(A, N)}{N^{1+\frac{s}{d}}} = \frac{C_{s,d}}{(\mathcal{H}_d(A))^{\frac{s}{d}}}, \quad (12)$$

where $C_{s,d}$ is a constant depending on s and d but not on the set A . Furthermore, for any sequence $\{\omega_N^s\}$ of configurations on A satisfying (12), we have

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{x \in \omega_N^s} \delta_x = \frac{\mathcal{H}_d(\cdot)|_A}{\mathcal{H}_d(A)}, \quad (13)$$

and the convergence is again understood in the weak-star topology of measures.

These results establish the order of growth of the energy for $s \geq d$ and further establish that configurations that are asymptotically optimal (in the sense that they satisfy (11) or (12)) are also asymptotically uniformly distributed on the set A , a

condition that is not generally satisfied in the potential theory case. The fact that Riesz s -optimal configurations are asymptotically uniformly distributed in the hyper-singular case will be used frequently in later chapters.

In ([3]), Borodachov, Hardin, and Saff were able to generalize Theorem II.4.5 to d -rectifiable sets. Another result of ([20]) that is noteworthy is the following:

Theorem II.4.6. ([20], Theorem 2.3) Let $A \subseteq \mathbb{R}^d$ be an infinite compact set, and let $s \geq d$, $N \geq 2$. Let ω_N^s an s -optimal configuration on A . Then there is a positive constant $C = C(A, s, d)$ so that

$$\min_{x_i \neq x_j \in \omega_N^s} \{|x_i - x_j|\} \geq \begin{cases} CN^{\frac{-1}{d}}, & s > d \\ C(N \log N)^{\frac{-1}{d}}, & s = d. \end{cases}$$

It should be noted that it is believed that the $\log N$ term above is not necessary in the case $s = d$. These separation results will be compared to remarks about circle-packing in section II.6.

Other cases where s is non-positive are also worth mentioning. Included among these is the case $s < 0$, in which one considers a maximization problem. Results in this case were obtained by Björck in ([2]). The case “ $s=0$ ” is not the Riesz kernel with exponent 0, but rather the Riesz kernel is replaced by the kernel $k_0(x, y) = -\log|x - y|$. The techniques of potential theory apply in this case; a standard text containing results is ([35]). Moreover, results for complex s were obtained recently by Brauchart, Hardin, and Saff; see ([4]) for more details.

II.5 Lattice Configurations

The increasingly local character of the Riesz kernel of exponent s together with the local homogeneity of lattice configurations makes lattice configurations natural candi-

dates to consider when searching for s -optimal configurations. Here an n -dimensional lattice L in \mathbb{R}^n will be defined to be

$$L = \left\{ \sum_{i=1}^n c_i v_i : c_i \in \mathbb{Z} \right\}, \quad (14)$$

where $\{v_i\}$ is a collection of n linearly independent unit vectors in \mathbb{R}^n , called the basis vectors of the lattice. Intersecting such a lattice with a compact set A on which a minimal energy problem is to be considered is natural, and scaling the lattice allows one to consider configurations with an increasing number of points and hence asymptotics. This matter will be discussed in greater detail in Chapter 3.

The question of what lattice configuration of points minimizes a certain energy is an important one and has been studied extensively. Important in such studies are the Epstein zeta function associated to a lattice:

$$\zeta_L(s) = \sum_{\substack{x \in L \\ x \neq 0}} \frac{1}{|x|^s}$$

and the theta function associated to a lattice:

$$\theta_L(s) = \sum_{\substack{x \in L \\ x \neq 0}} e^{-2\pi s|x|}.$$

Cassels ([6]) and Rankin ([31]) gave partial results about minimizing the Epstein zeta function over all two-dimensional lattices subject to the constraint that the fundamental cell have area 1. Here the fundamental cell of a lattice L is defined to be the closed convex hull of

$$\left\{ \sum_{i=1}^n c_i v_i : c_i = 0 \text{ or } 1 \right\},$$

where again v_i denotes a basis vector of the lattice.

Montgomery observed in ([27]) that if $\xi_L(s) = \zeta_L(s)\Gamma(s)(2\pi)^{-s}$, then

$$\xi_L(s) = \frac{1}{s-1} + \frac{1}{s} + \int_1^\infty (\theta_L(\alpha) - 1)(\alpha^s + \alpha^{1-s})d\alpha,$$

which provides a link between solving the problem of finding the minimal lattice for theta functions and for zeta functions. Using this approach, in ([27]) he was able to show that the hexagonal lattice in \mathbb{R}^2 , which has basis vectors $(1, 0)$ and $(\frac{1}{2}, \frac{\sqrt{3}}{2})$, minimizes the theta function and the zeta function over all lattices subject to the same constraint on the fundamental cell for all real $s > 0$.

In ([9]), Cohn and Kumar generalized the problem slightly and sought to find periodic point configurations (unions of finitely many translates of a lattice) that are “universally optimal,” where they define universally optimal in the following way: Suppose we are given a function

$$f := f(|x - y|^2) : (0, \infty) \rightarrow \mathbb{R},$$

called the potential function, which is completely monotone; that is, the function is positive, decreasing, and its subsequent derivatives alternate signs (and are all defined). Then a periodic point configuration \mathcal{P} is called universally optimal if it minimizes

$$\sum_{\substack{x, y \in \mathcal{P} \\ x \neq y}} f(|x - y|^2)$$

for all completely monotone functions f . Numerical evidence found in ([8]), and their own work in ([9]) cause Cohn and Kumar to conjecture that the hexagonal lattice is universally optimal in \mathbb{R}^2 , that the E_8 root lattice is universally optimal in \mathbb{R}^8 ,

and that the Leech lattice is universally optimal \mathbb{R}^{24} . (For more details on these second two lattices, the reader is referred to ([8]) and ([10]), respectively.) Sarnak and Strombergsson were able to show in ([34]) that these lattices are local minima for energy (as defined by Cohn and Kumar) amongst lattice configurations, and recent work by Coulangeon and Schürmann in ([11]) shows that these lattices are indeed local minima for this energy for more general perturbations of the lattice. The numerical evidence in ([8]) seems to indicate that in dimensions other than 2, 8, and 24, there are no universally optimal configurations; Cohn and Kumar remark in ([9]) that there are certainly no universally optimal configurations in dimensions 3, 5, 6, and 7.

II.6 Voronoi Diagrams

As mentioned earlier, because the discrete minimum energy problem is so difficult to solve, relatively little is known about the geometric structure of s -optimal configurations. This section introduces the Voronoi diagram associated to an N -point configuration, after which a few facts that shall be used in the following chapters are demonstrated in order to give some restrictions on the Voronoi diagram of an s -optimal N -point configuration.

First formally define the Voronoi cells and Voronoi diagram associated to any N -point configuration in \mathbb{R}^2 :

Definition II.6.1. Let $\omega_N = \{x_1, x_2, \dots, x_n\}$ be a collection of N points in \mathbb{R}^2 . Then for any $i = 1, 2, \dots, n$, the **Voronoi cell** associated to x_i is given by

$$V(x_i) = \bigcap_{1 \leq j \neq i \leq n} \{x \in \mathbb{R}^2 : |x - x_i| \leq |x - x_j|\} \quad (15)$$

The points x_i are called the **centers** of their respective Voronoi cells. Each set in the intersection in (15) is the half-space (containing x_i) whose boundary is the

perpendicular bisector of the segment connecting x_i to x_j . Since there are finitely many points in the configuration, and each Voronoi cell is an intersection of half-spaces, one readily sees that $V(x_i)$ is a convex polygon containing x_i . If two Voronoi cells share an edge, then the centers of those cells are said to be **nearest neighbors**.

Definition II.6.2. With ω_N and $\{V(x_i) : 1 \leq i \leq n\}$ defined as in the previous definition, the **Voronoi diagram** associated to ω_N is given by

$$\mathcal{V}(\omega_N) = \{V(x_1), V(x_2), \dots, V(x_n)\}.$$

For a compact subset $A \subseteq \mathbb{R}^2$, the Voronoi diagram on A associated to $\omega_N \subseteq A$ is simply

$$\mathcal{V}(\omega_N) \cap A.$$

It is a standard fact that the Voronoi diagram is the dual graph of the Delaunay triangulation. For more details on Voronoi diagrams, the reader is referred to ([37]).

The following is a simplified version of a theorem found in the text of Fejes-Toth ([16]):

Theorem II.6.3. ([16]) Let H denote a convex polygon of no more than 6 sides. Then, given $r > 0$, the number N of discs of radius r that can be placed without overlapping into H satisfies the inequality

$$N \leq \frac{\text{Area}(H)}{\text{Area}(h)},$$

where h is a regular hexagon circumscribed about the disc of radius r .

The proof of Theorem II.6.3 rests on a pair of lemmas, which will be stated shortly. First, recall that a real-valued function $f(x)$ defined on an interval I is said to be **convex** if, for all $t \in [0, 1]$ and all $x, y \in I$,

$$f((1-t)x + ty) \leq (1-t)f(x) + tf(y). \quad (16)$$

Graphically, we view this as follows: Given any two points $(x, f(x))$, $(y, f(y))$ on the graph of f , every point on the graph of f whose abscissa lies between x and y lies below (or possibly on) the segment connecting $(x, f(x))$ to $(y, f(y))$. When the inequality in (16) is strict, the function f is said to be **strictly convex**. A sufficient condition for a function to be (strictly) convex on an interval is for the second derivative to be non-negative (positive) on that interval.

A useful fact about convex functions of which we will make use is the following:

Jensen's Inequality (Special Case). Suppose that $f : I \rightarrow \mathbb{R}$ is a convex function on an interval I . Then for any x_1, x_2, \dots, x_n in I ,

$$\sum_{i=1}^n \frac{1}{n} f(x_i) \geq f\left(\frac{\sum_{i=1}^n x_i}{n}\right). \quad (17)$$

The **inradius** of a polygon is the radius of the largest circle that can be inscribed in that polygon. It is a simple exercise in geometry to show that the area of a regular n -gon of inradius 1 is given by

$$a(n) = n \cdot \tan(\pi/n).$$

It is known (see [16]) that the n -gon of minimal area with inradius 1 is the regular n -gon circumscribed about a circle of radius 1. This fact will be useful in what follows.

Lemma II.6.4. Let $a(x) = x \cdot \tan(\pi/x)$. Then $a(x)$ is strictly convex on $[3, \infty)$.

Proof. The proof is an exercise in basic calculus:

$$\begin{aligned}
 a'(x) &= \tan(\pi/x) - \pi \frac{\sec^2(\pi/x)}{x} \\
 a''(x) &= -\pi \frac{\sec^2(\pi/x)}{x^2} + \pi \frac{\sec^2(\pi/x)}{x^2} + \left(\frac{\pi^2}{x^3}\right) (2\sec^2(\pi/x)\tan(\pi/x)) \\
 &= \left(\frac{\pi^2}{x^3}\right) (2\sec^2(\pi/x)\tan(\pi/x)),
 \end{aligned}$$

which is positive for $x \geq 3$. □

The next lemma gives an upper bound on the number of edges contained in a Voronoi diagram on a polygon of six or fewer sides.

Lemma II.6.5. ([16]) Let $\mathcal{V}(\omega_N) = \{V(x_1), V(x_2), \dots, V(x_N)\}$ be the Voronoi diagram on a convex polygon $H \subseteq \mathbb{R}^2$ with at most six sides associated to $\omega_N \subseteq H$, and for all $1 \leq i \leq N$, let ν_i denote the number of sides of $V(x_i)$. Then

$$\sum_{i=1}^N \nu_i \leq 6N.$$

Proof. Denote by v and e the number of vertices and edges of the Voronoi diagram on H . Ignoring the unbounded face of the planar graph determined by the Voronoi diagram on H , apply Euler's formula for planar graphs:

$$v - e + N = 1. \tag{18}$$

Denote now by a the number of vertices on the boundary of H from which at least three edges emanate and by b the number of vertices on the boundary of H from which two edges emanate. Notice that $2e$ will count each vertex from which at least three

edges emanate at least three times and each vertex from which two edges emanate twice. Hence,

$$3v \leq 2e + b. \tag{19}$$

Notice further that, since every edge in the interior of H is shared by precisely two Voronoi cells, $\sum_{i=1}^N \nu_i$ will count each edge of the Voronoi diagram twice except for those on the boundary. Since the number of vertices on the boundary equals the number of edges on the boundary, we have:

$$\sum_{i=1}^N \nu_i = 2e - (a + b). \tag{20}$$

Now (18), (19), and (20) will be combined. (18) gives

$$3v = 3e + 3 - 3N,$$

whence (19) implies

$$3e + 3 - 3N \leq 2e + b,$$

implying

$$2e \leq 2b + 6N - 6.$$

Combining this with (20) gives

$$\sum_{i=1}^N \nu_i = 2e - a - b \leq 6N - a + b - 6.$$

Notice now that if a vertex has only two edges emanating from it, it must be a vertex of the polygon H . It follows that $b \leq 6$, from which it follows that

$$\sum_{i=1}^N \nu_i \leq 6N.$$

□

The previous two lemmas now give the result of Theorem II.6.3 rather quickly:

Proof of Theorem II.6.3. Suppose N discs are packed into the convex polygon H . Let $\omega_N = \{x_i\}_{i=1}^N$ denote the centers of these discs. Form the Voronoi diagram $\mathcal{V}(\omega_N) = \{V(x_1), V(x_2), \dots, V(x_N)\}$ on H associated to the configuration ω_N , and suppose the Voronoi cell $V(x_i)$ has ν_i sides. By construction, each Voronoi cell will have an inradius of at least r , whence

$$\text{Area}(H) = \sum_{i=1}^N \text{Area}(V(x_i)) \geq r^2 \sum_{i=1}^N a(\nu_i).$$

Now apply the convexity result of Lemma II.6.4:

$$\text{Area}(H) \geq r^2 \sum_{i=1}^N a(\nu_i) \geq r^2 N a\left(\frac{\sum_{i=1}^N \nu_i}{N}\right) \geq r^2 N a(6), \quad (21)$$

where the last inequality is a consequence of Lemma II.6.5. To conclude we simply observe that the area of a regular hexagon circumscribed about a disc of radius r is $r^2 a(6)$.

□

Theorem II.6.3 has a natural application to best-packing. Let A denote the unit square in \mathbb{R}^2 . We wish to maximize the following quantity over all N -point configurations $\omega_N \subseteq A$:

$$\delta(\omega_N) = \min\{|x - y| : x \neq y \in \omega_N\}$$

Call this maximum $\delta(N)$. Then solving (21) for r , one has that $\delta(N) \leq \frac{2}{\sqrt{Na(6)}}$, and taking N sufficiently large, one can make this inequality as close to an equality as desired. (The factor 2 reflects the difference between the inradius of a Voronoi cell and the distance between points whose Voronoi cells share an edge.) This indicates that the packing radius of N points into the unit square is, for N large, close to $\frac{2}{\sqrt{Na(6)}}$. (Notice the concordance of this result with the separation estimates of Theorem II.4.6.) This result will be seen again in Chapter 4.

II.7 Bonnesen Inequalities

The utility of considering the concept of Voronoi diagram presented in the previous section as a means of investigating a minimal energy problem is quite simple: Since the distances between certain points (nearest neighbors) in a configuration is double the perpendicular distances from the center of a Voronoi cell to its respective edges, the question of finding a configuration that minimizes energy on a planar set can be studied (particularly for a kernel with predominantly local behavior) by finding a convex polygon that is, in a certain sense, optimal. Geometric questions of this type go back as far as the classical isoperimetric inequality: Given a simple closed planar curve \mathcal{C} with length L and enclosed area A ,

$$L^2 - 4\pi A \geq 0,$$

with equality if and only if \mathcal{C} is a circle. The following is known as the Bonnesen Inequality (see e.g. ([29])):

$$L^2 - 4\pi A \geq \pi^2(R - r)^2,$$

where $R = \inf \{\text{radii of circles containing } \mathcal{C}\}$, and $r = \sup \{\text{radii of circles contained in } \mathcal{C}\}$.

In general, a Bonnesen-style inequality is of the form

$$L^2 - 4\pi A \geq B,$$

where $B \geq 0$ with equality only if \mathcal{C} is a circle, and B has some geometric significance.

The following isoperimetric inequality for polygons is also well-known; see e.g. ([21]), ([30]): For an n -sided polygon P_n with perimeter L_n and area A_n ,

$$L_n^2 - 4n \tan\left(\frac{\pi}{n}\right)A_n \geq 0, \tag{22}$$

with equality if and only if P_n is regular. Notice that the classical isoperimetric inequality can be viewed as a limiting case of (22).

In 1997, Zhang in ([39]) proved some Bonnesen-style isoperimetric inequalities for polygons using basic analytic inequalities. These inequalities are of the form

$$L_n^2 - 4n \tan\left(\frac{\pi}{n}\right)A_n \geq B_n,$$

where $B_n \geq 0$ with equality only if P_n is regular, and B_n has some geometric significance. As an example, he demonstrates that

$$L_n^2 - 4n \tan\left(\frac{\pi}{n}\right)A_n \geq (l_n - L_n)^2,$$

where l_n is the perimeter of the regular n -gon with the same circumradius as P_n . Equality holds only when P_n is regular.

Since the interest for one considering minimal energy problems concerns the lengths of altitudes rather than perimeter, another result of Zhang in ([39]) that merits consideration is the following inequality: Let $\{r_i\}_{i=1}^n$ denote the n altitudes of a polygon P_n , and set $R_n = \sum_{i=1}^n r_i$. Then

$$R_n^2 - n \cot\left(\frac{\pi}{n}\right) \geq (\bar{R}_n - R_n)^2,$$

where \bar{R}_n is the value of R_n for the regular n -gon having the same circumradius as P_n . Equality holds only when P_n is regular.

Inequalities of this type could prove useful since they not only describe a polygon that is, in various senses, optimal, but they also describe and quantify any deviations from optimality. In the minimal energy setting, this could prove useful in the description of configurations that are not only optimal configurations but merely near-optimal.

In Chapter 3, certain inequalities will be established relating to the minimization of the quantity

$$\left(\sum_{i=1}^n r_i^{-s}\right) (A(P_n))^{\frac{s}{2}}$$

over all convex n -gons P_n (for fixed n). Zhang's results do not immediately give any bounds on this quantity; in fact, in Chapter 3 we will see that there are settings in which the regular n -gon is not the minimizer for this quantity.

CHAPTER III

NEW GEOMETRIC INEQUALITIES AND A LOWER BOUND FOR $c_{s,2}$

III.1 Geometric Inequalities

For large values of s , information about s -optimal configurations' geometry and energy can be gotten by considering only nearest neighbors, due to the increasingly local character of the Riesz s -energy kernel for these values of s . The natural question then is the question of what nearest-neighbor structure is optimal in some appropriate sense. This is the question considered in this section.

For a given $M \in \mathbb{N}$, $M \geq 3$, $s \geq 2$, and a convex polygon P of M sides, let p be any point interior to P , and label the vertices of P $\{v_1, v_2, \dots, v_M\}$ in a counterclockwise manner. In what follows we shall identify a polygon P simply as the M -tuple of its vertices (v_1, \dots, v_M) . Then let h_i be the segment from p perpendicular to the line coinciding with the edge with endpoints v_i and v_{i+1} (here $v_{M+1} = v_1$). Let $A(P)$ be the area of P .

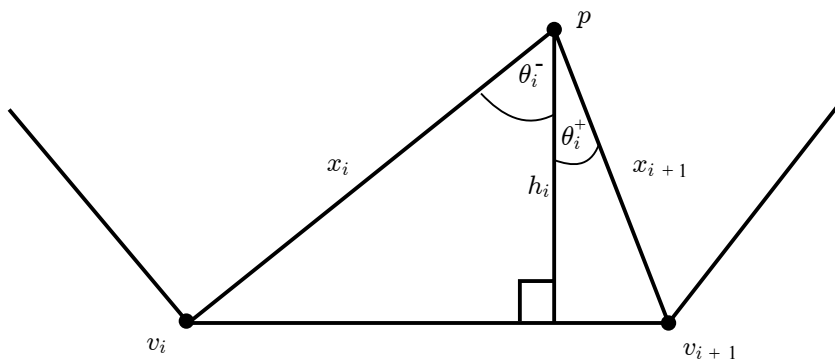


Figure 1: A portion of a polygon and its quantities of interest

Consider the following (scale-invariant) quantity:

$$F(P) := F(v_1, \dots, v_M) := \left(\sum_{i=1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}}. \quad (23)$$

where r_i denotes the length of the segment h_i . Notice that this quantity is also translation-invariant, and so without loss of generality, we place p at the origin. As implied at the beginning of this section, it is of interest to get a lower bound for $F(P)$ over all convex polygons P of M sides containing the origin.

Notice that the value of the quantity in (23) when P is the regular M -gon and p is the center of P is

$$\left(\sum_{i=1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}} = Ma(M)^{\frac{s}{2}},$$

where $a(n) = n \tan\left(\frac{\pi}{n}\right)$, which is the area of a regular n -gon with inradius 1. Preliminary analysis initially seems to indicate that this may be the desired lower bound; however, this is only partially the case, as will be discussed in Theorem 1.

Let now x_i be the segment from p to v_i . Denote by θ_i^- the angle formed by h_i and x_i , and by θ_i^+ the angle formed by h_i and x_{i+1} . Then we have that

$$A(P) = \frac{1}{2} \sum_{i=1}^{2M} s_i^2 \tan t_i,$$

where $\mathbf{s} = (r_1, r_1, r_2, r_2, \dots, r_M, r_M)$ and $\mathbf{t} = (\theta_1^-, \theta_1^+, \theta_2^-, \theta_2^+, \dots, \theta_M^-, \theta_M^+)$. Notice that it is possible that either θ_i^- or θ_i^+ is negative, but both cannot be; indeed $\theta_i^- + \theta_i^+ \in (0, \pi)$.

Notice further that $\tan \theta_i^- + \tan \theta_i^+ \geq 2 \tan\left(\frac{\theta_i^- + \theta_i^+}{2}\right)$. Indeed, if both θ_i^- and θ_i^+ are positive, this follows from the convexity of the tangent function on $(0, \frac{\pi}{2})$. If one of these two angles is negative, then one can consider the function

$$d(\theta) = \tan \theta_0 + \tan \theta - 2 \tan \left(\frac{\theta_0 + \theta}{2} \right),$$

where θ_0 is negative and $\theta \in [-\theta_0, \frac{\pi}{2})$. Then $d(-\theta_0) = 0$ and

$$d'(\theta) = \sec^2 \theta - \sec^2 \left(\frac{\theta_0 + \theta}{2} \right) > 0,$$

since the secant function is increasing. We therefore have that

$$A(P) = \frac{1}{2} \sum_{i=1}^{2M} s_i^2 \tan t_i \geq \sum_{i=1}^M r_i^2 \tan \theta_i,$$

where $\theta_i = \frac{1}{2}(\theta_i^- + \theta_i^+) \in (0, \frac{\pi}{2})$. This allows us to bound the quantity in (23) from below:

$$\left(\sum_{i=1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}} \geq \left(\sum_{i=1}^M r_i^{-s} \right) \left(\sum_{i=1}^M r_i^2 \tan \theta_i \right)^{\frac{s}{2}}. \quad (24)$$

This preliminary lower bound will be used in what follows. It will also be necessary to consider degenerate cases in which adjacent vertices coincide, and so not all vertices of the polygon will be required to be distinct. This motivates the following formulation of the same minimization problem for polygons in this degenerate case:

If $v_i \neq v_{i+1}$, then h_i will be defined as before. However, if $v_i = v_{i+1}$, we let h_i be the segment from p to v_i , and r_i be the length of h_i . Then we simply view the minimization of (23) as the minimization of a function $F : \mathbb{R}^{2M} \rightarrow \mathbb{R}$.

If $r_i = 0$ then we will say that $F(P) = \infty$. In addition, the scale-invariance of the problem assures us that we can keep the vertices inside a compact subset of the plane (for example, the unit disc). Therefore we will define the minimization problem on the set of all M -tuples of vertices (v_1, \dots, v_M) satisfying the condition that the vertices (v_1, \dots, v_M) form a counterclockwise-ordered list of (not necessarily distinct)

vertices of a convex M -gon contained in the unit disc and containing the origin. We will call this set \mathcal{V}_M .

For collections of vertices $V := (v_1, \dots, v_M)$ and $W := (w_1, \dots, w_M)$, define a metric D to be

$$D(V, W) = \sum_{i=1}^n |v_i - w_i|,$$

where $|\cdot|$ denotes the usual Euclidean norm in \mathbb{R}^2 . Then we have the following:

Lemma III.1.1. $F(P)$ is lower semicontinuous on \mathcal{V}_M . Hence it attains a minimum in \mathcal{V}_M .

Proof. Fix $P = (v_1, \dots, v_M) \in \mathcal{V}_M$, and let $P_n \in \mathcal{V}_M$ converge to P in the metric defined above. If none of the vertices coincide, lower semicontinuity is a consequence of the continuity of all the functions appearing in (24). If a pair of vertices v_i and v_{i+1} do coincide, lower semicontinuity follows from the fact that r_i is at least as large as any perpendicular length drawn from p to any line through v_i . That is, for a sequence of polygons $P_n \in \mathcal{V}_M$, $P_n = (v_{1,n}, \dots, v_{M,n})$, the quantity

$$\left(\sum_{i=1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}}$$

is less than or equal to the value obtained by choosing r_i to be the distance from p to v_i rather than the limiting value of distances from p to any line formed by distinct points $v_{i,n}$ and $v_{i+1,n}$. This establishes lower semicontinuity; the second statement is a standard fact from real analysis.

□

For a natural number $M \geq 3$,

$$f_s(M) := \inf \left\{ \left(\sum_{i=1}^M r_i^{-s} \right) (A(P))^{s/2} \right\} = \min_{P \in \mathcal{V}_M} F(P), \quad (25)$$

where the infimum is taken over all convex M -gons P and all interior points p , as before.

Before proceeding, we note the following useful proposition and lemma:

Proposition III.1.2. The function $g_s(\theta) := (\tan \theta)^{\frac{s}{s+2}}$ is convex on $(\tan^{-1}(\frac{1}{\sqrt{s+1}}), \pi/2)$ and concave on $(0, \tan^{-1}(\frac{1}{\sqrt{s+1}}))$.

Proof. It suffices to check the sign of the second derivative of g_s :

$$g_s(\theta) = \tan^{\frac{s}{s+2}} \theta$$

$$g'_s(\theta) = \frac{s}{s+2} \tan^{\frac{-2}{s+2}} \theta \sec^2 \theta$$

$$\begin{aligned} g''_s(\theta) &= \frac{2s}{s+2} \sec^2 \theta \tan^{\frac{-s-4}{s+2}} \theta \left(\tan^2 \theta - \frac{1}{s+2} \sec^2 \theta \right) \\ &= \frac{2s}{(s+2)^2} \sec^2 \theta \tan^{\frac{-s-4}{s+2}} \theta \left((s+1) \tan^2 \theta - 1 \right), \end{aligned}$$

whence the result follows. □

In the following, let $\gamma_s := \tan^{-1}(\frac{1}{\sqrt{s+1}})$.

Lemma III.1.3. For $M \in \mathbb{N}$, $M \geq 3$, let $h(\theta, \phi) : [0, \gamma_s] \times [\frac{\pi}{M}, \frac{\pi}{2}] \rightarrow \mathbb{R}$ be defined to be

$$h(\theta, \phi) = \frac{\tan^{\frac{s}{s+2}} \theta + \tan^{\frac{s}{s+2}} \phi}{2} - \tan^{\frac{s}{s+2}} \left(\frac{\theta + \phi}{2} \right).$$

Then for s sufficiently large, h attains its minimum value at $(\theta_1, \theta_M) = (0, \frac{\pi}{M})$, and this minimum value is positive.

Proof. First fix θ . Taking the derivative of h with respect to ϕ gives

$$\frac{\partial h}{\partial \phi} = \frac{s}{2(s+2)} \tan^{\frac{-2}{s+2}} \phi \sec^2 \phi - \frac{s}{2(s+2)} \tan^{\frac{-2}{s+2}} \left(\frac{\theta + \phi}{2} \right) \sec^2 \left(\frac{\theta + \phi}{2} \right).$$

For large s , the tangent terms are approaching 1 since ϕ is bounded away from 0. Since the secant function is increasing, and $\phi > \frac{\theta + \phi}{2}$, this partial derivative is positive for s sufficiently large, so for any fixed θ , $h(\theta, \phi)$ has its minimum at $\phi = \frac{\pi}{M}$.

Now minimize $h\left(\theta, \frac{\pi}{M}\right)$ over θ :

$$\frac{\partial h}{\partial \theta} = \frac{s}{2(s+2)} \tan^{\frac{-2}{s+2}} \theta \sec^2 \theta - \frac{s}{2(s+2)} \tan^{\frac{-2}{s+2}} \left(\frac{\theta + \frac{\pi}{M}}{2} \right) \sec^2 \left(\frac{\theta + \frac{\pi}{M}}{2} \right).$$

This is infinite at $\theta = 0$ and so the function $h(\theta, \frac{\pi}{M})$ is increasing at first. What we will show is that the derivative has a unique zero, which must be the location of a local maximum for $h(\theta, \frac{\pi}{M})$. This will mean that the minimum value of $h(\theta, \frac{\pi}{M})$ occurs either at $\theta = 0$ or $\theta = \gamma_s$. Notice that the function

$$m(x) = \sec^2 x \tan^{\frac{-2}{s+2}} x$$

has derivative

$$\frac{2 \sec^2 x \tan^{\frac{-s-4}{s+2}} x}{s+2} ((s+1) \tan^2 x - 1),$$

which implies that $h'(\theta, \frac{\pi}{M})$ is one-to-one on $[0, \gamma_s]$. Now if the minimum of $h(\theta, \frac{\pi}{M})$ occurs at γ_s , then convexity of g_s (where g_s is defined in the previous proposition) concludes the proof. What remains therefore is to show that $h(0, \frac{\pi}{M})$ is positive.

We have that

$$h\left(0, \frac{\pi}{M}\right) = \frac{1}{2} \tan^{\frac{s}{s+2}}\left(\frac{\pi}{M}\right) - \tan^{\frac{s}{s+2}}\left(\frac{\pi}{2M}\right).$$

This is positive precisely when

$$\frac{1}{2} \tan^{\frac{s}{s+2}}\left(\frac{\pi}{M}\right) > \tan^{\frac{s}{s+2}}\left(\frac{\pi}{2M}\right)$$

$$\left(\frac{1}{2}\right)^{\frac{s+2}{s}} \tan\left(\frac{\pi}{M}\right) > \tan\left(\frac{\pi}{2M}\right)$$

$$\left(\frac{1}{2}\right)^{\frac{s+2}{s}} > \frac{\tan\left(\frac{\pi}{2M}\right)}{\tan\left(\frac{\pi}{M}\right)}.$$

and this inequality is satisfied for s sufficiently large, since the quantity on the right increases to $\frac{1}{2}$ as M increases to infinity (i.e. it is always less than $\frac{1}{2}$).

□

We are now in a position to prove:

Theorem III.1.4. Let $M \in \mathbb{N}$ be given. Then there is an $s_0 = s_0(M)$ so that for all $s > s_0$, the infimum in (25) is attained uniquely by the regular M -gon; that is, $f_s(M) = Ma(M)^{\frac{s}{2}}$.

Proof. Fix $M \in \mathbb{N}$. Proceeding as in the beginning of this chapter,

$$\left(\sum_{i=1}^M r_i^{-s} \right) (A(P))^{s/2} \geq \left(\sum_{i=1}^M r_i^{-s} \right) \left(\sum_{i=1}^M r_i^2 \tan \theta_i \right)^{s/2}$$

where θ_i is the average of θ_i^+ and θ_i^- .

$$\begin{aligned} &= \left(\sum_{i=1}^M r_i^{-s} \right) \left(\sum_{i=1}^M r_i^2 \tan \theta_i \right)^{s/2} \\ &= \left[\left(\sum_{i=1}^M r_i^{-s} \right)^{\frac{2}{s+2}} \cdot \left(\sum_{i=1}^M r_i^2 \tan \theta_i \right)^{\frac{s}{s+2}} \right]^{\frac{s+2}{2}}. \end{aligned}$$

Using Hölder's inequality,

$$\left[\left(\sum_{i=1}^M r_i^{-s} \right)^{\frac{2}{s+2}} \cdot \left(\sum_{i=1}^M r_i^2 \tan \theta_i \right)^{\frac{s}{s+2}} \right]^{\frac{s+2}{2}} \geq \left(\sum_{i=1}^M (\tan \theta_i)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}}. \quad (26)$$

The idea now is to take advantage of the fact that the interval of concavity of $g_s(x) = \tan^{\frac{s}{s+2}} x$ is small when s is large together with the fact that the average of the angles is π/M (and π/M is far from γ_s for s large) to show that even though g_s is not convex on $(0, \pi/2)$, (17) still holds. Applying (17) to our current lower bound in (26) will give

$$\left(\sum_{i=1}^M (\tan \theta_i)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}} \geq M^{1+s/2} (\tan \pi/M)^{s/2} = Ma(M)^{s/2}.$$

Therefore our goal is to establish (17) for the sum

$$\sum_{i=1}^M \tan^{\frac{s}{s+2}} \theta_i.$$

Relabel the angles so that $\theta_1 < \theta_2 < \dots < \theta_M$; that is, the central angles of P are now listed in increasing order. If $\theta_1 \geq \gamma_s$, then all the angles are in the region of

convexity, and Jensen's inequality applies. If $\theta_1 < \gamma_s$, then the previous lemma gives that, for s sufficiently large,

$$\frac{\tan^{\frac{s}{s+2}} \theta_1 + \tan^{\frac{s}{s+2}} \theta_M}{2} \geq \tan^{\frac{s}{s+2}} \left(\frac{\theta_1 + \theta_M}{2} \right). \quad (27)$$

Since θ_M must be at least the average $\frac{\pi}{M}$, this will be sufficient provided s is chosen large enough such that it ensures that $\gamma_s < \frac{\pi}{2M}$. Indeed, if (27) holds, replace the configuration $(\theta_1, \dots, \theta_M)$ by the configuration $(\frac{\theta_1 + \theta_M}{2}, \theta_2, \dots, \theta_{M-1}, \frac{\theta_1 + \theta_M}{2})$, which decreases the quantity in (23); and if $\theta_2 < \gamma_s$, then there still must be another angle that is greater than the average of $\frac{\pi}{M}$, so repeat the procedure above. This concludes the proof. □

Remark III.1.5. The quantity in (23) is not optimized by the regular M -gon and central point for all values of s . To see this, notice that the M -gon is determined, up to scaling, by the angles $(\theta_1^-, \theta_1^+, \dots, \theta_M^-, \theta_M^+)$. Since the quantity in (23) is scale-invariant, it is completely determined by these angles. In light of the relations

$$x_i = r_i \sec \theta_i^- = r_{i-1} \sec \theta_{i-1}^+,$$

if $\theta_i^- = \theta_i^+$ for all $i = 1, 2, \dots, M$, the quantity in (23) simplifies to

$$\left(\sum_{i=1}^M \sec^s \theta_i \right) \left(\sum_{i=1}^M \sin \theta_i \cos \theta_i \right)^{\frac{s}{2}}, \quad (28)$$

where $\theta_i := \theta_i^- = \theta_i^+$. For $M = 6$ and $s = 2$, using the expression in (28) and the configuration of angles $(.809193, .0147173, .740205, .0241505, .774331, .778996)$ returns a value of 20.089, which is lower than $6a(6) \approx 20.785$.

The next theorem gives a lower bound for the quantity in (23) that will be useful in later sections.

Theorem III.1.6. For any M and any $s \geq 2$, we have

$$f_s(M) \geq \min_{\nu \leq M} \nu a(\nu)^{\frac{s}{2}}.$$

Furthermore, this inequality is strict unless $f_s(M) = Ma(M)^{\frac{s}{2}}$.

Proof. As in Theorem III.1.4, the idea is to work with the expression

$$\sum_{i=1}^M \tan^{\frac{s}{s+2}} \theta_i$$

by arranging the central angles in increasing order. Specifically, consider the function

$$j(\theta_1, \theta_M) = \tan^{\frac{s}{s+2}} \theta_1 + \tan^{\frac{s}{s+2}} \theta_M$$

with the idea of holding the other angles fixed. This means that, for some k , the above can be written as

$$j(\theta_1) = \tan^{\frac{s}{s+2}} \theta_1 + \tan^{\frac{s}{s+2}} (k - \theta_1).$$

The domain of this function is $[0, \min\{\gamma_s, \frac{\pi}{M}, k - \frac{\pi}{M}\}]$, with the added restriction that $k - \theta_1 < \frac{\pi}{2}$, since each central half-angle has measure at most $\frac{\pi}{2}$. Similar to the function h in Theorem III.1.4, this function is first increasing because its derivative is infinite at $\theta_1 = 0$. It has a unique maximum for the same reason that the function h in Theorem III.1.4 has a unique maximum.

This means that the minimum of j occurs at either 0 or the right endpoint of its domain of definition. If it occurs at the right endpoint, that means the minimum of j occurs at either

- $\theta_1 = \gamma_s$, in which case convexity applies;
- $\theta_1 = \frac{\pi}{M}$; or
- $\theta_M = \frac{\pi}{M}$.

If the minimum occurs at the left endpoint; that is, when $\theta_1 = 0$, then recast the problem in terms of $M - 1$ angles and repeat the above procedure until the function j has its minimum at the right endpoint of its domain for all the angles that have measure less than $\frac{\pi}{M}$. This means that, for some n , either by convexity or by this procedure one has that

$$\left(\sum_{i=1}^N \tan^{\frac{s}{s+2}} \theta_i \right)^{1+\frac{s}{2}} \geq (M-n)a(M-n)^{\frac{s}{2}} \geq \min_{\nu \leq M} \nu a(\nu)^{\frac{s}{2}}.$$

The remark about strict inequality in the statement of this theorem follows from the technique just demonstrated together with the remarks at the beginning of this chapter. More precisely, suppose that in the above technique, the angles $\theta_1, \dots, \theta_n$ are replaced by $0, \dots, 0$. (The other angles will also be reassigned in order to satisfy the constraint.) Then for the polygon generated by these new central angles we have that

$$\left(\sum_{i=1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}} = \left(\sum_{i=1}^n r_i^{-s} \right) A(P)^{\frac{s}{2}} + \left(\sum_{i=n+1}^M r_i^{-s} \right) A(P)^{\frac{s}{2}},$$

and using Hölder's inequality on the second term,

$$\left(\sum_{i=1}^n r_i^{-s}\right) A(P)^{\frac{s}{2}} + \left(\sum_{i=n+1}^M r_i^{-s}\right) A(P)^{\frac{s}{2}} \geq \left(\sum_{i=1}^n r_i^{-s}\right) A(P)^{\frac{s}{2}} + \left(\sum_{i=n+1}^M \tan^{\frac{s}{s+2}} \theta_i\right)^{\frac{s+2}{2}},$$

and this last quantity is strictly greater than the lower bound given in the statement of the theorem. \square

III.2 The Constant $C_{s,d}$

The constant $C_{s,d}$ appearing in the asymptotic result (12) of Hardin and Saff is worthy of study because it is indicative of the local structure of s -optimal configurations when $s > d$. The proof of Theorem III.2.3 will reflect this fact most concretely in the case $d = 2$, but intuitively one can think of this as a reflection of the local character of the Riesz kernel when $s > d$, since the first term in the asymptotic expansion should reflect the nearest neighbor structure of an optimal configuration.

Since selecting any N -point configuration on a set A and computing its Riesz s -energy gives an upper bound for $\mathcal{E}_s(A, N)$, upper bounds for $C_{s,d}$ can be readily attained. In this section lattices will be used to give an upper bound for the constant $C_{s,d}$ defined by (12). The computation is instructive and provides some intuition concerning the order of growth of $\mathcal{E}_s(A, N)$ as N approaches infinity. This argument can be found in [23] and references therein.

Consider any d -dimensional lattice $L \subseteq \mathbb{R}^d$ with fundamental cell F . Given N , shrink the lattice by a factor of $1/(N-1)$:

$$\frac{1}{N-1}L = \left\{ \frac{1}{N-1}x : x \in L \right\}.$$

Consider now $(\frac{1}{N-1}L) \cap F$. Then it is easy to see that this set contains N^d points of the entire scaled lattice. Call these N^d points ω_{N^d} and estimate the quantity

$$\frac{E_s(\omega_{N^d})}{(N^d)^{1+\frac{s}{d}}}$$

for a fixed $s > d$. The difficulty in computing the energy $E_s(\omega_{N^d})$ arises from the different local structures of the individual points in the lattice restricted to the fundamental domain F . To alleviate this problem, estimate the energy for each point in $(\frac{1}{N-1}L) \cap F$ by estimating

$$\sum_{\substack{x,y \in (\frac{1}{N-1}L) \cap F \\ x \neq y}} \frac{1}{|x-y|^s}$$

from above by

$$\sum_{x \in (\frac{1}{N-1}L) \cap F} \left(\sum_{\substack{y \in \frac{1}{N-1}L \\ y \neq x}} \frac{1}{|x-y|^s} \right).$$

It therefore follows that

$$E_s(\omega_{N^d}) = \sum_{\substack{x,y \in (\frac{1}{N-1}L) \cap F \\ x \neq y}} \frac{1}{|x-y|^s} \leq \sum_{x \in (\frac{1}{N-1}L) \cap F} \left(\sum_{\substack{y \in \frac{1}{N-1}L \\ y \neq x}} \frac{1}{|x-y|^s} \right) = N^d \zeta_L(s) (N-1)^s.$$

The factor $(N-1)^s$ comes from the scaling of the lattice by the factor $1/(N-1)$.

Hence

$$\frac{E_s(\omega_{N^d})}{(N^d)^{1+\frac{s}{d}}} \leq \frac{N^d \zeta_L(s) (N-1)^s}{N^{d+s}} \leq \zeta_L(s).$$

The existence of the limit in (12) now implies that

$$C_{s,d} = \lim_{N \rightarrow \infty} \frac{\mathcal{E}_s(F, N)}{N^{1+\frac{s}{d}}} |F|^{\frac{s}{d}} \leq \limsup_{N \rightarrow \infty} \frac{E_s(\omega_{N^d})}{(N^d)^{1+\frac{s}{d}}} |F|^{\frac{s}{d}} \leq \zeta_L(s) |F|^{\frac{s}{d}}, \quad (29)$$

where $|F|$ denotes the d -dimensional Lebesgue measure of F (in this case, equal to the d -dimensional Hausdorff measure of F).

The natural question that follows is to ask which lattice gives the best estimate for $C_{s,d}$. When $d = 1$, the integer lattice \mathbb{Z} gives the best bound, and in fact in ([25]) it was shown that

$$C_{s,1} = 2\zeta(s),$$

where $\zeta(s)$ denotes the classical Riemann zeta function. The value of $C_{s,d}$ is not known for any other values of d , but the results of Montgomery, Cohn, and Kumar mentioned in section II.5 serve as a starting point in dimensions 2, 8, and 24.

The efforts made in this thesis have had as their objective progress toward a computation of $C_{s,2}$. For this reason much of the work of the thesis concerns results from plane geometry.

Denoting by Λ the hexagonal lattice in the plane as defined a section ago, in ([23]) it was conjectured that, for $s > 2$,

$$C_{s,2} = \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}} \cdot \zeta_{\Lambda}(s).$$

The result of (29) gives

$$C_{s,2} \leq \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}} \cdot \zeta_{\Lambda}(s). \quad (30)$$

Before proceeding, we require the following lemmas:

Lemma III.2.1. Let $\{\omega_N\}$ be a sequence of s -optimal configurations on the unit square, where $s > 2$. Then the number of points whose Voronoi cell meets the boundary of the unit square is $o(N)$ as $N \rightarrow \infty$.

Proof. Let $\varepsilon > 0$ be a fixed small number. Let S_ε denote the complement in the unit square of the points inside the open square centered at $(1/2, 1/2)$ with area $1 - \frac{\varepsilon}{2}$. Let δ be the perpendicular distance from $(1/2, 1)$ to the open square just described. Choose $m \in \mathbb{N}$ so that $m > 32/\delta^2$. Partition then the upper strip of S_ε into $4m$ equal rectangles of height $\delta/4$ and width $\frac{1}{m}$. For N sufficiently large, each of the $4m$ rectangles just constructed will have points from ω_N in them, by (13). Notice then that any point in the third row of these rectangles cannot have a Voronoi cell that meets the upper boundary of the unit square, since the perpendicular bisector of any point in the third row of rectangles and any point in the corresponding rectangle two above it does not touch that boundary, by choice of m . Similarly for points in the fourth row of rectangles and below, and similarly in turn for points in the other strips of S_ε .

This implies that all of the points that have a Voronoi cell meeting the boundary of the unit square lie in the outer half of S_ε . Since Theorem II.4.4 implies that

$$\lim_{N \rightarrow \infty} \frac{|S_\varepsilon \cap \omega_N|}{N} < \varepsilon,$$

and ε was arbitrarily small, we have the claim. □

Remark III.2.2. Lemma III.2.1 also holds for compact sets $A \subseteq \mathbb{R}^2$ satisfying the following condition: For every $\varepsilon > 0$, there is a polygon $P \subseteq A$ whose area is within ε of the area of A . The proof is similar and involves choosing a polygon as just described, then fattening each edge into a small rectangle and proceeding as in the lemma.

Lemma III.2.3.

$$\lim_{s \rightarrow \infty} \zeta_{\Lambda}(s) = 6,$$

where Λ denotes the hexagonal lattice in \mathbb{R}^2 as defined in Chapter 2.

Proof. Let \mathcal{H}_0 denote the counting measure on \mathbb{R}^2 . As all points in $\Lambda - \{0\}$ are at a distance of at least 1 from the origin, one has that

$$\zeta_{\Lambda}(s) = \sum_{\substack{y \in \Lambda \\ y \neq 0}} \frac{1}{|y|^s} = \int_{\Lambda - \{0\}} \frac{1}{|y|^s} d\mathcal{H}_0(y),$$

and the integrand is monotonically decreasing with s . Therefore, by the monotone convergence theorem,

$$\lim_{s \rightarrow \infty} \zeta_{\Lambda}(s) = \lim_{s \rightarrow \infty} \int_{\Lambda - \{0\}} \frac{1}{|y|^s} d\mathcal{H}_0(y) = 6,$$

as the quantity $\frac{1}{|y|^s}$ approaches 0 as s approaches infinity for all points at a distance strictly greater than 1 from the origin.

□

We now have the following:

Theorem III.2.4. $\lim_{s \rightarrow \infty} \frac{C_{s,2}}{\left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}} = 6.$

Proof. In light of the upper estimate for $C_{s,2}$ in (30), it follows from Lemma III.2.3 that

$$\lim_{s \rightarrow \infty} \frac{C_{s,2}}{\left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}} \leq 6.$$

Therefore, it is only necessary to show the reverse inequality.

By Theorem III.1.4, choose s big enough so that $f_s(M)$ is given by $Ma(M)^{\frac{s}{2}}$ for $M \leq 7$. Then $(xa(x)^{s/2})^{\frac{2}{s+2}}$ is convex and decreasing on $[3, \beta_s]$, where β_s is the place where f_s takes its minimum. Let $M \in \mathbb{N}$ be the value such that $Ma(M)^{\frac{s}{2}}$ takes its least value, and let N' be the number of points in an s -optimal configuration ω_N^s on the unit square whose Voronoi cells do not meet the boundary, and let ν_i be the number of edges of the i -th Voronoi cell. Relabel ω_N^s so that $\{\omega_N^s\}_{i=1}^{N'}$ is the collection of points in ω_N^s whose Voronoi cells do not meet the boundary. Then by Theorem III.1.6,

$$\begin{aligned} 2^s E_s(\omega_N^s) \cdot A([0, 1]^2)^{\frac{s}{2}} &\geq \left(\sum_{i=1}^N \sum_{j=1}^{\nu_i} r_{ij}^{-s} \right) \left(\sum_{i=1}^N A(V_i) \right)^{\frac{s}{2}} \geq \left(\sum_{i=1}^{N'} \frac{f_s(\nu_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}} \\ &\geq \left(\sum_{i=1}^{N'} \frac{\phi_s(\nu_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}}, \end{aligned} \quad (31)$$

where

$$\phi_s(x) = \begin{cases} xa(x)^{\frac{s}{2}}, & x \leq M \\ Ma(M)^{\frac{s}{2}}, & x > M \end{cases}.$$

Using Hölder's inequality in (31) gives

$$\left(\left(\sum_{i=1}^{N'} \frac{\phi_s(\nu_i)}{A(V_i)^{\frac{s}{2}}} \right)^{\frac{2}{s+2}} \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}} \geq \left(\sum_{i=1}^{N'} \phi_s(\nu_i)^{\frac{2}{s+2}} \right)^{\frac{s+2}{2}},$$

and by convexity, choice of s , and Lemmas II.6.4 and II.6.5, for N sufficiently large one has

$$\left(\sum_{i=1}^{N'} \phi_s(\nu_i)^{\frac{2}{s+2}} \right)^{\frac{s+2}{2}} \geq (N')^{1+\frac{s}{2}} \phi_s \left(\frac{\sum_{i=1}^{N'} \nu_i}{N'} \right) = (N')^{1+\frac{s}{2}} \phi_s \left(\frac{6N}{N'} \right) = \frac{6N}{N'} (N')^{1+\frac{s}{2}} a \left(\frac{6N}{N'} \right)^{\frac{s}{2}}.$$

In light of Lemma III.2.1,

$$\lim_{N \rightarrow \infty} \frac{N'}{N} = 1.$$

Thus,

$$C_{s,2} = \lim_{N \rightarrow \infty} \frac{\mathcal{E}_s([0, 1]^2, N)}{N^{1+\frac{s}{2}}} \geq 6 \cdot 2^{-s} a(6)^{\frac{s}{2}} = 6 \left(\frac{\sqrt{3}}{2} \right)^{\frac{s}{2}},$$

whence the result follows. □

Let V_i denote the i -th Voronoi cell. In what follows, we will set

$$\Delta_s(V_i) := \left(\sum_{i=1}^{\nu_i} r_i^{-s} \right) A(V_i)^{\frac{s}{2}} - \phi_s(\nu_i)$$

so that $\Delta_s(V_i)$ gives a difference between the value of $\left(\sum_{i=1}^{\nu_i} r_i^{-s} \right) A(V_i)^{s/2}$ and the lower bound used in Theorem III.2.4.

CHAPTER IV

GEOMETRIC CONSTRAINTS ON CERTAIN CONFIGURATIONS

IV.1 Some Results Concerning the Geometry of s -Optimal Configurations for Large s

Given a compact set $A \subseteq \mathbb{R}^p$, one can relate a portion of the energy of an N -point configuration ω_N to the structure of the Voronoi diagram. In this section, it will be shown that, for large values of the exponent s , certain types of Voronoi cells associated to s -optimal configurations will comprise a small proportion of the total number of Voronoi cells. The aim of this strategy is then to estimate the energy from below by considering only the nearest neighbors of points whose Voronoi cells are in some sense desirable.

Results are first demonstrated for the unit square $[0, 1] \times [0, 1]$ in \mathbb{R}^2 , and then for a larger class of sets in the plane. Results for sets of Hausdorff dimension 2 embedded in higher-dimensional sets are then discussed.

Let ω_N^s denote an s -optimal configuration in the unit square in \mathbb{R}^2 , and fix $\gamma \in (0, 1)$. It shall be shown that the points whose closest neighbor is at a distance of less than $\delta(N) = \frac{2}{\sqrt{Na(6)}}$ form a small proportion of the s -optimal configuration ω_N^s .

To this end, define

$$A_{N,\gamma}^s = \{x \in \omega_N^s : r(x) < \gamma\delta(N)\},$$

where $r(x) = \min\{|x - y| : y \in \omega_N^s \text{ and } y \neq x\}$. If $y \in \omega_N^s$ satisfies $r(x) = |x - y|$, we shall call y a **closest neighbor** of x .

Let $C > 6$. Since, by Lemma III.2.3,

$$\lim_{s \rightarrow \infty} \zeta_\Lambda(s) = 6,$$

there is s_0 sufficiently large such that

$$\zeta_\Lambda(s) < C,$$

for all $s > s_0$.

Theorem IV.1.1. Let $\gamma \in (0, 1)$, $C > 6$, and choose s_0 as above. Then for all $s > s_0$, there is $N_0 = N_0(s)$ such that for all $N > N_0$,

$$\frac{|A_{N,\gamma}^s|}{N} \leq C\gamma^s.$$

Proof. It was shown in an earlier section that

$$\lim_{N \rightarrow \infty} \frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \leq \zeta_\Lambda(s) \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}.$$

Thus, if $s > s_0$, there is N_0 such that for all $N > N_0$,

$$\frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \leq C \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}. \quad (32)$$

To achieve a lower estimate, restrict the sum to only those points in $A_{N,\gamma}^s$ and sum only over one closest neighbor to each of those points, giving

$$\frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \geq \frac{|A_{N,\gamma}^s| \gamma^{-s} 2^{-s} (Na(6))^{\frac{s}{2}}}{N^{1+\frac{s}{2}}} = \frac{|A_{N,\gamma}^s|}{N} \gamma^{-s} \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}, \quad (33)$$

since $a(6) = 2\sqrt{3}$. Combining (32) and (33), for all $N > N_0$,

$$\frac{|A_{N,\gamma}^s|}{N} \gamma^{-s} \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}} \leq \frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \leq C \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}},$$

whence

$$\frac{|A_{N,\gamma}^s|}{N} \leq C\gamma^s.$$

□

Next the results from the previous section will be used to show that the proportion of Voronoi cells that do not have precisely six sides is also small for large s .

Theorem IV.1.2 Let $\gamma \in (0, 1)$ and $C > 6$. If $B_{N,\gamma}$ denotes the set of points whose Voronoi cell has an inradius of at least $\frac{\gamma\delta(N)}{2}$ but does not have exactly six sides, then there is a positive constant D such that, for $N = N(s)$ and s sufficiently large,

$$\frac{|B_{N,\gamma}|}{N} \leq D \cdot \left(\frac{1}{\gamma^2} - 1 + C\gamma^s \right).$$

(From now on, the dependence of sets such as $B_{N,\gamma}$ on s will be suppressed.)

Proof. Form a Voronoi decomposition for the configuration ω_N^s , but ignore the cells whose centers are in the set $A_{N,\gamma}^s$. Then every Voronoi cell considered will have an inradius of at least $\frac{\gamma\delta(N)}{2}$. Denote by $V(x)$ the Voronoi cell centered at x by $A(V(x))$ the area of $V(x)$. Then,

$$1 \geq \sum_{x \in \omega_N^s \setminus A_{N,\gamma}^s} A(V(x)) = \sum_{x \in G_{N,\gamma}} A(V(x)) + \sum_{x \in B_{N,\gamma}} A(V(x)), \quad (34)$$

where $G_{N,\gamma}$ denotes those points $x \in \omega_N^s \setminus A_{N,\gamma}^s$ whose Voronoi cell has exactly six sides, and $B_{N,\gamma}$ denotes those points $x \in \omega_N^s \setminus A_{N,\gamma}^s$ whose Voronoi cell does not have exactly six sides. We have that

$$\sum_{x \in G_{N,\gamma}} A(V(x)) \geq |G_{N,\gamma}| \left(\frac{\gamma\delta(N)}{2} \right)^2 a(6). \quad (35)$$

Set now

$$\tilde{a}(x) = \begin{cases} a(x), & x \in [3, 5] \cup [7, \infty) \\ a(5) + \frac{(a(7)-a(5))}{2}(x-5), & x \in [5, 7]. \end{cases}$$

Notice that $\tilde{a}(x)$ is also convex and agrees with $a(x)$ when $x \notin (5, 7)$. If $V(x)$ is a $\nu(x)$ -gon, it follows from Lemmas II.6.4 and II.6.5 that

$$\begin{aligned} \sum_{x \in B_{N,\gamma}} A(V(x)) &\geq \left(\frac{\gamma\delta(N)}{2} \right)^2 |B_{N,\gamma}| \cdot \tilde{a} \left(\sum_{x \in B_{N,\gamma}} \frac{\nu(x)}{|B_{N,\gamma}|} \right) \geq \left(\frac{\gamma\delta(N)}{2} \right)^2 |B_{N,\gamma}| \cdot \tilde{a}(6) \\ &= \left(\frac{\gamma\delta(N)}{2} \right)^2 |B_{N,\gamma}| \cdot (a(6) + \Delta_a), \end{aligned} \quad (36)$$

where $\Delta_a = \tilde{a}(6) - a(6)$. Since $|B_{N,\gamma}| + |G_{N,\gamma}| + |A_{N,\gamma}^s| = N$, inserting (35) and (36) into (40) gives

$$\begin{aligned} 1 &\geq \left(\frac{\gamma\delta(N)}{2} \right)^2 \left((N - |A_{N,\gamma}^s|) a(6) + |B_{N,\gamma}| \Delta_a \right), \\ &\geq \gamma^2 \left(1 - C\gamma^s + \frac{|B_{N,\gamma}|}{N} \frac{\Delta_a}{a(6)} \right), \end{aligned}$$

and one notices the use of Theorem IV.1.1, with C defined as in that theorem. Hence,

$$\frac{|B_{N,\gamma}|}{N} \leq \left(\frac{1}{\gamma^2} - 1 + C\gamma^s \right) \left(\frac{a(6)}{\Delta_a} \right).$$

□

What we have shown thus far is that a fraction, as close to 1 as desired, of all the Voronoi cells of an s -optimal configuration are hexagons with at least a radius $\gamma\delta(N)/2$ for sufficiently large N and s . The next logical result will be to form an upper bound on the area on the Voronoi cells.

Theorem IV.1.3. Let $\Gamma > 1$, $\gamma \in (0, 1)$ be fixed, and let $D_{N,\gamma,\Gamma}$ denote those points in ω_N^s whose Voronoi cells have six sides, an inradius at least $\gamma\delta(N)/2$, and area more than Γ/N . Then for any $C > 6$, there are N_0 (again depending on s) and s_0 sufficiently large such that, for $N > N_0$ and $s > s_0$,

$$\frac{|D_{N,\gamma,\Gamma}|}{N} \leq \frac{1 - \gamma^2(1 - C\gamma^s)}{\Gamma - \gamma^2}.$$

Proof. We proceed in a similar way to the previous theorem. Denote by $V(x)$ the Voronoi cell with center $x \in \omega_N^s$, and by $B_{N,\gamma}$ those points in ω_N^s whose Voronoi cells do not have six sides and do have inradius at least $\gamma\delta(N)/2$. Then one has

$$\begin{aligned} 1 &\geq \sum_{x \in B_{N,\gamma}} A(V(x)) + \sum_{x \in G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}} A(V(x)) + \sum_{x \in D_{N,\gamma,\Gamma}} A(V(x)) \\ &\geq \left(\frac{\gamma\delta(N)}{2} \right)^2 \left(|B_{N,\gamma}| \sum_{x \in B_{N,\gamma}} \frac{a(\nu(x))}{|B_{N,\gamma}|} + |G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}| \cdot a(6) \right) + |D_{N,\gamma,\Gamma}| \frac{\Gamma}{N}. \end{aligned}$$

As in Theorem IV.1.2, the first term inside the large parentheses above is bounded below by $|B_{N,\gamma}| \cdot a(6)$. Hence, the above quantity is bounded below by

$$\begin{aligned}
&\geq \left(\frac{\gamma\delta(N)}{2}\right)^2 (|B_{N,\gamma}| \cdot a(6) + |G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}| \cdot a(6)) + |D_{N,\gamma,\Gamma}| \frac{\Gamma}{N} \\
&\geq \gamma^2 \left(\frac{|B_{N,\gamma}|}{N} + \frac{|G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}|}{N}\right) + |D_{N,\gamma,\Gamma}| \frac{\Gamma}{N}.
\end{aligned}$$

As $N = |A_{N,\gamma}^s| + |B_{N,\gamma}| + |G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}| + |D_{N,\gamma,\Gamma}|$, it follows from the previous theorems of this section that, for N and s sufficiently large,

$$1 \geq \gamma^2 (1 - C\gamma^s) + \frac{|D_{N,\gamma,\Gamma}|}{N} \cdot (\Gamma - \gamma^2),$$

whence

$$\frac{|D_{N,\gamma,\Gamma}|}{N} \leq \frac{1 - \gamma^2 (1 - C\gamma^s)}{\Gamma - \gamma^2}.$$

□

Again notice that the right side of this inequality can be made as small as desired for any fixed Γ by appropriate choices of γ and s .

Remark IV.1.4. Suppose that $\{\omega_N\}$ is a sequence of asymptotically uniformly distributed N -point configurations on the unit square satisfying

$$\frac{E_s(\omega_N)}{N^{1+\frac{s}{2}}} \leq \lambda \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}$$

for some $\lambda > 6$ and N sufficiently large. Then Theorems IV.1.1, IV.1.2, and IV.1.3 all hold with C replaced by λ . This remark extends analogously to the results in the following two sections that are analogues of Theorems IV.1.1, IV.1.2, and IV.1.3.

IV.2 Analogous Results for S^2

Only a small amount of effort is required to extend the results of the previous section to the two-dimensional manifold $S^2 \subseteq \mathbb{R}^3$. First, observe that in the formation of Voronoi cells, the plane that perpendicularly bisects any pair of points will intersect S^2 in a great circle. Therefore, the Voronoi cells on S^2 will be spherical polygons rather than the Euclidean polygons seen in the previous section.

For simplicity, in what follows we will denote by S^2 the sphere in \mathbb{R}^3 centered at the origin and having unit area rather than unit radius. Also, it must be recalled that the energy is calculated using Euclidean distance in all cases; geodesic distance on the sphere is not used in the following calculations.

Let ω_N^s be an s -optimal configuration on S^2 . As in the previous, denote

$$A_{N,\gamma}^s = \{x \in \omega_N^s : r(x) < \gamma\delta(N)\},$$

where $r(x) = \min\{|x - y| : y \in \omega_N^s \text{ and } y \neq x\}$, and $\delta(N) = \frac{2}{\sqrt{Na(6)}}$. Then we have the following:

Theorem IV.2.1. Let $C > 6$, and choose s_0 so that $\zeta_\Lambda(s) < C$ for all $s > s_0$. Then if $s > s_0$, there is N_0 (depending on s) such that for all $N > N_0$,

$$\frac{|A_{N,\gamma}^s|}{N} \leq C\gamma^s.$$

Proof. The proof follows exactly the proof of Theorem IV.1.1. Summing only over one closest neighbor of each point in $A_{N,\gamma}^s$, then for N sufficiently large,

$$\frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \geq \frac{|A_{N,\gamma}^s| \gamma^{-s} 2^{-s} (Na(6))^{\frac{s}{2}}}{N^{1+\frac{s}{2}}} = \frac{|A_{N,\gamma}^s|}{N} \gamma^{-s} \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}}.$$

Using again the upper estimate on $C_{s,2}$ from an earlier section and recalling that S^2 has unit area, it follows that, for s sufficiently large,

$$\frac{|A_{N,\gamma}^s|}{N} \gamma^{-s} \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}} \leq \frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \leq C \left(\frac{\sqrt{3}}{2}\right)^{\frac{s}{2}},$$

whence

$$\frac{|A_{N,\gamma}^s|}{N} \leq C \gamma^s.$$

□

To extend the results of the previous section concerning Voronoi cells, we need analogues of the lemmas due to Fejes-Toth. First note that Lemma II.6.5 holds also for spherical graphs, since Euler's formula holds for those graphs. Our analogue of Lemma II.6.4 requires the computation of the area of a regular spherical n -gon of spherical inradius a .

Lemma IV.2.2 The area of a regular spherical n -gon of spherical inradius a is given by

$$\alpha_a(n) = R^2 \left[2n \cdot \cos^{-1} \left(\cos \left(\frac{a}{R} \right) \cdot \sin \left(\frac{\pi}{n} \right) \right) - (n-2)\pi \right],$$

where R is the radius of the sphere.

Proof. It is well-known that the area of a spherical n -gon is equal to the so-called angular deficiency; that is, it is the difference between the sum of all the spherical angles, denoted θ , and $(n-2)\pi$, scaled appropriately:

$$\text{Area} = (\theta - (n-2)\pi) R^2$$

The strategy then is to triangulate the regular spherical n -gon. Ratcliffe observed in [32] that in a right spherical triangle, if one of the angles β , other than the right angle, and the length of the adjacent leg a are known, then the third angle α is given by

$$\cos \alpha = \cos \left(\frac{a}{R} \right) \sin \beta.$$

Triangulating the n -gon gives us $2n$ right spherical triangles each having one angle with measure π/n . Hence the third angle of each of the $2n$ spherical triangles is

$$\alpha = \cos^{-1} \left(\cos \left(\frac{a}{R} \right) \sin \left(\frac{\pi}{n} \right) \right),$$

whence the result follows. □

Again it is a basic computation as in Lemma II.6.4 to show that

$$\alpha_a(x) = 2xR^2 \cdot \cos^{-1} \left(\cos \left(\frac{a}{R} \right) \sin \left(\frac{\pi}{x} \right) \right)$$

is a strictly convex function of x . Now let $a(N)$ denote the radius of a spherical cap formed by intersecting S^2 with another sphere centered at a point on S^2 with radius $\frac{\gamma\delta(N)}{2}$. One now has the following:

Theorem IV.2.3 Let $B_{N,\gamma} \subseteq \omega_N^s$ denote those points not in $A_{N,\gamma}^s$ and not having a six-sided Voronoi cell. Then for $N = N(s)$ and s sufficiently large, there are positive constants C and D such that

$$\frac{|B_{N,\gamma}|}{N} \leq D \left(\frac{1}{\gamma^2 \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right)} - 1 + C\gamma^s \right).$$

Proof. Let $G_{N,\gamma}$ denote those points in ω_N^s but neither in $A_{N,\gamma}$ nor $B_{N,\gamma}$. First notice that

$$1 \geq \sum_{x \in B_{N,\gamma}} A(V(x)) + \sum_{x \in G_{N,\gamma}} A(V(x)). \quad (37)$$

Now proceed as in the proof of Theorem IV.1.2. Let

$$\tilde{\alpha}_a(x) = \begin{cases} \alpha_a(x), & x \in [3, 5] \cup [7, \infty) \\ \alpha_a(5) + \frac{(\alpha_a(7) - \alpha_a(5))}{2}(x - 5), & x \in [5, 7]. \end{cases}$$

As before, this function is convex and decreasing on $[3, \infty)$. In [16] it was shown that the spherical n -gon with minimum area and a fixed spherical inradius is the regular spherical n -gon circumscribed about a spherical cap of that radius. Returning to (37) and applying the previous results of this section,

$$1 \geq |B_{N,\gamma}| \cdot \sum_{x \in B_{N,\gamma}} \frac{\tilde{\alpha}_{a(N)}(\nu(x))}{|B_{N,\gamma}|} + |G_{N,\gamma}| \cdot \alpha_{a(N)}(6),$$

where $\nu(x)$ denotes the number of sides of $V(x)$. The convexity of $\tilde{\alpha}_{a(N)}$ gives

$$\begin{aligned} 1 &\geq |B_{N,\gamma}| \cdot \tilde{\alpha}_{a(N)} \left(\frac{\sum_{x \in B_{N,\gamma}} \nu(x)}{|B_{N,\gamma}|} \right) + |G_{N,\gamma}| \cdot \alpha_{a(N)}(6) \\ &\geq |B_{N,\gamma}| \cdot \tilde{\alpha}_{a(N)}(6) + |G_{N,\gamma}| \cdot \alpha_{a(N)}(6), \end{aligned}$$

Since $|A_{N,\gamma}^s| + |B_{N,\gamma}| + |G_{N,\gamma}| = N$,

$$1 \geq |B_{N,\gamma}| \cdot \tilde{\alpha}_{a(N)}(6) + (N - |A_{N,\gamma}^s| - |B_{N,\gamma}|) \cdot \alpha_{a(N)}(6)$$

$$= |B_{N,\gamma}| \cdot \left(\tilde{\alpha}_{a(N)}(6) - \alpha_{a(N)}(6) \right) + (N - |A_{N,\gamma}^s|) \cdot \alpha_{\frac{\gamma\delta(N)}{2}}(6). \quad (38)$$

since $a(N)$ is greater than the straight line distance $\frac{\gamma\delta(N)}{2}$. To understand better the behavior of $\alpha_{a(N)}(6)$ for large N , look at the power expansion of $\alpha_{a(N)}(6)$ (as a function of $a(N)$) about $a = 0$. The power series expansion of $\cos^{-1}(x)$ about $x = \sin(\pi/6) = 1/2$ is

$$\cos^{-1}(x) = \frac{\pi}{3} - \frac{2}{\sqrt{3}}\left(x - \frac{1}{2}\right) + \mathcal{O}(x^2),$$

and the power series expansion of $\frac{1}{2}\cos(a)$ about $a = 0$ is

$$\frac{1}{2}\cos(a) = \frac{1}{2} - \frac{1}{4}a^2 + \mathcal{O}(a^4).$$

It follows that the power series expansion of $\alpha_{a(N)}(6)$ about $a = 0$ is given by

$$\alpha_{a(N)}(6) = 2\sqrt{3}a^2 - \mathcal{O}(a^4).$$

Notice now that

$$\alpha_{\frac{\gamma\delta(N)}{2}}(6) = \frac{\gamma^2}{N} \left(1 - \mathcal{O}\left(\frac{1}{N}\right) \right).$$

This last result together with (38) now imply that

$$1 \geq |B_{N,\gamma}| \cdot \left(\tilde{\alpha}_{a(N)}(6) - \alpha_{a(N)}(6) \right) + \gamma^2 \left(1 - \frac{|A_{N,\gamma}|}{N} \right) \left(1 - \mathcal{O}\left(\frac{1}{N}\right) \right),$$

dividing and multiplying the first term on the right by $\alpha_{\frac{\gamma\delta(N)}{2}}(6)$ it follows that

$$1 \geq \gamma^2 \frac{|B_{N,\gamma}|}{N} \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right) \cdot \frac{(\tilde{\alpha}_{a(N)}(6) - \alpha_{a(N)}(6))}{\alpha_{\frac{\gamma\delta(N)}{2}}(6)} + \gamma^2 \left(1 - \frac{|A_{N,\gamma}|}{N}\right) \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right),$$

whence Theorem IV.2.1 gives

$$\frac{1}{\gamma^2 \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right)} \geq \frac{|B_{N,\gamma}|}{N} \cdot \frac{(\tilde{\alpha}_{a(N)}(6) - \alpha_{a(N)}(6))}{\alpha_{\frac{\gamma\delta(N)}{2}}(6)} + 1 - C\gamma^s,$$

with C defined as in that theorem. Hence,

$$\frac{|B_{N,\gamma}|}{N} \leq \frac{\alpha_{\frac{\gamma\delta(N)}{2}}(6)}{(\tilde{\alpha}_{a(N)}(6) - \alpha_{a(N)}(6))} \left(\frac{1}{\gamma^2 \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right)} - 1 + C\gamma^s \right).$$

It must be mentioned that, as N approaches infinity, a computation shows that the term outside parentheses approaches roughly 91.7, so it is finite for all N . This concludes the proof. □

The next result is the direct analogue of Theorem IV.2.3:

Theorem IV.2.4 Let $\Gamma > 1$ be fixed, and let $D_{N,\gamma,\Gamma}$ denote those points in $G_{N,\gamma}$ (as defined in the previous theorem) whose Voronoi cells have area more than Γ/N . Then for any $C > 6$, there are N_0 (depending on s) and s_0 sufficiently large such that, for $N > N_0$ and $s > s_0$,

$$\frac{|D_{N,\gamma,\Gamma}|}{N} \leq \frac{1 - \gamma^2 (1 - C\gamma^s) \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right)}{\Gamma - 1}$$

Proof. Proceeding as in the proof of Theorem IV.1.3,

$$1 \geq \sum_{x \in B_{N,\gamma}} A(V(x)) + \sum_{x \in G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}} A(V(x)) + \sum_{x \in D_{N,\gamma,\Gamma}} A(V(x))$$

$$\geq |B_{N,\gamma}| \cdot \alpha_a(6) + |G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}| \cdot \alpha_a(6) + \frac{\Gamma}{N} |D_{N,\gamma,\Gamma}|.$$

As $|A_{N,\gamma}^s| + |B_{N,\gamma}| + |G_{N,\gamma} \setminus D_{N,\gamma,\Gamma}| + |D_{N,\gamma,\Gamma}| = N$ and $a \geq \frac{\gamma\delta(N)}{2}$, it follows that

$$1 \geq \left(N - |A_{N,\gamma}^s| - |D_{N,\gamma,\Gamma}| \right) \cdot \alpha_{\frac{\gamma\delta(N)}{2}}(6) + \frac{\Gamma}{N} |D_{N,\gamma,\Gamma}|,$$

whence

$$\frac{|D_{N,\gamma,\Gamma}|}{N} \leq \frac{1 - \alpha_{\frac{\gamma\delta(N)}{2}}(6) \cdot (N - |A_{N,\gamma}^s|)}{\Gamma - \alpha_{\frac{\gamma\delta(N)}{2}}(6)} \leq \frac{1 - \gamma^2 (1 - C\gamma^s) \left(1 - \mathcal{O}\left(\frac{1}{N}\right)\right)}{\Gamma - 1}.$$

□

Again these results reflect that the sets $A_{N,\gamma}^s$, $B_{N,\gamma}$, and $D_{N,\gamma,\Gamma}$ make up a small proportion of all the points in ω_N^s . This gives very good constraints on the Voronoi cells: An arbitrarily large fraction of them are hexagons of area arbitrarily close to $1/N$ (in the unit square and the sphere of unit area) with the appropriate choice of s .

IV.3 Results in the Plane

The first and simplest extension of the theorems IV.1.1, IV.1.2, and IV.1.3 are to all convex polygons of six or fewer sides, because the essential results of Fejes-Toth (see [16]) that were used in Theorem IV.1.2 all apply to such polygons. The only subtlety to which one must pay some attention is the area of the polygon, which requires only a slight adjustment. That adjustment is to change the packing radius $\delta(N)$. For a figure of unit area, the packing radius is $\delta(N) = \frac{2}{\sqrt{Na(6)}}$, but for figures P of arbitrary

area, the packing radius becomes $\delta_P(N) = \frac{2(\text{Area}(P))^{\frac{1}{2}}}{\sqrt{Na(6)}}$. Indeed, here is how the results are extended to these polygons:

Theorem IV.3.1 Let P be a convex polygon of six or fewer sides and area $A(P)$. Define the sets $A_{N,\gamma,s}$, $B_{N,\gamma}$, and $D_{N,\gamma,\Gamma}$ as in section 1, but replacing $\delta(N)$ with $\delta_P(N)$ where appropriate. Then the same inequalities given in Theorems IV.1.1, IV.1.2, and IV.1.3 hold.

Proof. The proof follows the proof of Theorem IV.1.1. Given $C > 6$, s can be chosen so that

$$\zeta_\Lambda(s) < C.$$

It follows from previous results then that for $N = N(s)$ sufficiently large,

$$\frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \leq C \left(\frac{\sqrt{3}}{2} \right)^{\frac{s}{2}} \cdot A(P)^{-\frac{s}{2}}.$$

We achieve a lower bound for $E_s(\omega_N^s)$ by summing over only one closest neighbor to each point in $A_{N,\gamma,s}$:

$$E_s(\omega_N^s) \geq |A_{N,\gamma,s}| \cdot \gamma^{-s} \cdot 2^{-s} \cdot A(P)^{-s/2} \cdot (Na(6))^{s/2},$$

and dividing now by $N^{1+\frac{s}{2}}$ gives us that

$$\begin{aligned} \frac{|A_{N,\gamma,s}| \cdot \gamma^{-s} \cdot 2^{-s} \cdot A(P)^{-s/2} \cdot (Na(6))^{s/2}}{N^{1+\frac{s}{2}}} &= \frac{|A_{N,\gamma,s}| \cdot \gamma^{-s} \cdot A(P)^{-s/2}}{N} \cdot \left(\frac{\sqrt{3}}{2} \right)^{\frac{s}{2}} \\ &\leq \frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \end{aligned}$$

$$\leq C \left(\frac{\sqrt{3}}{2} \right)^{\frac{s}{2}} \cdot A(P)^{\frac{-s}{2}},$$

whence the first result follows. The other results have exactly the same proofs as section IV.1, with a similar cancellation of the term $A(P)$.

□

An important and natural question to ask is to what class of sets $A \subseteq \mathbb{R}^2$ we hope to be able to extend the results of section IV.1. First it is important to note that an important tool in the proof of Theorem IV.1.1 is the asymptotic result of Theorem 2.4 in [20] (Theorem II.4.4), which requires only that the set A be compact. On the other hand, it would be convenient to restrict the Voronoi diagrams to the set A itself and to make use of the concept of area. Therefore, the sets considered will be connected and compact with nonempty interior. However, to extend the results of section 1, it was also necessary to add a restriction on A that is something of a rectifiability condition; this condition is precisely the condition given in the Remark III.2.2. Namely, for every $\epsilon > 0$, there must be a polygon P inside A such that

$$\text{Area}(A \setminus P) < \epsilon.$$

Admitting these conditions gives the following:

Theorem IV.3.2 Let K be a compact set of area $A(K)$ satisfying the rectifiability condition above and $\epsilon > 0$, $\gamma \in (0, 1)$ be given. Let $C > 6$ be given, choose s as in Theorem IV.1.1, and let ω_N^s be an s -optimal configuration on K . Then given the usual definition of the set

$$A_{N,\gamma,s} = \{x \in \omega_N^s : r(x) < \gamma \delta_K(N)\},$$

for all $N = N(s)$ sufficiently large we have

$$\frac{|A_{N,\gamma,s}|}{N} < C\gamma^s.$$

Proof. The proof is exactly the same as the proof of Theorem IV.3.1 shown above. □

Theorem IV.3.3 Under the same conditions of Theorem IV.3.2, given $\varepsilon > 0$, and given the usual definition of the set

$$B_{N,\gamma} = \{x \in \omega_N^s \setminus A_{N,\gamma,s} : \text{The Voronoi cell of } x \text{ is not a 6-sided polygon}\},$$

there is $N = N(s, \varepsilon)$ sufficiently large and $\gamma \in (0, 1)$ so that

$$\frac{|B_{N,\gamma}|}{N} < \varepsilon.$$

Proof. For any $\varepsilon > 0$, by hypothesis one constructs a polygon P in the interior of K whose area is within ε of the area of K . Given this polygon, it can then be decomposed into a union of triangles. Define now F_ρ to be those points in K that are within a distance ρ of the boundary of one of these triangles or outside of the polygon P . Given now $\varepsilon > 0$, choose P , corresponding triangles $\{T_i\}_{i=1}^m$, and ρ such that

$$\text{Area}(F_\rho) < \frac{\varepsilon \cdot \text{Area}(K)}{4}.$$

By Theorem II.4.4, for all N sufficiently large, the number of points in ω_N^s that are in F_ρ is no more than $\frac{\varepsilon N}{2}$. In addition, choose N sufficiently large so that those points not in F_ρ do not have Voronoi cells that would gain an edge by the superposition of the triangles on the Voronoi diagram (here again Lemma III.2.2 is being used). Then

$$A(K) \geq \sum_{x \in \omega_N^s \setminus A_{N,\gamma,s}} A(V(x)) = \sum_{x \in B_{N,\gamma} \cap F_\rho} A(V(x)) + \sum_{x \in B_{N,\gamma} \setminus F_\rho} A(V(x)) + \sum_{x \in G_{N,\gamma}} A(V(x)),$$

where $G_{N,\gamma}$ is the set of those points not in $A_{N,\gamma,s} \cup F_\rho$ whose Voronoi cell is a hexagon.

Now work in each triangle T_i individually, proceeding as in Theorem IV.1.2 above:

$$\begin{aligned} A(T_i) &\geq \sum_{x \in G_{N,\gamma} \cap T_i} A(V(x)) + \sum_{x \in (B_{N,\gamma} \setminus F_\rho) \cap T_i} A(V(x)) \\ &\geq |G_{N,\gamma} \cap T_i| \left(\frac{\gamma \delta_K(N)}{2} \right)^2 \cdot a(6) + \left(\frac{\gamma \delta_K(N)}{2} \right)^2 |(B_{N,\gamma} \setminus F_\rho) \cap T_i| \cdot \tilde{a} \left(\sum_{x \in (B_{N,\gamma} \setminus F_\rho) \cap T_i} \frac{\nu(x)}{|(B_{N,\gamma} \setminus F_\rho) \cap T_i|} \right), \end{aligned}$$

where $\tilde{a}(x)$ is the convex, decreasing function defined in Theorem IV.1.2. Again proceeding as in that theorem,

$$\tilde{a} \left(\sum_{x \in (B_{N,\gamma} \setminus F_\rho) \cap T_i} \frac{\nu(x)}{|(B_{N,\gamma} \setminus F_\rho) \cap T_i|} \right) \geq \tilde{a}(6),$$

whence

$$A(T_i) \geq \left(\frac{\gamma \delta_K(N)}{2} \right)^2 [|G_{N,\gamma} \cap T_i| \cdot a(6) + |(B_{N,\gamma} \setminus F_\rho) \cap T_i| \cdot \tilde{a}(6)].$$

Summing both sides over i ,

$$A(K) \geq A(P) \geq \left(\frac{\gamma^2 A(K)}{Na(6)} \right) (|G_{N,\gamma}| \cdot a(6) + |B_{N,\gamma} \setminus F_\rho| \cdot \tilde{a}(6)).$$

as $N = |A_{N,\gamma,s}| + |B_{N,\gamma} \setminus F_\rho| + |F_\rho| + |G_{N,\gamma}|$,

$$A(K) \geq \left(\frac{\gamma^2 A(K)}{Na(6)} \right) ((N - |A_{N,\gamma,s}| - |B_{N,\gamma} \setminus F_\rho| - |F_\rho|) \cdot a(6) + |B_{N,\gamma} \setminus F_\rho| \cdot \tilde{a}(6))$$

$$= (\gamma^2 A(K)) \left(1 - \frac{|A_{N,\gamma,s}|}{N} - \frac{|F_\rho|}{N} + \left(\frac{|B_{N,\gamma \setminus F_\rho}|}{N} \right) \left(\frac{\tilde{a}(6) - a(6)}{a(6)} \right) \right),$$

whence

$$\frac{|B_{N,\gamma \setminus F_\rho}|}{N} \leq D \cdot \left(\frac{1}{\gamma^2} - 1 + C\gamma^s + \frac{|F_\rho|}{N} \right),$$

which can be made arbitrarily small for appropriate choices of s and γ , and since $\frac{|F_\rho|}{N} < \frac{\varepsilon}{2}$, giving the result. \square

The next theorem is the natural extension of Theorem IV.1.3.

Theorem IV.3.4 Let $\Gamma > 1$, $\varepsilon > 0$ be fixed, and let $D_{N,\gamma,\Gamma}$ denote those points in $G_{N,\gamma}$ (as defined in the previous theorem) whose Voronoi cells have area more than $\frac{\Gamma \cdot A(K)}{N}$. Then for all s and $N = N(s)$ sufficiently large, there is γ sufficiently close to 1 so that

$$\frac{|D_{N,\gamma,\Gamma}|}{N} < \varepsilon.$$

Proof. The proof again uses a decomposition of the region as in Theorem IV.3.3, and again the fact that one can choose a set arbitrarily small measure inside which only a small proportion of the minimal energy points can lie, proceeding as in the proof of Theorem IV.1.3. \square

IV.4 Hölder Inequality Techniques and Refined Estimates

Given a compact set $A \subseteq \mathbb{R}^2$, some of the upper bounds for certain classes of Voronoi cells given in a previous chapter can be improved by using lower estimates of the en-

ergy given by considering only the nearest neighbors of points away from the boundary of A . In addition, similar techniques give an improvement on estimates for the quantity $C_{s,2}$ described in an earlier chapter.

Lemma IV.4.1. Let $a(x) = x \tan \frac{\pi}{x}$, which is a decreasing, convex function on $[3, \infty)$ satisfying $\lim_{x \rightarrow \infty} a(x) = \pi$. Then, furthermore, $a(x)^{\frac{s}{s+2}}$ is convex and decreasing on $[3, \infty)$ for $s \geq 2$.

Proof. $a'(x) = \tan \frac{\pi}{x} - \frac{\pi}{x} \sec^2 \frac{\pi}{x}$, and

$$a''(x) = \frac{2\pi^2}{x^3} \sec^2 \frac{\pi}{x} \tan \frac{\pi}{x}. \text{ In more generality, if } b(x) = a(x)^{\frac{s}{s+2}},$$

$$b'(x) = \frac{s}{s+2} a(x)^{\frac{-2}{s+2}} \cdot a'(x).$$

This is negative on $[3, \infty)$ since $a'(x)$ is negative on $[3, \infty)$. In addition,

$$\begin{aligned} b''(x) &= \frac{-2s}{(s+2)^2} a(x)^{\frac{-s-4}{s+2}} \cdot (a'(x))^2 + \frac{s}{s+2} a(x)^{\frac{-2}{s+2}} \cdot a''(x). \\ &= \frac{s}{s+2} a(x)^{\frac{-s-4}{s+2}} \left(a(x)a''(x) - \frac{2}{s+2} (a'(x))^2 \right). \end{aligned}$$

The quantity outside the parentheses above is always positive. Therefore, $b(x)$ will be convex if the quantity inside parentheses is positive. Notice that the quantity inside parentheses is increasing as s increases. Therefore, it suffices to check that the quantity inside parentheses is positive for all x in $[3, \infty)$ when $s = 2$.

To that end, it suffices to verify that

$$\left(x \tan \frac{\pi}{x} \right) \left(\frac{2\pi^2}{x^3} \sec^2 \frac{\pi}{x} \tan \frac{\pi}{x} \right) - \frac{1}{2} \left(\tan \frac{\pi}{x} - \frac{\pi}{x} \sec^2 \frac{\pi}{x} \right)^2 \geq 0.$$

This will hold precisely when

$$\left(x \tan \frac{\pi}{x}\right) \left(\frac{2\pi^2}{x^3} \sec^2 \frac{\pi}{x} \tan \frac{\pi}{x}\right) \geq \frac{1}{2} \left(\tan \frac{\pi}{x} - \frac{\pi}{x} \sec^2 \frac{\pi}{x}\right)^2,$$

$$\frac{2\pi}{x} \left(\sec \frac{\pi}{x} \tan \frac{\pi}{x}\right) \geq \frac{\pi}{x} \sec^2 \frac{\pi}{x} - \tan \frac{\pi}{x}.$$

Notice the reversal of signs on the right side since $a'(x)$ is negative, and a positive quantity belongs on the right. The above inequality leads to the corresponding inequality

$$2\pi \sec \frac{\pi}{x} \tan \frac{\pi}{x} + x \tan \frac{\pi}{x} \geq \pi \sec^2 \frac{\pi}{x},$$

which will certainly hold if

$$2\pi \sec \frac{\pi}{x} \tan \frac{\pi}{x} + \pi \geq \pi \sec^2 \frac{\pi}{x},$$

since $x \tan \frac{\pi}{x} = a(x) \geq \pi$. Now multiplying on both sides by $\cos^2 \frac{\pi}{x}/\pi$ gives

$$2 \sin \frac{\pi}{x} + \cos^2 \frac{\pi}{x} \geq 1.$$

This inequality is certainly true, since $2 \sin \frac{\pi}{x} \geq \sin \frac{\pi}{x} \geq \sin^2 \frac{\pi}{x}$.

□

Theorem IV.4.2. Let $C > 6$. Choose s_0 so that $\zeta_\Lambda(s_0) < C$. Let $B_6 \subseteq \omega_N^s$ denote the set of points in the unit square whose Voronoi cell does not have six sides and does not meet the boundary of the unit square. Then for every $s > s_0$, there is $N_0 = N_0(s)$ and a constant D such that for all $N > N_0$,

$$\frac{|B_6|}{N} \leq D \left(C^{\frac{2}{s+2}} - 1\right).$$

Proof. Let $\xi_N^s \subseteq \omega_N^s$ be those points whose Voronoi cells do not meet the boundary of the unit square. Say that $|\xi_N^s| = N'$. For a point $x_i \in \xi_N^s$, let $\{r_{ij}\}_{j=1}^{\nu_i}$ denote the collection of perpendicular distances from x_i to the ν_i edges of its Voronoi cell. Then

$$\mathcal{E}_s([0, 1]^2, N)(A([0, 1]^2)) \geq 2^{-s} \left(\sum_{i=1}^{N'} \sum_{j=1}^{\nu_i} r_{ij}^{-s} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}},$$

where $A(V_i)$ denotes the area of the i -th Voronoi cell. For convenience, set $R_i^{-s} = \sum_{j=1}^{\nu_i} r_{ij}^{-s}$. It follows then that

$$\mathcal{E}_s([0, 1]^2, N)(A([0, 1]^2)) \geq 2^{-s} \left(\sum_{i=1}^{N'} R_i^{-s} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}} = 2^{-s} \left\{ \left(\sum_{i=1}^{N'} R_i^{-s} \right)^{\frac{2}{s+2}} \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{s+2}} \right\}^{\frac{s+2}{2}}.$$

Applying Hölder's inequality then gives

$$2^{-s} \left\{ \left(\sum_{i=1}^{N'} R_i^{-s} \right)^{\frac{2}{s+2}} \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{s+2}} \right\}^{\frac{s+2}{2}} \geq 2^{-s} \left\{ \sum_{i=1}^{N'} \left(R_i^{-2} A(V_i) \right)^{\frac{s}{s+2}} \right\}^{\frac{s+2}{2}}.$$

Let now $r_i = \min_j r_{ij}$. In light of the obvious inequalities

$$R_i^{-2} \geq r_i^{-2}$$

$$A(V_i) \geq r_i^2 a(\nu_i),$$

it follows that

$$2^{-s} \left\{ \sum_{i=1}^{N'} \left(R_i^{-2} A(V_i) \right)^{\frac{s}{s+2}} \right\}^{\frac{s+2}{2}} \geq 2^{-s} \left(\sum_{i=1}^{N'} a(\nu_i)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}}. \quad (39)$$

By the previous lemma, $a(x)^{\frac{s}{s+2}}$ is convex and decreasing for all $s \geq 2$. Set now

$$\tilde{a}(x) = \begin{cases} a(x)^{\frac{s}{s+2}}, & x \in [3, 5] \cup [7, \infty) \\ a(5)^{\frac{s}{s+2}} + \frac{(a(7)^{\frac{s}{s+2}} - a(5)^{\frac{s}{s+2}})}{2}(x - 5), & x \in [5, 7]. \end{cases}$$

Notice that \tilde{a} is also convex and decreasing on $[3, \infty)$. Let now $N_6 = N' - |B_6|$.

Picking up from (39), notice that

$$2^{-s} \left(\sum_{i=1}^{N'} a(\nu_i)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}} = 2^{-s} \left(N_6 a(6)^{\frac{s}{s+2}} + \sum_{x_i \in B_6} \tilde{a}(\nu_i)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}}.$$

The convexity of \tilde{a} and Fejes-Toth's result now give us a lower bound:

$$\begin{aligned} 2^{-s} \left(N_6 a(6)^{\frac{s}{s+2}} + \sum_{x_i \in B_6} \tilde{a}(\nu_i)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}} &\geq 2^{-s} \left(N_6 a(6)^{\frac{s}{s+2}} + (N' - N_6) \tilde{a} \left(\frac{6(N - N_6)}{N' - N_6} \right)^{\frac{s}{s+2}} \right)^{\frac{s+2}{2}} \\ &= 2^{-s} \left(N' a(6)^{\frac{s}{s+2}} + (N' - N_6) \left(\tilde{a} \left(\frac{6(N - N_6)}{N' - N_6} \right)^{\frac{s}{s+2}} - a(6)^{\frac{s}{s+2}} \right) \right)^{\frac{s+2}{2}}. \end{aligned}$$

(Notice that $\tilde{a} \left(\frac{6(N - N_6)}{N' - N_6} \right)$ approaches $\tilde{a}(6)$ as N approaches ∞ , by Lemma III.2.1 of the previous chapter.) The upper bound for $C_{s,2}$ given earlier together with these inequalities now imply that, for N sufficiently large,

$$Ca(6)^{\frac{s}{2}} N^{1+\frac{s}{2}} \geq \mathcal{E}_s([0, 1]^2, N) \geq (N')^{1+\frac{s}{2}} a(6)^{\frac{s}{2}} \left(1 + \left(1 - \frac{N_6}{N'} \right) \Delta_s \right)^{\frac{s+2}{2}}, \quad (40)$$

where $\Delta_s = \Delta_s(N) = \frac{\tilde{a} \left(\frac{6(N - N_6)}{N' - N_6} \right)^{\frac{s}{s+2}} - a(6)^{\frac{s}{s+2}}}{a(6)^{\frac{s}{s+2}}}$. Proceeding from (40) now gives that

$$1 + \left(1 - \frac{N_6}{N'}\right)\Delta_s \leq C^{\frac{2}{s+2}} \left(\frac{N}{N'}\right),$$

whence

$$1 - \frac{N_6}{N'} \leq D \left(C^{\frac{2}{s+2}} \left(\frac{N}{N'}\right) - 1 \right),$$

where $D = \frac{1}{\Delta_s}$. Hence

$$\frac{|B_6|}{N} \leq D \left(C^{\frac{2}{s+2}} - \frac{N'}{N} \right) - \frac{N}{N'} + 1 \leq D' \left(C^{\frac{2}{s+2}} - 1 \right),$$

for a suitable choice of a slightly-adjusted D' . □

Computations of the quantity Δ_s show that, for N sufficiently large, the constant D in the theorem above can always be chosen (regardless of s) to be less than 100. Notice that the upper bound on $|B_6|/N$ given here has no dependence on the inradius of any of the cells, a difference from Theorem IV.1.2. This result can also be generalized from the unit square to compact sets in the plane:

Corollary IV.4.3. Given $C > 6$, choose s_0 as in Theorem IV.1.1. Let $A \subseteq \mathbb{R}^2$ be a compact set such that for any $\varepsilon > 0$, there is a polygon $P \subseteq A$ whose area is within ε of the area of A . Then with B_6 as defined in Theorem IV.4.2, for every $s > s_0$ there is $N_0 = N_0(s)$ and a constant D so that for all $N > N_0$,

$$\frac{|B_6|}{N} \leq D \left(C^{\frac{2}{s+2}} - 1 \right).$$

Proof. Given $\varepsilon > 0$, choose a polygon $P \subseteq A$ whose area is within ε of the area of A . By Lemma III.2.1 of the previous chapter and Remark III.2.2, the number of

Voronoi cells that meet the boundary is $o(N)$ as $N \rightarrow \infty$. Therefore, one can proceed precisely as in Theorem IV.4.2 to gain the desired result. □

Recall that in Chapter 3, we defined

$$\Delta_s(V_i) := \left(\sum_{i=1}^{\nu_i} r_i^{-s} \right) A(V_i)^{\frac{s}{2}} - \phi_s(\nu_i)$$

Then proceeding as in Theorem III.2.4, for any N -point configuration ω_N on the unit square,

$$\begin{aligned} E_s(\omega_N) \cdot A([0, 1]^2)^{\frac{s}{2}} &\geq 2^{-s} \left(\sum_{i=1}^{N'} \frac{\phi_s(\nu_i) + \Delta_s(V_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}} \\ &= 2^{-s} \left(\sum_{i=1}^{N'} \frac{\phi_s(\nu_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}} + 2^{-s} \left(\sum_{i=1}^{N'} \frac{\Delta_s(V_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}}. \end{aligned} \quad (41)$$

This motivates the following:

Theorem IV.4.4. Let $\{\omega_N^s\}$ be a sequence of s -optimal configurations on the unit square for $s > 2$. Then

$$\limsup_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right) \leq (\zeta_\Lambda(s) - 6)^{\frac{2}{s+2}} \cdot a(6)^{\frac{s}{s+2}}.$$

Proof. Let ω_N^s be an s -optimal configuration, and $s > 2$. Proceeding from (41), applying Hölder's inequality to the last term gives

$$2^{-s} \left(\sum_{i=1}^{N'} \frac{\Delta_s(V_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}} \geq 2^{-s} \left(\sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right)^{\frac{s+2}{2}}.$$

Applying Hölder's inequality followed by Jensen's inequality on the other term in the last expression of (41) gives the expression of Theorem III.2.4:

$$2^{-s} \left(\sum_{i=1}^{N'} \frac{\phi_s(\nu_i)}{A(V_i)^{\frac{s}{2}}} \right) \left(\sum_{i=1}^{N'} A(V_i) \right)^{\frac{s}{2}} \geq 2^{-s} (N')^{1+\frac{s}{2}} \phi_s \left(\frac{6N}{N'} \right) = 2^{-s} \frac{6N}{N'} (N')^{1+\frac{s}{2}} a \left(\frac{6N}{N'} \right)^{\frac{s}{2}}.$$

Thus,

$$E_s(\omega_N^s) \cdot A([0, 1]^2)^{\frac{s}{2}} \geq 2^{-s} \frac{6N}{N'} (N')^{1+\frac{s}{2}} a \left(\frac{6N}{N'} \right)^{\frac{s}{2}} + 2^{-s} \left(\sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right)^{\frac{s+2}{2}}.$$

Let Λ again denote the hexagonal lattice in the plane. Then recalling that, by the optimality of ω_N^s ,

$$\lim_{N \rightarrow \infty} \frac{E_s(\omega_N^s)}{N^{1+\frac{s}{2}}} \leq \zeta_\Lambda(s) \cdot \left(\frac{\sqrt{3}}{2} \right)^{\frac{s}{2}},$$

we have that

$$\frac{6N}{N'} \left(\frac{N'}{N} \right)^{1+\frac{s}{2}} a \left(\frac{6N}{N'} \right)^{\frac{s}{2}} + \left(\frac{1}{N} \sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right)^{\frac{s+2}{2}} \leq \zeta_\Lambda(s) \cdot a(6)^{\frac{s}{2}} + \mathcal{O}_s(N),$$

where $\mathcal{O}_s(N)$ indicates an expression that is $\mathcal{O}(N)$ but with some dependence on s .

Letting N tend to infinity gives

$$\limsup_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right)^{\frac{s+2}{2}} \leq (\zeta_\Lambda(s) - 6) \cdot a(6)^{\frac{s}{2}},$$

whence

$$\limsup_{N \rightarrow \infty} \left(\frac{1}{N} \sum_{i=1}^{N'} \Delta_s(V_i)^{\frac{2}{s+2}} \right) \leq (\zeta_\Lambda(s) - 6)^{\frac{2}{s+2}} \cdot a(6)^{\frac{s}{s+2}}.$$

□

Recall that Theorem III.1.4 and Theorem III.1.6 state that if the lower bound given by the function $\phi(\nu_i)$ is attained, then it is uniquely attained by the regular ν_i -gon. Therefore, one can interpret the above result as a sense in which the Voronoi cells “approach” regular polygons. To be a bit more precise, for a given Voronoi cell V_i , let us now analyze the quantity $\Delta_s(V_i)$. Let $r_{i,\min}$ be the minimum altitude length drawn from the fixed point p , and let $\beta_i = \frac{A(V_i)}{r_{i,\min}^2 a(\nu_i)}$. Then we have

$$\left(\sum_{i=1}^{\nu_i} r_i^{-s} \right) (A(V_i))^{\frac{s}{2}} \geq r_{i,\min}^{-s} \cdot \beta_i^{\frac{s}{2}} r_{i,\min}^s a(\nu_i)^{\frac{s}{2}} = \beta_i^{\frac{s}{2}} a(\nu_i)^{\frac{s}{2}}.$$

Thus, we have

$$\Delta_s(V_i)^{\frac{2}{s+2}} \geq \left(\beta_i^{\frac{s}{2}} - \nu_i \right)_+^{\frac{2}{s+2}} \cdot a(\nu_i)^{\frac{s}{s+2}},$$

where $(\cdot)_+$ denotes the positive part of (\cdot) . Theorem IV.4.4 now gives

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^{N'} \left(\beta_i^{\frac{s}{2}} - \nu_i \right)_+^{\frac{2}{s+2}} \cdot a(\nu_i)^{\frac{s}{s+2}} \leq (\zeta_\Lambda(s) - 6) \cdot a(6)^{\frac{s}{2}}. \quad (42)$$

Again relabel the points so that $\{\omega_N^s\}_{i=1}^{N''}$ is the set of all points in ω_N^s whose Voronoi cell does not meet the boundary and is a hexagon. Then considering only those points in (42) whose Voronoi cell is a hexagon gives

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^{N''} \left(\beta_i^{\frac{s}{2}} - 6 \right)_+^{\frac{2}{s+2}} \cdot a(6)^{\frac{s}{s+2}} \leq (\zeta_\Lambda(s) - 6)^{\frac{2}{s+2}} \cdot a(6)^{\frac{s}{s+2}},$$

whence

$$\limsup_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^{N''} \left(\beta_i^{\frac{s}{2}} - 6 \right)_+^{\frac{2}{s+2}} \leq (\zeta_\Lambda(s) - 6)^{\frac{2}{s+2}},$$

which can be viewed as another geometric constraint.

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